

Compendium of Theoretical Meteorology

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1 INTRODUCTION

There are many good textbooks in the different areas of meteorology, especially in dynamics the amount of literature is large and constantly growing. But there are also extensive standard works on cloud physics and radiation and a certain number of books that are somewhat thin in terms of content, but have been prepared in a didactic manner. However, as is typical of textbooks, some derivations are presented in simplified or at least shortened form, just like in many lectures. This can leave a theoretically interested reader or listener with a feeling of doubt about the correctness of the theory. In addition, there are numerous different notations of the quantities, so that a literature search, for example on the derivations and prerequisites of certain concepts, sometimes does not provide any clarity. This book aims to close this gap. It should not be understood as a pure textbook, because in such a book the linguistic explanations would probably have been a little less condensed; on the other hand, it is not a pure collection of formulas, because such a collection would not contain any derivations.

The reader should find answers to questions like

- How do you come up with the different forms of the divergence equation in the p-system?,
- Under what conditions is the quasi-geostrophic theory a suitable approximation?

and will find a mathematically rigorous (at least for a physicist) but not didactically broken down presentation of the content; all requirements and limitations of a concept are clearly stated as such. The derivations are so small that additional calculations should not be necessary for a reader who is confident in high school mathematics.

Dynamics, radiation, cloud microphysics and numerical science are covered. In part I the physical basics that are important for understanding the atmosphere are compiled. In part II an attempt is made to put together a system of equations that describes all processes in the atmosphere. The basic knowledge gained is then applied to specific areas of atmospheric theory. In part III, theoretical tools are prepared for the treatment of air flows in a planetary atmosphere, which is referred to as *dynamics*. In the following part IV this theory is applied to concrete atmospheric and oceanic problems. In contrast to this, part V deals with the additional areas of radiation and cloud microphysics. *Numerical problems* are discussed in the sixth part. In the seventh part a *dynamic core* is developed. Mathematical basics are explained in the appendix.

The SI system is used as the system of units.

1.1 Important literature

The following books are relevant in the different areas:

- collection of mathematical formulas: *Abramowitz et al.* [1]
- Canon of Theoretical Physics: e.g. *Fließbach* [10], [9], [11], [12]
- Fluid mechanics: *Kundu* [22]
- Radiation transfer: *Chandrasekhar* [6]
- Cloud microphysics: *Pruppacher and Klett* [21]
- Water surface waves: *Massel* [27]

1.2 Scales

The word *scales* denotes orders of magnitude. The goal of scale analysis is to simplify equations. Different scales are characterized by different phenomena that typically occur on them. Tab. 1.3 provides an overview of the time and length scales typically used in meteorology, their names and typical phenomena. Some important quantities of the synoptic scale are listed in table 1.3.

Symbol / Bezeichnung	Bedeutung	evtl. Wert
k_B	Boltzmann-Konstante	$1,380649 \cdot 10^{-23} \text{ JK}^{-1}$ [29]
N_A	Avogadro-Konstante	$6,0221409 \cdot 10^{23} \text{ mol}^{-1} = 1$ [29]
$R = k_B \cdot N_A$	universelle Gaskonstante	$8,314463 \text{ Jmol}^{-1}\text{K}^{-1}$
R_s	spezifische Gaskonstante	
$c^{(p)}$	isobaric specific heat capacity	
$c^{(V)}$	isochoric specific heat capacity	
Index d	Bezug auf trockene Luft	
Index v	Bezug auf Wasserdampf	
index g	reference to the gaseous portion of the air	
M_d	molare Masse trockener Luft	$0,028964420 \text{ kg/mol}$ [23]
M_v	molare Masse von Wasser	$0,01801527 \text{ kg/mol}$ [32]
ω	Winkelgeschwindigkeit der Erddrotation	$7,292115 \cdot 10^{-5} \text{ 1/s}$ [28]
a	Earth's radius at the equator	6378137.0 m [20]
$1/\tilde{f}$	Abplattung	$298,257223563$ [20]
β	<i>Obliquity</i> of the Earth's axis	23.439279° [28]
S_o	Solarkonstante	1361 W/m^2 [2]
Ω	Winkelgeschwindigkeit der Erdrevolution	$1,99099 \cdot 10^{-7} \text{ s}^{-1}$ [2]
M	Masse der Erde	$5,9723 \cdot 10^{24} \text{ kg}$ [2]
spezifisch	pro Masse	

Table 1.1: Symbols with the same meaning as long as this is not defined differently in the respective location.

name	alternative name	length scale / m	time scale / s	typical phenomena
synoptic scale	large scale	$> 1 \cdot 10^6$	$> 1 \cdot 10^5$	Rossby waves, extratropical depressions
Meso- α -Skala		$2 \cdot 10^5 -$ $2 \cdot 10^6$	$2 \cdot 10^4 -$ $2 \cdot 10^5$	tropische Zyklonen, Fronten
Meso- β -Skala		$2 \cdot 10^4 -$ $2 \cdot 10^5$	$2 \cdot 10^3 -$ $2 \cdot 10^4$	Land-Seewind- Zirkulation
Meso- γ - scale	storm scale, convective scale	$2 \cdot 10^3 - 2 \cdot 10^4$	$2 \cdot 10^2 - 2 \cdot 10^3$	convection, leeward waves, Kelvin-Helmholtz instability
microscale		$2 \cdot 10^{-3} - 2 \cdot 10^3$	$2 \cdot 10^{-4} -$ $2 \cdot 10^2$	turbulence, flow around houses and trees etc.
molekulare Skala		$< 2 \cdot 10^{-3}$	$< 2 \cdot 10^{-4}$	Impuls- und Stoffdiffusion, Strahlung

Table 1.2: Definitions of typical scales in meteorology. Of course, these lengths and times are not to be understood technically and in most cases the phenomena listed can also occur on the neighboring scales.

size	magnitude
synoptic length scale L	10^6 m
Horizontalwind u, v	10^1 ms $^{-1}$
Vertikalwind w	10^{-2} ms $^{-1}$
Schwere g	10^1 ms $^{-2}$
characteristic height H	10^4 m
Zeitskala $T = L/u$	10^5 s
Erdradius a	10^7 m
Dichte ρ	10^0 kgm $^{-3}$
Coriolis-Parameter f	10^{-4} s $^{-1}$
horizontale Druckschwankung δp	10^3 Pa
vertikale Druckschwankung δp	10^5 Pa
Rossby-Parameter β	10^{-11} m $^{-1}$ s $^{-1}$
relative Vorticity ζ	10^{-5} s $^{-1}$
Horizontaldivergenz δ	10^{-5} s $^{-1}$
p –Vertikalgeschwindigkeit ω	10^{-1} Pas $^{-1}$

Table 1.3: Orders of magnitude of the synoptic scale, see [18].

Abk.	Aussprache	Bedeutung
P	peta	10^{15}
T	tera	10^{12}
G	giga	10^9
M	mega	10^6
k	kilo	10^3
h	hekto	10^2
da	deka	10^1
d	dezi	10^{-1}
c	zenti	10^{-2}
m	milli	10^{-3}
μ	mikro	10^{-6}
n	nano	10^{-9}
p	piko	10^{-12}
f	femto	10^{-15}
a	atto	10^{-18}

Table 1.4: Decimal prefixes.

Part I

Physical basics

2 CLASSIC MECHANICS

Classical mechanics deals with mass points, i.e. masses without spatial extension, which move at speeds $\ll c$ (transition to relativity theory) and are not too light (transition to quantum mechanics).

2.1 Newtonian mechanics

Classical mechanics is based on Newton's axioms [10]. The most important axiom is *Newton's Second Axiom*:

Let a point mass m with momentum $\mathbf{p}$ be given, on which the force $\mathbf{F}$ acts, then the following applies

$$\frac{d\mathbf{p}}{dt} = \mathbf{F}. \quad (2.1)$$

The impulse is defined by

$$\mathbf{p} := m \frac{d\mathbf{r}}{dt}, \quad (2.2)$$

where $\mathbf{r} = \mathbf{r}(t)$ is the trajectory of the mass point. The First Axiom is a special case of the Second and is therefore insignificant. Newton's Third Axiom is:

Let two masses m_1 and m_2 be given. Let $\mathbf{F}_1$ and $\mathbf{F}_2$ be the forces on the masses due to the pairwise interaction (WW). Then applies

$$\mathbf{F}_1 = -\mathbf{F}_2. \quad (2.3)$$

To complete the theory, two additions to Newton's axioms are introduced. First, one determines that if $N \geq 1$ forces $\mathbf{F}_j$ act on a mass point, in Eq. (2.1) to use the sum of these forces is:

$$m \frac{d^2 \mathbf{r}}{dt^2} = \sum_{j=1}^N \mathbf{F}_j \quad (2.4)$$

Furthermore, it is assumed that the force $\mathbf{F}_1$ is parallel to the connecting line $\mathbf{r}_1 - \mathbf{r}_2$:

$$\mathbf{F}_1 \parallel \mathbf{r}_1 - \mathbf{r}_2 \quad (2.5)$$

Let two point masses m_1, m_2 be given at the locations $\mathbf{r}_1, \mathbf{r}_2$. One defines the *center of gravity* $\mathbf{R}$ by

$$\mathbf{R} := \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{M} \quad (2.6)$$

with the total mass

$$M := m_1 + m_2. \quad (2.7)$$

Newton's Second Axiom applies to the acceleration of the center of gravity

$$\frac{d^2 \mathbf{R}}{dt^2} = \frac{m_1 \frac{d^2 \mathbf{r}_1}{dt^2} + m_2 \frac{d^2 \mathbf{r}_2}{dt^2}}{M} = \frac{1}{M} (\mathbf{F}_1 + \mathbf{F}_2), \quad (2.8)$$

where $\mathbf{F}_1$ represents the total force acting on m_1 and $\mathbf{F}_2$ represents the total force acting on m_2 . These can be divided into an internal and an external force:

$$\mathbf{F}_1 = \mathbf{F}_1^{(\text{int})} + \mathbf{F}_1^{(\text{ext})}, \quad \mathbf{F}_2 = \mathbf{F}_2^{(\text{int})} + \mathbf{F}_2^{(\text{ext})} \quad (2.9)$$

The internal force arises from interactions within the system. Due to Newton's third axiom,

$$\mathbf{F}_1^{(\text{int})} = -\mathbf{F}_2^{(\text{int})}. \quad (2.10)$$

So you get

$$\frac{d^2 \mathbf{R}}{dt^2} = \frac{1}{M} \left(\mathbf{F}_1^{(\text{ext})} + \mathbf{F}_2^{(\text{ext})} \right). \quad (2.11)$$

So a kind of Newton's second axiom applies

$$M \frac{d^2 \mathbf{R}}{dt^2} = \sum_i \mathbf{F}_i^{(\text{ext})} \quad (2.12)$$

for the movement of the center of gravity coordinate. The relative coordinate is carried out in the same way

$$\mathbf{r} := \mathbf{r}_2 - \mathbf{r}_1 \quad (2.13)$$

a. This satisfies the equation of motion

$$\frac{d^2 \mathbf{r}}{dt^2} = \frac{d^2 \mathbf{r}_2}{dt^2} - \frac{d^2 \mathbf{r}_1}{dt^2} = \frac{\mathbf{F}_1}{m_1} - \frac{\mathbf{F}_2}{m_2} \Leftrightarrow \frac{m_1 m_2}{m_1 + m_2} \frac{d^2 \mathbf{r}}{dt^2} = \frac{m_2}{m_1 + m_2} \mathbf{F}_1 - \frac{m_1}{m_1 + m_2} \mathbf{F}_2. \quad (2.14)$$

If you now only assume internal WW, you get

$$\mu \frac{d^2 \mathbf{r}}{dt^2} = \mathbf{F}_1^{(\text{int})}. \quad (2.15)$$

This was the reduced mass

$$\mu := \frac{m_1 m_2}{M} \quad (2.16)$$

introduced. With vanishing external forces, a mass μ effectively moves in the force field of the pairwise WW, its position vector is $\mathbf{r}$. Some of the results also hold for $N \in \mathbb{N}$ with $N \geq 1$ particles. First you can get a total mass

$$M := \sum_{i=1}^N m_i \quad (2.17)$$

and a center of gravity coordinate

$$\mathbf{R} := \frac{\sum_{i=1}^N m_i \mathbf{r}_i}{M} \quad (2.18)$$

define. You derive this twice in time and get

$$M \frac{d^2 \mathbf{R}}{dt^2} = \sum_{i=1}^N m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{i=1}^N \mathbf{F}_i. \quad (2.19)$$

It applies again

$$\mathbf{F}_i = \mathbf{F}_i^{(\text{int})} + \mathbf{F}_i^{(\text{ext})} = \sum_{\substack{j=1, \\ j \neq i}}^N \mathbf{F}_i^{(j)} + \mathbf{F}_i^{(\text{ext})}. \quad (2.20)$$

Here $\mathbf{F}_i^{(j)}$ is the force that the j th particle exerts on the i th particle. Thus you get

$$\sum_{i=1}^N \mathbf{F}_i = \sum_{\substack{i,j=1, \\ i \neq j}}^N \mathbf{F}_i^{(j)} + \sum_{i=1}^N \mathbf{F}_i^{(\text{ext})} = \sum_{\substack{i,j=1, \\ i > j}}^N \mathbf{F}_i^{(j)} + \mathbf{F}_j^{(i)} + \sum_{i=1}^N \mathbf{F}_i^{(\text{ext})} = \sum_{\substack{i,j=1, \\ i > j}}^N \mathbf{F}_i^{(j)} - \mathbf{F}_i^{(j)} + \sum_{i=1}^N \mathbf{F}_i^{(\text{ext})} = \sum_{i=1}^N \mathbf{F}_i^{(\text{ext})}. \quad (2.21)$$

This became Newton's third axiom

$$\mathbf{F}_i^{(j)} = -\mathbf{F}_j^{(i)} \quad (2.22)$$

used. This means: The internal WWs have no influence on the trajectory of the center of gravity. If no external forces act, the total momentum is constant; this is called *law of conservation of momentum*.

There is a formulation of Newtonian mechanics for rotations (rotational movements). The *angular momentum* L of a particle is defined by

$$\mathbf{L} := \mathbf{r} \times \mathbf{p}. \quad (2.23)$$

The *torque* $\mathbf{F}$ is defined as

$$\mathbf{D} := \mathbf{r} \times \mathbf{F}. \quad (2.24)$$

By deriving Eq. (2.23) follows

$$\frac{d}{dt} \mathbf{L} = \frac{d\mathbf{r}}{dt} \times \mathbf{p} + \mathbf{r} \times \frac{d\mathbf{p}}{dt} = \mathbf{r} \times \mathbf{F} = \mathbf{D}. \quad (2.25)$$

This is also called *Newton's Second Axiom of Rotation*. For $N \in \mathbb{N}$ with $N \geq 1$ particles one obtains a total angular momentum of

$$\mathbf{L} = \sum_{i=1}^N \mathbf{L}_i = \sum_{i=1}^m \mathbf{r}_i \times \mathbf{p}_i. \quad (2.26)$$

This applies to this one

$$\begin{aligned} \frac{d\mathbf{L}}{dt} &= \sum_{i=1}^N \mathbf{r}_i \times \left(\mathbf{F}_i^{(\text{int})} + \mathbf{F}_i^{(\text{ext})} \right) = \sum_{\substack{i,j=1, \\ i \neq j}}^N \mathbf{r}_i \times \mathbf{F}_i^{(j)} + \sum_{i=1}^N \mathbf{r}_i \times \mathbf{F}_i^{(\text{ext})} \\ &= \sum_{\substack{i,j=1, \\ i > j}}^N \mathbf{r}_i \times \mathbf{F}_i^{(j)} + \mathbf{r}_j \times \mathbf{F}_j^{(i)} + \sum_{i=1}^N \mathbf{r}_i \times \mathbf{F}_i^{(\text{ext})} = \sum_{\substack{i,j=1, \\ i > j}}^N \mathbf{F}_i^{(j)} \times (\mathbf{r}_i - \mathbf{r}_j) + \sum_{i=1}^N \mathbf{r}_i \times \mathbf{F}_i^{(\text{ext})} \\ &= \sum_{i=1}^N \mathbf{r}_i \times \mathbf{F}_i^{(\text{ext})}. \end{aligned} \quad (2.27)$$

Newton's third axiom was used again as well as the additional statement that the force between two particles acts along the line connecting them. If no external forces act, the angular momentum is conserved; this is called *law of conservation of angular momentum*.

The concept of *energy* should be introduced. A force field is a function $\mathbf{F} = \mathbf{F}(\mathbf{r})$, which assigns to each point $\mathbf{r}$ a force $\mathbf{F}(\mathbf{r})$ acting there. A mass point moves along the trajectory $\mathbf{r} = \mathbf{r}(t)$. Then you define the *work* W that the force field does at the mass point in the time interval $[t_1, t_2]$ by

$$W := \int_{t_1}^{t_2} \mathbf{F}(\mathbf{r}(t)) \cdot \frac{d\mathbf{r}}{dt} dt. \quad (2.28)$$

Using Newton's Second Axiom and partial integration follows

$$\begin{aligned}
 W &= \int_{t_1}^{t_2} m \frac{d^2 \mathbf{r}}{dt^2} \cdot \frac{d\mathbf{r}}{dt} dt = \left[m \frac{d\mathbf{r}}{dt} \cdot \frac{d\mathbf{r}}{dt} \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} m \frac{d\mathbf{r}}{dt} \cdot \frac{d^2 \mathbf{r}}{dt^2} dt \\
 &\Leftrightarrow W = \frac{1}{2} m \mathbf{v}(t_2)^2 - \frac{1}{2} m \mathbf{v}(t_1)^2.
 \end{aligned} \tag{2.29}$$

Define the *kinetic energy* E_{kin} by

$$E_{\text{kin}} := \frac{1}{2} m \mathbf{v}^2, \tag{2.30}$$

follows

$$W = \Delta E_{\text{kin}}. \tag{2.31}$$

So the work done by the field becomes kinetic energy. Furthermore, a force field is called *conservative*, if a *potential* $U = U(\mathbf{r})$ exists with

$$\mathbf{F} = -\nabla U. \tag{2.32}$$

In this case, according to Eq. (B.47)

$$\nabla \times \mathbf{F} = \mathbf{o}, \tag{2.33}$$

Thus, using Stokes' theorem, Eq. (15.26)

$$\int_{\partial A} \mathbf{F} \cdot d\mathbf{s} = \mathbf{o} \tag{2.34}$$

for each surface A , so that the work done is independent of the path. Define the total energy of the particle by

$$E := E_{\text{kin}} + U, \tag{2.35}$$

so this size is obtained:

$$\begin{aligned}
 \frac{dE}{dt} &= \frac{dE_{\text{kin}}}{dt} + \frac{dU}{dt} = \frac{1}{2} m \frac{d\mathbf{r}}{dt} \cdot \frac{d^2 \mathbf{r}}{dt^2} + \nabla U \cdot \frac{d\mathbf{r}}{dt} \\
 &= \left(m \frac{d^2 \mathbf{r}}{dt^2} + \nabla U \right) \cdot \frac{d\mathbf{r}}{dt} = (\mathbf{F} + \nabla U) \cdot \frac{d\mathbf{r}}{dt} = (-\nabla U + \nabla U) \cdot \frac{d\mathbf{r}}{dt} = \mathbf{o}
 \end{aligned} \tag{2.36}$$

$$\Rightarrow \frac{dE}{dt} = \mathbf{o} \tag{2.37}$$

The energy of a particle moving under the influence of a conservative force is therefore constant.

There are two other formulations of classical mechanics, the *Lagrange formalism* and the Hamilton formalism. Both can be derived from Newton's axioms.

2.2 Lagrange formalism

Newtonian mechanics is practical for flying points of mass (atoms in a gas, planets in a solar system) or rigid bodies (ships, airplanes). In principle, these can move freely in any direction. However, situations in which a mass point is restricted in its freedom of movement are common, for example a marble in a marble run, a billiard ball on a table or a train on a track. Such systems are subject to *constraints*. If the system consists of exactly one particle with the trajectory $\mathbf{r} = \mathbf{r}(t)$, then one can have a constraint in the form

$$g(\mathbf{r}, t) = \mathbf{o} \tag{2.38}$$

write. g is some scalar field. The condition $g = 0$ can be imagined as a surface. This surface can also be explicitly time-dependent, such as a vertically accelerated pool table. Eq. (2.38) is called *holonomic constraint*, all other constraints are called nonholonomic. This would be the case, for example, if g were a function of $\frac{d\mathbf{r}}{dt}$. Explicitly time-dependent constraints are called *rheonomie*, while time-independent constraints are called *skleronomie*. In general you have N particles, in this case you can set up R constraints

$$g_a(\mathbf{r}_1, \dots, \mathbf{r}_N, t) = 0 \quad (2.39)$$

with $1 \leq a \leq R$ and $R \leq 3N - 1$. At $R = 3N$ no movement could occur since each constraint eliminates one degree of freedom.

2.2.1 Lagrange equations 1st Art

Compliance with the constraint conditions is ensured by the so-called coercive forces. These are perpendicular to the surface specified by the constraint - this can easily be seen when moving on a table, for example. Although the friction force acts tangentially to the table, the friction force has nothing to do with compliance with the constraint and is therefore not a constraint. So you can use a constraint force $\mathbf{Z}$

$$\mathbf{Z}(\mathbf{r}, t) = \lambda(t) \nabla g(\mathbf{r}, t). \quad (2.40)$$

The multiplier λ is time dependent because the forcing force depends on the time dependent trajectory. You can now write it down as an equation of motion

$$m \frac{d^2}{dt^2} \mathbf{r} = \mathbf{F} + \lambda(t) \nabla g(\mathbf{r}, t), \quad (2.41)$$

here $\mathbf{F}$ is the sum of all non-constraint forces (gravity, friction force, etc.). If you have given two constraints, you can generalize this to:

$$m \frac{d^2}{dt^2} \mathbf{r} = \mathbf{F} + \sum_{a=1}^2 \lambda_a(t) \nabla g_a(\mathbf{r}, t). \quad (2.42)$$

This is plausible: $g_1 = 0$ and $g_2 = 0$ define two areas in which the trajectory runs. ∇g_1 and ∇g_2 are each perpendicular to the corresponding surface and thus also to the trajectory, and they are also linearly independent. Therefore $\sum_{a=1}^2 \lambda_a(t) \nabla g_a(\mathbf{r}, t)$ is a general approach for a force perpendicular to the trajectory, i.e. for a general forcing force. Together with $g_1(\mathbf{r}, t) = g_2(\mathbf{r}, t) = 0$ you now have five equations for the five unknown functions $x(t), y(t), z(t), \lambda_1(t), \lambda_2(t)$. So there is a chance of solvability. In general, one has given N particles with the Cartesian coordinates x_n with $1 \leq n \leq 3N$, here x_1, x_2, x_3 are the coordinates of the first particle x_4, x_5, x_6 are those of the second, etc. If one has $R \leq 3N - 1$ holonomic constraints $g_j(\mathbf{r}, t) = 0$ can be written down as equations of motion

$$m_n \frac{d^2 x_n}{dt^2} = F_n + \sum_{a=1}^R \lambda_a(t) \frac{\partial g_a(x_1, \dots, x_{3N}, t)}{\partial x_n}. \quad (2.43)$$

Here, $m_1 = m_2 = m_3$ is the mass of the first particle, etc. Together with the constraints, you get $3N + R$ equations for the $3N + R$ functions $x_n(t), \lambda_a(t)$. These $3N + R$ equations are called *Lagrange equations of the first kind*.

2.2.2 Lagrange equations 2nd kind

If you are not interested in calculating the forcing forces, eliminating them is a good idea. This is now being done. As noted, each of the constraints g_a eliminates one degree of freedom

$$f = 3N - R \quad (2.44)$$

here is the number of numbers necessary to determine the location of all N particles. These numbers are called *generalized coordinates* $q_1, \dots, q_f$. You must meet two conditions:

1. You need to set the Cartesian coordinates, $x_n = x_n(q_1, \dots, q_f, t)$ for all $1 \leq n \leq 3N$.

2. You have to consider the constraints: $g_a(q_1, \dots, q_f, t) = 0$ for $1 \leq a \leq R$ and all possible q_i .

The second condition can be expressed formally as:

$$\frac{dg_a}{dq_k} = \sum_{n=1}^{3N} \frac{\partial g_a}{\partial x_n} \frac{\partial x_n}{\partial q_k} = 0. \quad (2.45)$$

If you multiply Eq. (2.43) with $\frac{\partial x_n}{\partial q_k}$, one obtains

$$m_n \frac{d^2 x_n}{dt^2} \frac{\partial x_n}{\partial q_k} = F_n \frac{\partial x_n}{\partial q_k} + \sum_{a=1}^R \lambda_a(t) \frac{\partial g_a(x_1, \dots, x_{3N}, t)}{\partial x_n} \frac{\partial x_n}{\partial q_k}. \quad (2.46)$$

If you sum this over n , it follows

$$\sum_{n=1}^{3N} m_n \frac{d^2 x_n}{dt^2} \frac{\partial x_n}{\partial q_k} = \sum_{n=1}^{3N} F_n \frac{\partial x_n}{\partial q_k}. \quad (2.47)$$

This equation applies to all $1 \leq k \leq f$. Coercive forces no longer appear here. The following notations are introduced:

$$x := (x_1, \dots, x_n), \quad \dot{x} := (\dot{x}_1, \dots, \dot{x}_n) \quad (2.48)$$

$$q := (q_1, \dots, q_n), \quad \dot{q} := (\dot{q}_1, \dots, \dot{q}_n) \quad (2.49)$$

The $\dot{q}_i$ is also referred to as *generalized velocities*. You now derive the transformation equation

$$x_n = x_n(q, t) \quad (2.50)$$

totally after the time:

$$\dot{x}_n = \frac{d}{dt} x_n(q, t) = \sum_{k=1}^f \frac{\partial x_n}{\partial q_k} \dot{q}_k + \frac{\partial x_n}{\partial t} = \dot{x}_n(q, \dot{q}, t) \quad (2.51)$$

It follows

$$\frac{\partial \dot{x}_n}{\partial \dot{q}_k} = \frac{\partial x_n}{\partial q_k}. \quad (2.52)$$

For the kinetic energy T applies

$$T = T(\dot{x}) = \sum_{n=1}^{3N} \frac{1}{2} m_n \dot{x}_n^2. \quad (2.53)$$

Here you set Eq. (2.51) on:

$$T = T(q, \dot{q}, t) = \sum_{i,k=1}^f m_{i,k}(q, t) \dot{q}_i \dot{q}_k + \sum_{k=1}^f b_k(q, t) \dot{q}_k + c(q, t) \quad (2.54)$$

From Eq. (2.53) follows

$$\frac{\partial T(q, \dot{q}, t)}{\partial q_k} = \sum_{n=1}^{3N} m_n \dot{x}_n \frac{\partial \dot{x}_n}{\partial q_k}. \quad (2.55)$$

Still applies

$$\frac{\partial T(q, \dot{q}, t)}{\partial \dot{q}_k} = \sum_{n=1}^{3N} m_n \dot{x}_n \frac{\partial \dot{x}_n}{\partial \dot{q}_k} = \sum_{n=1}^{3N} m_n \dot{x}_n \frac{\partial x_n}{\partial q_k}. \quad (2.56)$$

If you derive this totally according to time, you get

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{q}_k} = \sum_{n=1}^{3N} m_n \frac{d^2 x_n}{dt^2} \frac{\partial x_n}{\partial q_k} + \sum_{n=1}^{3N} m_n \dot{x}_n \frac{\partial \dot{x}_n}{\partial q_k}. \quad (2.57)$$

In the last term the following identity was exploited:

$$\frac{d}{dt} \frac{\partial x_n}{\partial q_k} = \sum_{l=1}^f \frac{\partial^2 x_n}{\partial q_l \partial q_k} \dot{q}_l + \frac{\partial^2 x_n}{\partial t \partial q_k} = \frac{\partial}{\partial q_k} \left(\sum_{l=1}^f \frac{\partial x_n}{\partial q_l} \dot{q}_l + \frac{\partial x_n}{\partial t} \right) = \frac{\partial}{\partial q_k} \frac{dx_n}{dt} \quad (2.58)$$

One now defines *generalized forces*:

$$Q_k := \sum_{n=1}^{3N} F_n \frac{\partial x_n}{\partial q_k} \quad (2.59)$$

This definition is combined with Eq. (2.57) and Eq. (2.55) in Eq. (2.47):

$$\begin{aligned} \sum_{n=1}^{3N} m_n \frac{d^2 x_n}{dt^2} \frac{\partial x_n}{\partial q_k} &= \sum_{n=1}^{3N} F_n \frac{\partial x_n}{\partial q_k} && \Leftrightarrow \sum_{n=1}^{3N} m_n \frac{d^2 x_n}{dt^2} \frac{\partial x_n}{\partial q_k} = Q_k \\ \Leftrightarrow \frac{d}{dt} \frac{\partial T}{\partial \dot{q}_k} - \sum_{n=1}^{3N} m_n \dot{x}_n \frac{\partial \dot{x}_n}{\partial q_k} &= Q_k && \Leftrightarrow \frac{d}{dt} \frac{\partial T}{\partial \dot{q}_k} - \frac{\partial T}{\partial q_k} = Q_k \end{aligned} \quad (2.60)$$

You bet on your strengths

$$F_n = -\frac{\partial U(x, \dot{x}, t)}{\partial x_n} + \frac{d}{dt} \frac{\partial U(x, \dot{x}, t)}{\partial \dot{x}_n} \quad (2.61)$$

with a potential $U = U(x, \dot{x}, t)$. In the case of a speed-independent conservative force, this reduces to the form known from Newtonian mechanics, the second term has been added to take the speed dependence into account. $(x, \dot{x})$ can be bijectively mapped to $(q, \dot{q})$, so you can note it down

$$U = U(q, \dot{q}, t). \quad (2.62)$$

Now you can write

$$Q_k = \sum_{n=1}^{3N} F_n \frac{\partial x_n}{\partial q_k} = - \sum_{n=1}^{3N} \frac{\partial U}{\partial x_n} \frac{\partial x_n}{\partial q_k} + \frac{d}{dt} \sum_{n=1}^{3N} \frac{\partial U}{\partial \dot{x}_n} \frac{\partial \dot{x}_n}{\partial q_k} = - \frac{\partial U}{\partial q_k} + \frac{d}{dt} \frac{\partial U}{\partial \dot{q}_k}. \quad (2.63)$$

The equation follows

$$\frac{d}{dt} \frac{\partial (T - U)}{\partial \dot{q}_k} = \frac{\partial (T - U)}{\partial q_k}. \quad (2.64)$$

One defines the *Lagrange function* L by

$$L(q, \dot{q}, t) := T(q, \dot{q}, t) - U(q, \dot{q}, t). \quad (2.65)$$

This gives you

$$\frac{d}{dt} \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}_k} = \frac{\partial L(q, \dot{q}, t)}{\partial q_k}. \quad (2.66)$$

For $1 \leq k \leq f$ these are the *Lagrange equations of the second kind*.

2.3 Hamilton formalism

First define the *canonical impulses* by

$$p_i := \frac{\partial L}{\partial \dot{q}_i} \quad (2.67)$$

for $1 \leq i \leq f$. One now eliminates the generalized velocities $\dot{q}$:

$$p_i = \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}_i} \rightarrow \dot{q}_j = \dot{q}_j(q, p, t) \quad (2.68)$$

The *Hamilton function* H is defined by

$$H(q, p, t) := \sum_{i=1}^f \dot{q}_i(q, p, t) p_i - L(q, \dot{q}(q, p, t), t). \quad (2.69)$$

The *Hamilton's equations* or also *canonical equations* follow by partial differentiation:

$$\frac{\partial H}{\partial q_k} = \sum_{i=1}^f \frac{\partial \dot{q}_i}{\partial q_k} p_i - \frac{\partial L}{\partial q_k} - \sum_{i=1}^f \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial q_k} = - \frac{\partial L}{\partial q_k} = - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_k} \right) = -\dot{p}_k \quad (2.70)$$

$$\frac{\partial H}{\partial p_k} = \sum_{i=1}^f \frac{\partial \dot{q}_i}{\partial p_k} p_i + \dot{q}_k - \sum_{i=1}^f \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial p_k} = \dot{q}_k \quad (2.71)$$

$$\frac{\partial H}{\partial t} = \sum_{i=1}^f \frac{\partial \dot{q}_i}{\partial t} p_i - \sum_{i=1}^f \frac{\partial L}{\partial \dot{q}_i} \frac{\partial \dot{q}_i}{\partial t} - \frac{\partial L}{\partial t} = - \frac{\partial L}{\partial t} \quad (2.72)$$

The space of (q, p) is called *phase space*.

2.3.1 Poisson bracket

Any two quantities F, K can only depend on (q, p, t) . One defines the *Poisson bracket* $\{F, K\}$ of F and K by

$$\{F, K\} := \sum_{i=1}^f \left(\frac{\partial F}{\partial q_i} \frac{\partial K}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial K}{\partial q_i} \right). \quad (2.73)$$

The following are immediate consequences:

$$\{F + G, K\} = \{F, K\} + \{G, K\}, \quad (2.74)$$

$$\{F, K\} = -\{K, F\}, \quad (2.75)$$

$$\{F, F\} = 0. \quad (2.76)$$

Apply in the Hamilton formalism

$$\frac{\partial q_i}{\partial q_j} = \delta_{i,j}, \quad \frac{\partial q_i}{\partial p_j} = 0, \quad \frac{\partial q_i}{\partial t} = 0, \quad (2.77)$$

$$\frac{\partial p_i}{\partial q_j} = 0, \quad \frac{\partial p_i}{\partial p_j} = \delta_{i,j}, \quad \frac{\partial p_i}{\partial t} = 0. \quad (2.78)$$

Furthermore are

$$\{F, q_j\} = -\frac{\partial F}{\partial p_j}, \quad \{F, p_j\} = \frac{\partial F}{\partial q_j}. \quad (2.79)$$

This follows further

$$\{q_i, q_j\} = 0, \quad \{p_i, p_j\} = 0, \quad \{p_i, q_j\} = -\delta_{i,j}. \quad (2.80)$$

For the total time derivative of F we now get

$$\frac{dF}{dt} = \sum_{i=1}^f \frac{\partial F}{\partial q_i} \dot{q}_i + \sum_{i=1}^f \frac{\partial F}{\partial p_i} \dot{p}_i + \frac{\partial F}{\partial t} = \sum_{i=1}^f \frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \sum_{i=1}^f \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial F}{\partial t} \quad (2.81)$$

$$\Leftrightarrow \frac{dF}{dt} = \{F, H\} + \frac{\partial F}{\partial t}. \quad (2.82)$$

This implies

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}. \quad (2.83)$$

The Hamilton function is constant if and only if it does not explicitly depend on time. From Eq. (2.82) follows the equations (2.70) - (2.71) in the form

$$\dot{p}_i = \{p_i, H\}, \quad \dot{q}_i = \{q_i, H\}. \quad (2.84)$$

2.4 Harmonic oscillator

The so-called *harmonic oscillator* is used as an example for the application of the theory of classical mechanics. This is about the evolution of a generalized coordinate $x = x(t)$ according to the differential equation

$$\frac{d^2 x}{dt^2} = -kx. \quad (2.85)$$

If x is the Cartesian coordinate of a mass point with mass m and k is the quotient of the spring constant and mass, then it is an undamped spring, but there are also other examples.

2.4.1 Undamped fall

If you put in Eq. (2.85) a solution $x = x_0 e^{-i\omega_0 t}$ follows

$$-\omega_0^2 = -k \Rightarrow \omega_0 = \pm \sqrt{k}. \quad (2.86)$$

ω bezeichnet man als *Eigenfrequenz*. For the kinetic energy K as a function of time applies

$$K = \frac{1}{2} m \left(\frac{dx}{dt} \right)^2 = \frac{1}{2} m x_0^2 \omega_0^2 \sin^2(\omega_0 t), \quad (2.87)$$

here m is the mass of the oscillating mass point. For the potential energy applies

$$U = \frac{1}{2} m k x^2 = \frac{1}{2} m k x_0^2 \cos^2(\omega_0 t). \quad (2.88)$$

This therefore applies to the total energy E

$$\begin{aligned} E = K + U &= \frac{1}{2} m x_0^2 \omega_0^2 \sin^2(\omega_0 t) + \frac{1}{2} m k x_0^2 \cos^2(\omega_0 t) \\ &= \frac{1}{2} m k x_0^2 [\sin^2(\omega_0 t) + \cos^2(\omega_0 t)] = \frac{1}{2} m k x_0^2 = \frac{1}{2} m \omega_0^2 x_0^2. \end{aligned} \quad (2.89)$$

Furthermore, on average half of the energy is stored in kinetic and potential energy:

$$\begin{aligned} \overline{K} &= \frac{1}{4} m x_0^2 \omega_0^2 = \frac{1}{4} m x_0^2 k = \frac{E}{2}, \\ \overline{U} &= \frac{1}{4} m k x_0^2 = \frac{1}{4} m \omega_0^2 x_0^2 = \frac{E}{2}. \end{aligned} \quad (2.90)$$

2.4.2 Dampened case

Now you dampen the oscillator linearly, modifying Eq. (2.85) accordingly

$$x'' = -kx - d x' \quad (2.91)$$

with a *damping* $d \geq 0$. If you insert a solution of the form $x = x_0 e^{-i\omega t}$ here, you get

$$-\omega^2 = -k + i d \omega \Leftrightarrow \omega^2 + i d \omega - k = 0. \quad (2.92)$$

From this it follows using the pq formula Eq. (A.5)

$$\omega = -i d \pm \sqrt{-d^2 + k}. \quad (2.93)$$

In the case $d = 0$, Eq. (2.86).

2.4.2.1 swing case

In the case

$$-d^2 + k > 0 \Leftrightarrow d^2 < k \quad (2.94)$$

applies

$$x(t) = \underbrace{x_0}_{\text{Anfangsamplitude}} \cdot \underbrace{\exp(-dt)}_{\text{Einhüllende}} \cdot \underbrace{\exp(\mp i t \sqrt{-d^2 + k})}_{\text{Oszillation}} \quad (2.95)$$

or

$$x(t) = x_0 \exp(-dt) \exp(-i t \sqrt{-d^2 + k}) + x_1 \exp(-dt) \exp(i t \sqrt{-d^2 + k}). \quad (2.96)$$

x_0 and x_1 result from the initial conditions. In this case, the damping has two consequences:

1. The natural frequency is now

$$\omega = \pm\sqrt{k - d^2}. \quad (2.97)$$

2. The initial amplitude decreases exponentially over time with the decay time $\tau = \frac{1}{d}$.

This case is called *swing case*.

2.4.2.2 creep case

In the case

$$-d^2 + k < 0 \Leftrightarrow d^2 > k \quad (2.98)$$

applies

$$\omega = -id \pm \sqrt{-d^2 + k} = -id \pm \sqrt{(-1) \cdot (d^2 - k)} = -id \pm \sqrt{-1} \underbrace{\sqrt{d^2 - k}}_{>0} = -id \pm i\sqrt{d^2 - k} = i \left(\underbrace{-d \pm \sqrt{d^2 - k}}_{<0} \right). \quad (2.99)$$

From this it follows

$$x(t) = x_0 \exp \left[-i^2 \left(-d \pm \sqrt{d^2 - k} \right) t \right] = x_0 \exp \left[\left(-d \pm \sqrt{d^2 - k} \right) t \right]. \quad (2.100)$$

or

$$x(t) = x_0 \exp \left[\left(-d + \sqrt{d^2 - k} \right) t \right] + x_1 \exp \left[\left(-d - \sqrt{d^2 - k} \right) t \right]. \quad (2.101)$$

So there is no longer any oscillation. This case is called *creep case*.

2.4.2.3 Aperiodic limit case

In borderline cases

$$-d^2 + k = 0 \Leftrightarrow d^2 = k \quad (2.102)$$

the two linearly independent solutions, which were found in the oscillating case and in the aperiodic limit case, shrink to one. Since it is based on a second-order differential equation, there must be another solution in this case. This is where the approach is made

$$x(t) = x_1 t \exp(-dt). \quad (2.103)$$

This implies

$$x'(t) = x_1 \exp(-dt) - dx_1 t \exp(-dt), \quad (2.104)$$

$$x''(t) = -dx_1 \exp(-dt) - dx_1 \exp(-dt) + d^2 x_1 t \exp(-dt) = -2dx_1 \exp(-dt) + d^2 x_1 t \exp(-dt). \quad (2.105)$$

From this it follows by inserting into Eq. (2.91)

$$\begin{aligned} -2dx_1 \exp(-dt) + d^2 x_1 t \exp(-dt) &= -kx_1 t \exp(-dt) - x_1 2d \exp(-dt) + 2d^2 x_1 t \exp(-dt) \\ \Leftrightarrow -2dx_1 + d^2 x_1 t &= -kx_1 t - 2x_1 d + 2d^2 x_1 t \\ \Leftrightarrow -2d + d^2 t &= -kt - 2d + 2d^2 t \\ \Leftrightarrow d^2 t &= -kt + 2d^2 t \\ \Leftrightarrow d^2 &= -k + 2d^2 \\ \Leftrightarrow -d^2 &= -k. \end{aligned}$$

This is according to Eq. (2.102) is met. Eq. (2.103) solves Equation (2.91). So the general solution in this case is:

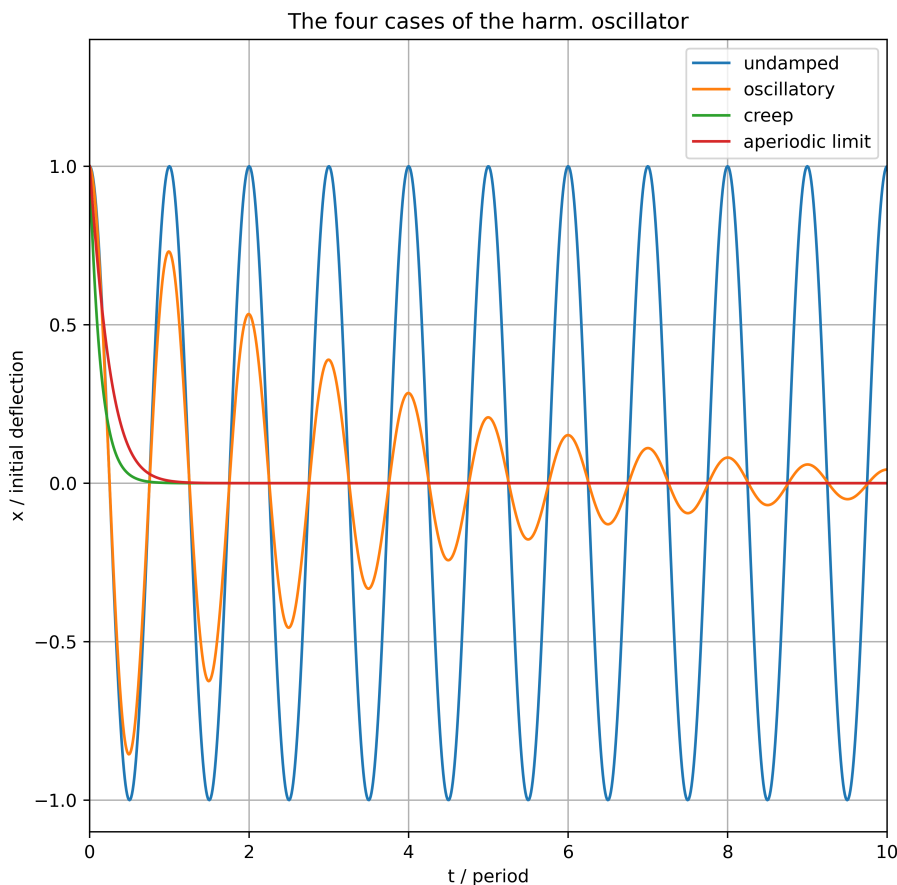


Figure 2.1: Solutions of the undriven harmonic oscillator.

$$x(t) = x_o \exp(-dt) + x_1 t \exp(-dt) = (x_o + x_1 t) \exp(-dt). \quad (2.106)$$

This case is called *aperiodic limit*. The four cases of the harmonic oscillator are shown in Fig. 2.1.

2.4.3 Powered case

Now you drive the system with the circular frequency ω , modifying Eq. (2.91) too

$$x'' + kx + \mathfrak{z}dx' = y_o \exp(-i\omega t) \quad (2.107)$$

with a real excitation amplitude $y_o > 0$. If you use the approach $x = x_o e^{-i\omega t}$ again, you get

$$\begin{aligned} -\omega^2 x_o + kx_o - \mathfrak{z}i\omega x_o &= y_o \\ \Leftrightarrow -\omega^2 + k - \mathfrak{z}i\omega &= \frac{y_o}{x_o} \end{aligned} \quad (2.108)$$

$$\Leftrightarrow \omega^2 - k + \mathfrak{z}i\omega = -\frac{y_o}{x_o} \quad (2.109)$$

$$\Leftrightarrow \omega^2 + \mathfrak{z}i\omega + \left(\frac{y_o}{x_o} - k \right) = 0. \quad (2.110)$$

The amplitude is independent of time, therefore ω is real. For x_o you now write down in polar coordinates

$$x_o = |x_o| \exp(i\varphi), \quad (2.111)$$

the real number φ is called the phase. If it is positive, the oscillator runs ahead of the excitation; if it is negative, the oscillator runs behind the excitation. Putting this into Eq. (2.110), you get

$$\omega^2 + 2id\omega + \left(\frac{y_o}{|x_o|} e^{-i\varphi} - k \right) = \omega^2 + 2id\omega + \left(\frac{y_o}{|x_o|} \cos(\varphi) - \frac{y_o}{|x_o|} i \sin(\varphi) - k \right) = 0. \quad (2.112)$$

ω is not an unknown here, it is given by the excitation. The unknowns are the reaction of the system $|x_o|, \varphi$. To determine this, write down the real and imaginary parts of Equation. (2.112):

$$\omega^2 + \left(\frac{y_o}{|x_o|} \cos(\varphi) - k \right) = 0, \quad (2.113)$$

$$2d\omega - \frac{y_o}{|x_o|} \sin(\varphi) = 0 \Rightarrow 2d\omega = \frac{y_o}{|x_o|} \sin(\varphi) \Rightarrow |x_o| = \frac{y_o}{2d\omega} \sin(\varphi). \quad (2.114)$$

If you put Eq. (2.114) in Eq. (2.113), you get

$$\begin{aligned} \omega^2 + \left(\frac{y_o}{\frac{y_o}{2d\omega} \sin(\varphi)} \cos(\varphi) - k \right) &= 0 \\ \Leftrightarrow \omega^2 + \left(\frac{2d\omega}{\tan(\varphi)} - k \right) &= 0 \\ \Leftrightarrow \omega^2 \tan(\varphi) + 2d\omega - k \tan(\varphi) &= 0 \\ \Leftrightarrow \tan(\varphi) (k - \omega^2) &= 2d\omega \\ \Leftrightarrow \tan(\varphi) &= \frac{2d\omega}{k - \omega^2}. \end{aligned} \quad (2.115)$$

The function

$$\varphi(\omega) = \arctan\left(\frac{2d\omega}{k - \omega^2}\right) \quad (2.116)$$

is called *phase spectrum*. Because $-\pi/2 < \varphi < \pi/2$ holds

$$\sin = \tan \cdot \cos = \tan \sqrt{1 - \sin^2} \Rightarrow \sin^2 = \tan^2 - \tan^2 \sin^2 \Rightarrow \sin^2 (1 + \tan^2) = \tan^2 \Rightarrow \sin = \frac{\tan}{\sqrt{1 + \tan^2}}. \quad (2.117)$$

If you now set Eq. (2.116) in Eq. (2.114), you get

$$|x_o| = \frac{y_o}{2d\omega} \sin(\varphi) = \frac{y_o}{2d\omega} \frac{\tan(\varphi)}{\sqrt{1 + \tan^2(\varphi)}} = \frac{y_o}{2d\omega} \frac{\frac{2d\omega}{k - \omega^2}}{\sqrt{1 + \frac{4d^2\omega^2}{(k - \omega^2)^2}}} = \frac{y_o}{(k - \omega^2) \sqrt{1 + \frac{4d^2\omega^2}{(k - \omega^2)^2}}}. \quad (2.118)$$

From this it follows

$$|x_o| = \frac{y_o}{\sqrt{(k - \omega^2)^2 + 4d^2\omega^2}}. \quad (2.119)$$

This function is called *amplitude spectrum*. One defines the auxiliary function h by

$$h(\omega) := (k - \omega^2)^2 + 4d^2\omega^2 \Rightarrow h'(\omega) = -4\omega(k - \omega^2) + 8d^2\omega = -4\omega k + 4\omega^3 + 8d^2\omega. \quad (2.120)$$

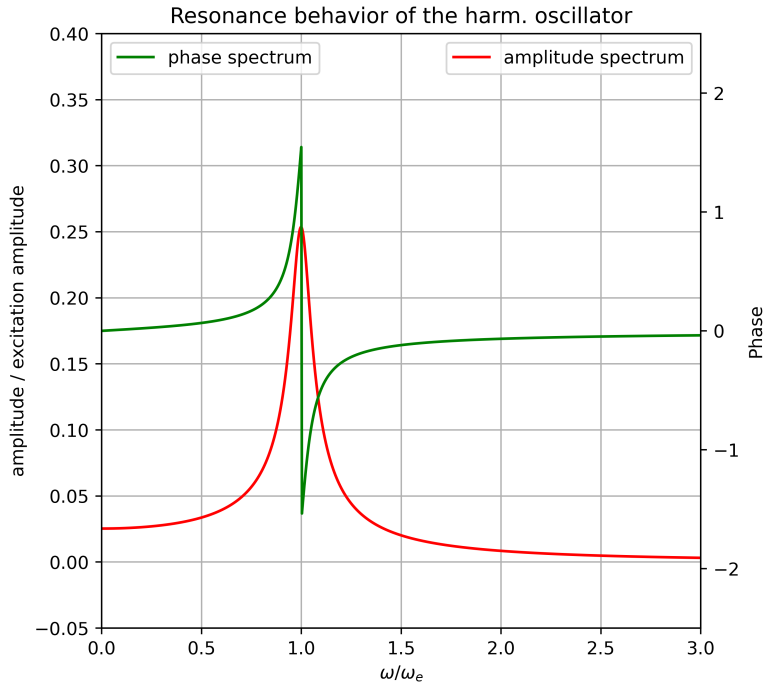


Figure 2.2: The resonance behavior of the driven harmonic oscillator.

Setting the derivative to zero results in

$$\begin{aligned} -4\omega k + 4\omega^3 + 8d^2\omega &\stackrel{!}{=} 0 \Rightarrow -4k + 4\omega^2 + 8d^2 = 0 \Rightarrow -k + \omega^2 + 2d^2 = 0 \\ &\Rightarrow \omega^2 = k - 2d^2. \end{aligned} \quad (2.121)$$

Here we limit ourselves to this case

$$k - 2d^2 > 0 \Leftrightarrow d < \sqrt{\frac{k}{2}}. \quad (2.122)$$

The frequency

$$\omega_{\text{res}} := \sqrt{k - 2d^2} \quad (2.123)$$

is called *resonance frequency*. For the second derivative of h one obtains

$$h''(\omega) = -4k + 12\omega^2 + 8d^2. \quad (2.124)$$

From this it follows

$$h''(\omega_{\text{res}}) = -4k + 12(k - 2d^2) + 8d^2 = -4k + 12k - 24d^2 + 8d^2 = 8k - 16d^2 = 8(k - 2d^2) > 0. \quad (2.125)$$

ω_{res} ist also die Frequenz maximaler Amplitude. Man beachte den Unterschied zwischen Eigenfrequenz Glg. (2.97) und Resonanzfrequenz Glg. (2.123). Das Resonanzverhalten ist in Abb. 2.2 dargestellt.

The system considered so far in this section has exactly one degree of freedom, namely the generalized deflection x . Conceptually, however, many of the findings can be generalized to systems with many degrees of freedom. Such complex systems (houses, circuits, the climate) also have their own modes.

3 ELECTRODYNAMICS

3.1 Lorentz force

For the force $\mathbf{F}$ on a particle with charge q , which moves with the speed $\mathbf{v}$ through the electromagnetic field $(\mathbf{E}, \mathbf{B})$, applies

$$\mathbf{F} = q \left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right). \quad (3.1)$$

This force is called *Lorentz force*.

3.2 Maxwell equations

The *Maxwell equations* (MWGen) for the electromagnetic field (EMF) $(\mathbf{E}, \mathbf{B})$ (ρ is the charge density and $\mathbf{j}$ is the current density) are

$$\nabla \cdot \mathbf{E} = 4\pi\rho, \quad (3.2)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (3.3)$$

$$\nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (3.4)$$

$$\nabla \times \mathbf{B} - \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \frac{4\pi}{c} \mathbf{j}. \quad (3.5)$$

Charges and currents are therefore sources of the electromagnetic field. The equations (3.1) - (3.5) are the basis of the ED, from which the theory follows. The MWGen have a memorable structure: They each consist of a differential equation for the divergent or rotational portion of the fields $\mathbf{E}, \mathbf{B}$. For each of the fields $\mathbf{E}$ and $\mathbf{B}$ there is a homogeneous and an inhomogeneous equation. With Gauss's and Stokes's theorems, the integral forms of Maxwell's equations result:

$$\int_{\partial V} \mathbf{E} \cdot d\mathbf{n} = 4\pi Q \quad (3.6)$$

$$\int_{\partial V} \mathbf{B} \cdot d\mathbf{n} = 0 \quad (3.7)$$

$$\int_{\partial A} \mathbf{E} \cdot d\mathbf{s} + \frac{1}{c} \frac{\partial}{\partial t} \int_A \mathbf{B} \cdot d\mathbf{n} = 0 \quad (3.8)$$

$$\int_{\partial A} \mathbf{B} \cdot d\mathbf{s} - \frac{1}{c} \frac{\partial}{\partial t} \int_A \mathbf{E} \cdot d\mathbf{n} = \frac{4\pi}{c} I \quad (3.9)$$

Here Q is the charge in V and I is the current passing through A . The corresponding experimental findings that led to the formulation of the equations are the following:

- Coulomb's Law
- There are no magnetic monopoles.
- Faraday's law of induction
- Ampère's law and Maxwell's displacement current

3.2.1 Formulation about potentials

If you write down the MWGen component by component, you get eight equations for the six components of the electromagnetic field. The question therefore arises as to whether the MWGen are overdetermined and do not have non-trivial solutions. This section shows that this is not the case.

Because of Eq. (3.3) exists a vector field $\mathbf{A}$ with

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad (3.10)$$

the field $\mathbf{A}$ is called *the vector potential*. This means that Eq. (3.3) according to Eq. (B.48) is met. Because of the third Maxwell equation Eq. (3.4) applies

$$\nabla \times \left(\mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right) = \mathbf{0}. \quad (3.11)$$

So there exists a potential φ with

$$\mathbf{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}, \quad (3.12)$$

φ is called *the scalar potential*. So Eq. (3.4) fulfilled. The definitions of the potentials are therefore obtained from the homogeneous Maxwell equations. If you put the previous specifications in Eq. (3.5), one obtains with Eq. (B.54)

$$-\Delta \mathbf{A} + \nabla (\nabla \cdot \mathbf{A}) + \frac{1}{c} \nabla \frac{\partial \varphi}{\partial t} + \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = \frac{4\pi}{c} \mathbf{j}. \quad (3.13)$$

If you add a conservative field $\nabla \varphi'$ to $\mathbf{A}$, $\mathbf{B}$ does not change. With the replacement

$$\varphi \rightarrow \varphi - \frac{1}{c} \frac{\partial \varphi'}{\partial t} \quad (3.14)$$

$\mathbf{E}$ does not change either.

This is called the gauge invariance of the MWGen. The calibration can be determined by any linear relationship between the potentials, with the *Lorenz calibration*

$$\nabla \cdot \mathbf{A} + \frac{1}{c} \frac{\partial \varphi}{\partial t} = \mathbf{0} \quad (3.15)$$

becomes the fourth MWG

$$\Delta \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\frac{4\pi}{c} \mathbf{j}. \quad (3.16)$$

The first MWG will be closed

$$-\Delta \varphi - \frac{1}{c} \frac{\partial}{\partial t} \nabla \cdot \mathbf{A} = 4\pi \rho \Leftrightarrow \Delta \varphi - \frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} = -4\pi \rho. \quad (3.17)$$

This gives four linear, independent differential equations for φ , $\mathbf{A}$, which replace the Maxwell equations. The EMF ($\mathbf{E}$, $\mathbf{B}$) can be determined from this using the equations (3.12) and (3.10).

3.2.2 Continuity equation of charge

If one forms the partial time derivative of Eq. (3.2), multiplies the divergence of Eq. (3.5) with c and adding the two resulting equations, you get

$$\nabla \cdot \frac{\partial \mathbf{E}}{\partial t} - \nabla \cdot \frac{\partial \mathbf{E}}{\partial t} = 4\pi \frac{\partial \rho}{\partial t} + 4\pi \nabla \cdot \mathbf{j}$$

$$\Leftrightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0. \quad (3.18)$$

This is the charge continuity equation.

3.2.3 Lagrange and Hamilton functions of a particle in the EMF

Now the Lagrange and Hamilton functions of a particle with mass m and charge q in the electromagnetic field $(\mathbf{E}, \mathbf{B})$ should be derived. If one sets the potential $U = U(\mathbf{r}, \dot{\mathbf{r}}, t)$

$$U(\mathbf{r}, \dot{\mathbf{r}}, t) = q\varphi(\mathbf{r}, t) - \frac{q}{c} \mathbf{A}(\mathbf{r}, t) \cdot \dot{\mathbf{r}}, \quad (3.19)$$

it follows from Eq. (2.61)

$$\begin{aligned} \mathbf{F}(\mathbf{r}, \dot{\mathbf{r}}, t) &\stackrel{\text{Glg. (B.52)}}{=} -q\nabla\varphi + \frac{q}{c}(\dot{\mathbf{r}} \cdot \nabla)\mathbf{A} + \frac{q}{c}\dot{\mathbf{r}} \times \mathbf{B} - \frac{q}{c} \frac{D}{Dt}\mathbf{A} = q \left(-\nabla\varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \frac{1}{c} \dot{\mathbf{r}} \times \mathbf{B} \right) \\ &= q \left(\mathbf{E} + \frac{\dot{\mathbf{r}}}{c} \times \mathbf{B} \right). \end{aligned} \quad (3.20)$$

This results in the Lorentz force according to Eq. (3.1), this shows the correctness of the approach Eq. (D.173). So the Lagrange function of a particle in the EMF is

$$L(\mathbf{r}, \dot{\mathbf{r}}, t) = \frac{m}{2} \dot{\mathbf{r}}^2 - q\varphi(\mathbf{r}, t) + \frac{q}{c} \dot{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}, t) \quad (3.21)$$

This follows for the canonical impulses

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + \frac{q}{c} A_i \Rightarrow \dot{x}_i = \frac{1}{m} \left(p_i - \frac{q}{c} A_i \right). \quad (3.22)$$

For the Hamilton function $H = H(\mathbf{r}, \mathbf{p}, t)$ therefore applies

$$\begin{aligned} H(\mathbf{r}, \mathbf{p}, t) &= \frac{1}{m} \left(\mathbf{p} - \frac{q}{c} \mathbf{A} \right) \cdot \mathbf{p} - \frac{m}{2} \frac{1}{m^2} \left(\mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 + q\varphi(\mathbf{r}, t) - \frac{q}{cm} \left(\mathbf{p} - \frac{q}{c} \mathbf{A} \right) \cdot \mathbf{A}(\mathbf{r}, t) \\ &= \frac{1}{m} \left(\mathbf{p} - \frac{q}{c} \mathbf{A} \right) \left(\mathbf{p} - \frac{1}{2} \left(\mathbf{p} - \frac{q}{c} \mathbf{A} \right) - \frac{q}{c} \mathbf{A} \right) + q\varphi(\mathbf{r}, t) = \frac{1}{2m} \left(\mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 + q\varphi(\mathbf{r}, t). \end{aligned} \quad (3.23)$$

3.3 Electromagnetic waves

In a vacuum the MWGen is

$$\nabla \cdot \mathbf{E} = 0, \quad (3.24)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (3.25)$$

$$\nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (3.26)$$

$$\nabla \times \mathbf{B} - \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = 0. \quad (3.27)$$

If you apply $\nabla \times$ to the equations (3.26) and (3.27), you get

$$-\Delta \mathbf{E} + \frac{1}{c} \frac{\partial}{\partial t} \nabla \times \mathbf{B} = 0 \Leftrightarrow \Delta \mathbf{E} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} = 0, \quad (3.28)$$

$$-\Delta \mathbf{B} - \frac{1}{c} \frac{\partial}{\partial t} \nabla \times \mathbf{E} = 0 \Leftrightarrow \Delta \mathbf{B} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{B} = 0, \quad (3.29)$$

so wave equations for the EMF $(\mathbf{E}, \mathbf{B})$. Approaches are now being made

$$\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}, \quad \mathbf{B} = \mathbf{B}_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t + \varphi)}. \quad (3.30)$$

More general waves can be obtained with the FT from the superposition of such plane waves. One immediately sees that electromagnetic waves in a vacuum are dispersion-free and have phase velocity c . One is interested in the ratio of the amplitudes $\mathbf{E}_0$, $\mathbf{B}_0$, as well as the phase shift φ . From the equations (3.24) and (3.25) it follows $\mathbf{E}_0, \mathbf{B}_0 \perp \mathbf{k}$. Electromagnetic waves are therefore transverse waves. One continues with Eq. (B.51)

$$\nabla \times \mathbf{E} = -i\mathbf{E} \times \mathbf{k}. \quad (3.31)$$

Also apply

$$\nabla \times \mathbf{B} = -i\mathbf{B} \times \mathbf{k}, \quad \frac{\partial \mathbf{E}}{\partial t} = -i\omega \mathbf{E}, \quad \frac{\partial \mathbf{B}}{\partial t} = -i\omega \mathbf{B}. \quad (3.32)$$

If you insert this into the equations (3.26) - (3.27), you get

$$-i\mathbf{E} \times \mathbf{k} - \frac{1}{c} i\omega \mathbf{B} = \mathbf{0}, \quad (3.33)$$

$$-i\mathbf{B} \times \mathbf{k} + \frac{1}{c} i\omega \mathbf{E} = \mathbf{0}. \quad (3.34)$$

With $c = \frac{\omega}{k}$ it follows

$$\mathbf{E} \times \mathbf{k} = -k\mathbf{B}. \quad (3.35)$$

Follow from this

$$\mathbf{E} \cdot \mathbf{B} = 0, \varphi = 0. \quad (3.36)$$

Since $\mathbf{E} \perp \mathbf{k}$,

$$E = B \quad (3.37)$$

and thus

$$E_0 = B_0. \quad (3.38)$$

3.4 Energy of the electromagnetic field

To determine the energy of the electromagnetic field, consider a system of N charges q_i at locations $\mathbf{r}_i$. The work that the electromagnetic field does on this system is, according to Eq. (3.1) given by

$$\begin{aligned} W &= \sum_{i=1}^N \int \mathbf{F}(\mathbf{r}_i) \cdot \frac{d\mathbf{r}_i}{dt} dt = \sum_{i=1}^N \int q_i \left(\mathbf{E}(\mathbf{r}_i) + \frac{1}{c} \frac{d\mathbf{r}_i}{dt} \times \mathbf{B} \right) \cdot \frac{d\mathbf{r}_i}{dt} dt \\ &= \sum_{i=1}^N \int q_i \mathbf{E}(\mathbf{r}_i) \cdot \frac{d\mathbf{r}_i}{dt} dt. \end{aligned} \quad (3.39)$$

It follows

$$\frac{dW}{dt} = \sum_{i=1}^N q_i \mathbf{E}(\mathbf{r}_i) \cdot \frac{d\mathbf{r}_i}{dt}. \quad (3.40)$$

Here you can see the current density

$$\mathbf{j}(\mathbf{r}, t) = \sum_{i=1}^N q_i \mathbf{v}_i \delta(\mathbf{r} - \mathbf{r}_i) \quad (3.41)$$

insert:

$$\frac{dW}{dt} = \int_{\mathbb{R}^3} \mathbf{j} \cdot \mathbf{E} d^3r \quad (3.42)$$

This can be transformed using Maxwell's equations,

$$\mathbf{j} \cdot \mathbf{E} = \frac{c}{4\pi} \mathbf{E} \cdot \nabla \times \mathbf{B} - \frac{1}{4\pi} \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t}. \quad (3.43)$$

With Eq. (B.55) is obtained

$$\mathbf{j} \cdot \mathbf{E} = -\frac{c}{4\pi} \nabla \cdot (\mathbf{E} \times \mathbf{B}) + \frac{c}{4\pi} \mathbf{B} \cdot \nabla \times \mathbf{E} - \frac{1}{8\pi} \frac{\partial \mathbf{E}^2}{\partial t} = -\frac{c}{4\pi} \nabla \cdot (\mathbf{E} \times \mathbf{B}) - \frac{1}{8\pi} \frac{\partial}{\partial t} (\mathbf{E}^2 + \mathbf{B}^2). \quad (3.44)$$

Now define the energy density w of the electromagnetic field by

$$w(\mathbf{r}, t) := \frac{1}{8\pi} (\mathbf{E}^2 + \mathbf{B}^2) \quad (3.45)$$

as well as the radiation flux density as

$$\mathbf{S}(\mathbf{r}, t) := \frac{c}{4\pi} (\mathbf{E} \times \mathbf{B}). \quad (3.46)$$

This follows

$$\frac{\partial w}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{j} \cdot \mathbf{E}. \quad (3.47)$$

Eq. (3.47) is the *Poynting theorem*. This can still be illustrated. One integrates Eq. (3.47) over a time-independent volume V :

$$\frac{\partial}{\partial t} \int_V w(\mathbf{r}, t) d^3r + \int_{\partial V} \mathbf{S} \cdot d\mathbf{n} = -\frac{dW}{dt}. \quad (3.48)$$

Is Eq. (9.33) is the energy density of the electromagnetic field, so is

$$U = \int_V w(\mathbf{r}, t) d^3r \quad (3.49)$$

the energy of the same. Thus follows

$$\frac{dU}{dt} + \frac{dW}{dt} = - \int_{\partial V} \mathbf{S} \cdot d\mathbf{n}. \quad (3.50)$$

3.4.1 Radiation quantities

Radiation means energy transport through electromagnetic waves. The physical quantities that describe radiation are called radiation quantities. The spectral quantities are to be understood as follows: Imagine a device that

Radiation size	SI unit	Definition
radiant energy	J	the energy transferred to a system in a specific time interval
spectral radiant energy	J/m	radiant energy per wavelength
Radiation flux	W	the temporal rate at which energy is transferred by radiation
spectral radiant flux	W/m	radiant flux per wavelength
radiant flux density	W/m ²	i. A. vector quantity, radiant energy that passes through a certain area per time
spectral radiant flux density	W/m ³	radiant flux density per wavelength
Strahldichte	W/m ²	Strahlungsflussdichte pro Raumwinkel
spectral radiance	W/m ³	radiance per wavelength
Energiedichte	J/m ³	Energie, die pro Volumen in Form elektromagnetischer Wellen vorhanden ist
spectral energy density	J/m ⁴	energy density per wavelength

Table 3.1: Summary of definitions of radiation quantities.

can measure the underlying quantity filtered by wavelength. For example, you measure a radiation flux φ that acts on a system, but the measurement stops at a wavelength $\lambda > \circ$. This is how you define the function $\varphi(\lambda)$. The derivative of this function $\varphi_\lambda := \frac{d\varphi}{d\lambda}$ after λ is called *spectral radiation flux*, since this quantity allows a statement about the spectral distribution of the energy. It applies

$$\varphi = \int_{\circ}^{\infty} \varphi_\lambda d\lambda. \quad (3.51)$$

Spectral radiation quantities can also be defined by deriving them from the frequency. The word *spectral* is sometimes omitted.

3.5 Special theory of relativity

The MWGen gives the phase velocity c for electromagnetic waves in vacuum in every IS. This is a contradiction to the Galileo transformation. This is therefore incorrect and should be replaced by the *Lorentz transformation*, which must contain the Galilei transformation as a limiting case for velocities $v \ll c$. This is the statement of the special theory of relativity.

An element $(x^{(a)})$ of the *spacetime* is defined by a *4-vector*

$$(x^{(a)}) := \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}, \quad (3.52)$$

spacetime is the set of all 4 vectors. x, y, z are Cartesian coordinates in an IS, t is the time coordinate determined by an arbitrary time zero point $t_{\circ}$. Greek indices are always supposed to run from zero to three. One further defines an *event* as a measurable physical process without temporal and spatial extension. Let two events be denoted by the indices 1 and 2, then they can be defined by their corresponding space-time coordinates:

$$\begin{aligned} (x_1^{(a)}) &= \begin{pmatrix} ct_1 \\ x_1 \\ y_1 \\ z_1 \end{pmatrix}, \\ (x_2^{(a)}) &= \begin{pmatrix} ct_2 \\ x_2 \\ y_2 \\ z_2 \end{pmatrix}. \end{aligned} \quad (3.53)$$

One defines the *distance* $s_{1,2}^2$ of the two events in spacetime by

$$s_{1,2}^2 := c^2 (t_2 - t_1)^2 - (x_2 - x_1)^2 - (y_2 - y_1)^2 - (z_2 - z_1)^2. \quad (3.54)$$

Now define an IS' whose axes are parallel to those of IS and which moves with a constant speed $\mathbf{v} = v\mathbf{e}_x$ relative to IS. At time $t = t' = 0$ the origins of the two KS are at the same place. Experimentally one finds

$$s_{1,2}^2 = s_{1,2}'^2. \quad (3.55)$$

For a photon (or an electromagnetic wavefront) moving in every IS with c , holds

$$s_{1,2}^2 = s_{1,2}'^2 = 0, \quad (3.56)$$

so the statement is clear. For a particle moving in a straight line and uniformly

$$s_{1,2}^2 = (c^2 - v^2) (t_2 - t_1)^2 = (c^2 - v'^2) (t'_2 - t'_1)^2 = s_{1,2}'^2 \quad (3.57)$$

to be verified experimentally. Now we further define the matrix η by

$$\eta := \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{I} \end{pmatrix}. \quad (3.58)$$

This allows the distance between two events ds to be developed linearly:

$$ds^2 = c^2 dt^2 - dx^2 - dy^2 - dz^2 = \sum_{a=0}^3 \sum_{\beta=0}^3 \eta_{a,\beta} dx^{(a)} dx^{(\beta)} =: \eta_{a,\beta} dx^{(a)} dx^{(\beta)} \quad (3.59)$$

Here, the *Einstein's sum convention* was introduced: Two identical indices, one of which is at the bottom and the other at the top, are summed. Now we start with the Lorentz transformation

$$x'^{(a)} = \Lambda_{\beta}^{(a)} x^{(\beta)} + b^{(a)}. \quad (3.60)$$

From this it follows

$$dx'^{(a)} = \Lambda_{\beta}^{(a)} dx^{(\beta)}. \quad (3.61)$$

Now you ask $ds^2 = ds'^2$ and get

$$\begin{aligned} ds'^2 &= \eta_{a,\beta} dx'^{(a)} dx'^{(\beta)} = \eta_{a,\beta} dx'^{(a)} \Lambda_{\delta}^{(\beta)} dx^{(\delta)} = \eta_{a,\beta} \Lambda_{\gamma}^{(a)} dx^{(\gamma)} \Lambda_{\delta}^{(\beta)} dx^{(\delta)} \\ &= \eta_{a,\beta} \Lambda_{\gamma}^{(a)} \Lambda_{\delta}^{(\beta)} dx^{(\gamma)} dx^{(\delta)} = \eta_{\gamma,\delta} dx^{(\gamma)} dx^{(\delta)} = ds^2. \end{aligned} \quad (3.62)$$

Since this is supposed to apply to all dx and dx' ,

$$\eta_{\gamma,\delta} = \eta_{a,\beta} \Lambda_{\gamma}^{(a)} \Lambda_{\delta}^{(\beta)}. \quad (3.63)$$

This means

$$\eta_{\gamma,\delta} = \sum_{a,\beta=0}^3 \eta_{a,\beta} \Lambda_{\gamma}^{(a)} \Lambda_{\delta}^{(\beta)} = \sum_{a=0}^3 \Lambda_{\gamma}^{(a)} \sum_{\beta=0}^3 \eta_{a,\beta} \Lambda_{\delta}^{(\beta)} = \sum_{a=0}^3 \left(\Lambda_{\gamma}^{(a)} \right)^T \sum_{\beta=0}^3 \eta_{a,\beta} \Lambda_{\delta}^{(\beta)} = (\Lambda^T \eta \Lambda)_{\gamma,\delta}, \quad (3.64)$$

so

$$\Lambda^T \eta \Lambda = \eta. \quad (3.65)$$

For the arrangement of two KS IS and IS' described above, $\mathbf{b} = \mathbf{o}$. Furthermore, the assumptions $y' = y$ and $z' = z$ make sense. The transformation between (x, t) and (x', t') cannot depend on the y or z coordinates, since rotating both CS around the x axis must not lead to any change. So the transformation matrix Λ has the form

$$\Lambda = \begin{pmatrix} \Lambda_o^{(o)} & \Lambda_I^{(o)} & \mathbf{o} & \mathbf{o} \\ \Lambda_o^{(i)} & \Lambda_I^{(i)} & \mathbf{o} & \mathbf{o} \\ \mathbf{o} & \mathbf{o} & \mathbf{1} & \mathbf{0} \\ \mathbf{o} & \mathbf{o} & \mathbf{0} & \mathbf{1} \end{pmatrix}. \quad (3.66)$$

Furthermore, the origin of IS'

$$x^{(o)} = ct \leftrightarrow x'^{(o)} = ct', \quad (3.67)$$

$$x^{(i)} = vt \leftrightarrow x'^{(i)} = \mathbf{o}, \quad (3.68)$$

$$x^{(2)} = \mathbf{o} \leftrightarrow x'^{(2)} = \mathbf{o}, \quad (3.69)$$

$$x^{(3)} = \mathbf{o} \leftrightarrow x'^{(3)} = \mathbf{o}. \quad (3.70)$$

From Eq. (3.65) follows

$$\begin{aligned} & \begin{pmatrix} \Lambda_o^{(o)} & \Lambda_o^{(i)} \\ \Lambda_I^{(o)} & \Lambda_I^{(i)} \end{pmatrix} \begin{pmatrix} \mathbf{1} & \mathbf{o} \\ \mathbf{o} & -\mathbf{1} \end{pmatrix} \begin{pmatrix} \Lambda_o^{(o)} & \Lambda_I^{(o)} \\ \Lambda_o^{(i)} & \Lambda_I^{(i)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{o} \\ \mathbf{o} & -\mathbf{1} \end{pmatrix} \\ & \Rightarrow \begin{pmatrix} \Lambda_o^{(o)} & -\Lambda_o^{(i)} \\ \Lambda_I^{(o)} & -\Lambda_I^{(i)} \end{pmatrix} \begin{pmatrix} \Lambda_o^{(o)} & \Lambda_I^{(o)} \\ \Lambda_o^{(i)} & \Lambda_I^{(i)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{o} \\ \mathbf{o} & -\mathbf{1} \end{pmatrix} \\ & \Rightarrow \begin{pmatrix} \left(\Lambda_o^{(o)}\right)^2 - \left(\Lambda_o^{(i)}\right)^2 & \Lambda_o^{(o)}\Lambda_I^{(o)} - \Lambda_o^{(i)}\Lambda_I^{(i)} \\ \Lambda_o^{(o)}\Lambda_I^{(o)} - \Lambda_o^{(i)}\Lambda_I^{(i)} & \left(\Lambda_o^{(i)}\right)^2 - \left(\Lambda_I^{(i)}\right)^2 \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{o} \\ \mathbf{o} & -\mathbf{1} \end{pmatrix}. \end{aligned} \quad (3.71)$$

From this follow the three conditions

$$\left(\Lambda_o^{(o)}\right)^2 - \left(\Lambda_o^{(i)}\right)^2 = \mathbf{1}, \quad (3.72)$$

$$\left(\Lambda_o^{(i)}\right)^2 - \left(\Lambda_I^{(i)}\right)^2 = -\mathbf{1}, \quad (3.73)$$

$$\Lambda_o^{(o)}\Lambda_I^{(o)} - \Lambda_o^{(i)}\Lambda_I^{(i)} = \mathbf{o}. \quad (3.74)$$

One can assume ψ, φ for two real numbers

$$\Lambda_o^{(i)} = -\sinh(\psi), \quad (3.75)$$

$$\Lambda_I^{(o)} = -\sinh(\varphi). \quad (3.76)$$

So they apply

$$\Lambda_o^{(o)} = \pm \cosh(\psi), \Lambda_I^{(i)} = \pm \cosh(\varphi). \quad (3.77)$$

The identical transformation should result for $\psi, \varphi \rightarrow \mathbf{o}$, so exclude the minus sign at this point. The third condition is

$$\cosh(\psi) \sinh(\varphi) = \cosh(\varphi) \sinh(\psi), \quad (3.78)$$

from this it follows $\psi = \varphi$. So it applies

$$\begin{pmatrix} \Lambda_o^{(o)} & \Lambda_I^{(o)} \\ \Lambda_o^{(i)} & \Lambda_I^{(i)} \end{pmatrix} = \begin{pmatrix} \cosh(\psi) & -\sinh(\psi) \\ -\sinh(\psi) & \cosh(\psi) \end{pmatrix}. \quad (3.79)$$

Therefore applies

$$x'^{(i)} = \mathbf{o} = -\sinh(\psi) ct + \cosh(\psi) x^{(i)} = [-\sinh(\psi) c + \cosh(\psi) v] t. \quad (3.80)$$

From this it follows

$$\tanh(\psi) = \frac{v}{c} \Rightarrow \psi = \operatorname{artanh}\left(\frac{v}{c}\right). \quad (3.81)$$

ψ is called *Rapidity*. One continues to define

$$\gamma := \cosh(\psi) = \frac{1}{\sqrt{1 - \tanh(\psi)^2}} = \frac{1}{\sqrt{1 - v^2/c^2}}, \quad (3.82)$$

then applies

$$\sinh(\psi) = \gamma \frac{v}{c}. \quad (3.83)$$

In this case the Lorentz transformation is complete

$$\begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma \frac{v}{c} & 0 & 0 \\ -\gamma \frac{v}{c} & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} \quad (3.84)$$

set.

3.6 Relativistic treatment of the electromagnetic field

The equations of the potentials (3.16) and (3.17) as well as the Lorenz calibration (3.15) are summarized again here:

$$\left(\Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \varphi = -4\pi \rho, \quad (3.85)$$

$$\left(\Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) \mathbf{A} = -4\pi \mathbf{j}, \quad (3.86)$$

$$\frac{1}{c} \frac{\partial \varphi}{\partial t} + \nabla \cdot \mathbf{A} = 0. \quad (3.87)$$

Now the 4-vector

$$\left(A^{(a)}\right) := \begin{pmatrix} \varphi \\ A_x \\ A_y \\ A_z \end{pmatrix} \quad (3.88)$$

defined. Define further

$$\left(j^{(a)}\right) := \begin{pmatrix} \rho \\ j_x \\ j_y \\ j_z \end{pmatrix} \quad (3.89)$$

It is defined as a shorthand notation for partial derivatives

$$\partial_0 = \partial^{(0)} := \frac{1}{c} \frac{\partial}{\partial t}, \quad (3.90)$$

$$\partial^{(i)} := \frac{\partial}{\partial x_i} = -\frac{\partial}{\partial x^{(i)}} = -\partial_i \quad (3.91)$$

for $1 \leq i \leq 3$. With the *d'Alembert operator*

$$\square := \partial_\beta \partial^{(\beta)} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta \quad (3.92)$$

you can do this as

$$\square A^{(a)} = \frac{4\pi}{c} j^{(a)} \quad (3.93)$$

note down. The Lorenz calibration is therefore written as:

$$\partial_a A^{(a)} = 0. \quad (3.94)$$

One defines the *field strength tensor* $F^{(a,\beta)}$ by

$$F^{(a,\beta)} = \partial^{(a)} A^{(\beta)} - \partial^{(\beta)} A^{(a)}. \quad (3.95)$$

This matrix is antisymmetric:

$$F^{(\beta,a)} = \partial^{(\beta)} A^{(a)} - \partial^{(a)} A^{(\beta)} = - \left(\partial^{(a)} A^{(\beta)} - \partial^{(\beta)} A^{(a)} \right) = -F^{(a,\beta)} \quad (3.96)$$

At this point it is still on

$$\mathbf{E} = -\nabla\varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A} \quad (3.97)$$

remembered. It applies

$$\begin{aligned} F^{(a,\beta)} &= \begin{pmatrix} 0 & \frac{1}{c} \frac{\partial A_x}{\partial t} + \frac{\partial \varphi}{\partial x} & \frac{1}{c} \frac{\partial A_y}{\partial t} + \frac{\partial \varphi}{\partial y} & \frac{1}{c} \frac{\partial A_z}{\partial t} + \frac{\partial \varphi}{\partial z} \\ -\frac{\partial \varphi}{\partial x} - \frac{1}{c} \frac{\partial A_x}{\partial t} & 0 & \frac{\partial}{\partial y} - \frac{\partial}{\partial x} & \frac{\partial}{\partial z} - \frac{\partial}{\partial x} \\ -\frac{\partial \varphi}{\partial y} - \frac{1}{c} \frac{\partial A_y}{\partial t} & \frac{\partial}{\partial x} - \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial z} - \frac{\partial}{\partial y} \\ -\frac{\partial \varphi}{\partial z} - \frac{1}{c} \frac{\partial A_z}{\partial t} & \frac{\partial}{\partial x} - \frac{\partial}{\partial z} & \frac{\partial}{\partial y} - \frac{\partial}{\partial z} & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix}. \end{aligned} \quad (3.98)$$

Consider again the two KS IS and IS', which were already worked with in Sect. 3.5. The electromagnetic fields in the systems are denoted by $(\mathbf{E}, \mathbf{B})$ and $(\mathbf{E}', \mathbf{B}')$. The field strength tensors transform with Eq. (3.84) like

$$\begin{aligned} F' &= \Lambda F \Lambda^T = \Lambda \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix} \begin{pmatrix} \gamma & -\gamma \frac{v}{c} & 0 & 0 \\ -\gamma \frac{v}{c} & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \gamma & -\gamma \frac{v}{c} & 0 & 0 \\ -\gamma \frac{v}{c} & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \gamma E_x \frac{v}{c} & -\gamma E_x & -E_y & -E_z \\ \gamma E_x & -\gamma E_x \frac{v}{c} & -B_z & B_y \\ \gamma E_x - \gamma B_z \frac{v}{c} & -\gamma E_y \frac{v}{c} + \gamma B_z & 0 & -B_x \\ \gamma E_z + \gamma B_y \frac{v}{c} & -\gamma E_z \frac{v}{c} - \gamma B_y & B_x & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -\gamma^2 E_x + \gamma^2 E_x \frac{v^2}{c^2} & -\gamma E_y + B_z \gamma \frac{v}{c} & -E_z \gamma - B_y \gamma \frac{v}{c} \\ -\gamma^2 E_x \frac{v^2}{c^2} + \gamma^2 E_x & 0 & E_y \gamma \frac{v}{c} - B_z \gamma & E_z \gamma \frac{v}{c} + \gamma B_y \\ \gamma E_x - \gamma B_z \frac{v}{c} & -\gamma E_y \frac{v}{c} + \gamma B_z & 0 & -B_x \\ \gamma E_z + \gamma B_y \frac{v}{c} & -\gamma E_z \frac{v}{c} - \gamma B_y & B_x & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -E_x & -\gamma E_y + B_z \gamma \frac{v}{c} & -E_z \gamma - B_y \gamma \frac{v}{c} \\ E_x & 0 & E_y \gamma \frac{v}{c} - B_z \gamma & E_z \gamma \frac{v}{c} + \gamma B_y \\ \gamma E_x - \gamma B_z \frac{v}{c} & -\gamma E_y \frac{v}{c} + \gamma B_z & 0 & -B_x \\ \gamma E_z + \gamma B_y \frac{v}{c} & -\gamma E_z \frac{v}{c} - \gamma B_y & B_x & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -E'_x & -E'_y & -E'_z \\ E'_x & 0 & -B'_z & B'_y \\ E'_y & B'_z & 0 & -B'_x \\ E'_z & -B'_y & B'_x & 0 \end{pmatrix}. \end{aligned} \quad (3.99)$$

Follow from this

$$E'_x = E_x, \quad E'_y = \gamma \left(E_y - B_z \frac{v}{c} \right), \quad E'_z = \gamma \left(E_z + B_y \frac{v}{c} \right), \quad (3.100)$$

$$B'_x = B_x, \quad B'_y = \gamma \left(B_y + E_z \frac{v}{c} \right), \quad B'_z = \gamma \left(B_z - E_y \frac{v}{c} \right). \quad (3.101)$$

This can be generalized vectorially to:

$$\mathbf{E}'_{\parallel} = \mathbf{E}_{\parallel}, \quad (3.102)$$

$$\mathbf{B}'_{\parallel} = \mathbf{B}_{\parallel}, \quad (3.103)$$

$$\mathbf{E}'_{\perp} = \gamma \left(\mathbf{E}_{\perp} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right), \quad (3.104)$$

$$\mathbf{B}'_{\perp} = \gamma \left(\mathbf{B}_{\perp} - \frac{\mathbf{v}}{c} \times \mathbf{E} \right), \quad (3.105)$$

where components parallel and perpendicular to $\mathbf{v}$ are meant. The inverse transformation is obtained with $\mathbf{v} \rightarrow \mathbf{v}'$

$$\mathbf{E}_{\parallel} = \mathbf{E}'_{\parallel}, \quad \mathbf{B}_{\parallel} = \mathbf{B}'_{\parallel}, \quad (3.106)$$

$$\mathbf{E}_{\perp} = \gamma \left(\mathbf{E}'_{\perp} - \frac{\mathbf{v}}{c} \times \mathbf{B}' \right), \quad \mathbf{B}_{\perp} = \gamma \left(\mathbf{B}'_{\perp} + \frac{\mathbf{v}}{c} \times \mathbf{E}' \right). \quad (3.107)$$

4 QUANTUM MECHANICS

Only the basics of quantum mechanics (QM) are explained here; for a more detailed explanation see [11]. In QM, the trajectory $\mathbf{r}(t)$ is replaced by the wave function $\psi(\mathbf{r}, t)$ to determine the state of a particle without spin. ψ is i. A. complex-valued and $|\psi(\mathbf{r}, t)|^2$ is the probability density of finding the particle at $\mathbf{r}$ at time t . For functions $f, g : \mathbb{R}^3 \rightarrow \mathbb{C}$ one defines the unitary product $\langle | \rangle$ by

$$\langle f | g \rangle := \int_{\mathbb{R}^3} f^* g d^3 r. \quad (4.1)$$

Since the particle is somewhere,

$$\langle \psi | \psi \rangle = 1. \quad (4.2)$$

The *Schrödinger equation* (SG) applies

$$\hat{H}\psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} \quad (4.3)$$

with the *Hamilton operator*

$$\hat{H} := -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}). \quad (4.4)$$

Here $\hbar := \frac{h}{2\pi}$ with the *Planck's constant* h . An operator turns a function into a new function and is identified by an umbrella symbol. Two further axiomatic assumptions of QM are the *de Broglie relation*

$$\mathbf{p} = \hbar \mathbf{k} \quad (4.5)$$

for the connection between momentum $\mathbf{p}$ and circular wave number $\mathbf{k}$ of a particle as well as the *Planck-Einstein relation*

$$E = \hbar \omega \quad (4.6)$$

for the connection between energy E and angular frequency ω . A plane wave can therefore pass through

$$\psi(\mathbf{r}, t) = \psi_{\circ} \exp(i(\mathbf{k} \cdot \mathbf{r} - \omega t)) = \psi_{\circ} \exp\left(\frac{i}{\hbar}(\mathbf{p} \cdot \mathbf{r} - Et)\right) \quad (4.7)$$

be noted. Here it is found that

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = E \psi(\mathbf{r}, t) \quad (4.8)$$

applies, so the right side of the SG pulls the energy forward. The same applies to the left side

$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r},t) = \frac{p^2}{2m}\psi(\mathbf{r},t) = E_{\text{kin}}\psi(\mathbf{r},t) \quad (4.9)$$

with the non-relativistic energy-momentum relationship $E_{\text{kin}} = \frac{p^2}{2m}$. The SG is therefore the law of conservation of energy for a plane probability wave. Because of

$$-i\hbar\nabla\psi(\mathbf{r},t) = \mathbf{p}\psi(\mathbf{r},t) \quad (4.10)$$

you define

$$\hat{\mathbf{p}} := -i\hbar\nabla \quad (4.11)$$

as the *momentum operator*. The term of the partial time derivative $i\hbar\frac{\partial}{\partial t}$ is used for wave functions $\psi(\mathbf{r},t)$, whose time dependence is trivial and can be separated from the position dependence, i.e

$$\psi(\mathbf{r},t) = \psi(\mathbf{r}) \exp\left(-i\frac{E}{\hbar}t\right), \quad (4.12)$$

to

$$i\hbar\frac{\partial}{\partial t} = E. \quad (4.13)$$

The Schrödinger equation then becomes *stationary Schrödinger equation*

$$\hat{H}\psi(\mathbf{r},t) = E\psi(\mathbf{r},t). \quad (4.14)$$

This is an eigenvalue problem, where E is the eigenvalue and $\psi(\mathbf{r},t)$ is the eigenvector.

4.1 Free particle

A free particle of mass m moves in the absence of a potential $\hat{v}_h = 0$ according to the equation

$$-\frac{\hbar^2}{2m}\Delta\psi = i\hbar\frac{\partial\psi}{\partial t}. \quad (4.15)$$

For $\psi(\mathbf{r},t)$ we again use the approach of a plane wave

$$\psi(\mathbf{r},t) = \psi_0 \exp(i(\mathbf{k} \cdot \mathbf{r} - \omega t)) = \psi_0 \exp\left(\frac{i}{\hbar}(\mathbf{p} \cdot \mathbf{r} - Et)\right), \quad (4.16)$$

The dispersion relation follows from this

$$\frac{\hbar^2 \mathbf{k}^2}{2m} = E = \hbar\omega \Leftrightarrow \omega(\mathbf{k}) = \frac{\hbar \mathbf{k}^2}{2m}. \quad (4.17)$$

Eq. (4.17) is called *dispersion relation*. The phase velocity c_{ph} of a matter wave thus becomes

$$c_{ph} = \frac{\omega}{k} = \frac{\hbar k}{2m}, \quad (4.18)$$

while c_{gr} applies to the group velocity

$$c_{\text{gr}} = \sum_{i=1}^3 \frac{\partial \omega}{\partial k_i} \mathbf{e}_i = \frac{\hbar \mathbf{k}}{m}. \quad (4.19)$$

Unlike electromagnetic waves, matter waves are not dispersion-free in a vacuum. The group speed is twice as large as the phase speed.

4.2 potential well

The *potential well* describes a potential $V(x)$ of the form

$$V(x) := \begin{cases} 0, & 0 \leq x \leq L, \\ \infty, & \text{sonst} \end{cases} \quad (4.20)$$

with $L > 0$. The Hamiltonian $\hat{H}$ of a particle in this potential is

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta + V(x). \quad (4.21)$$

The boundary conditions arise from the fact

$$\psi(x) = 0 \text{ f\"ur } x \notin (0, L). \quad (4.22)$$

You make the approach

$$\psi(x) = C \exp(ik_1 x) + C_2 \exp(ik_2 x) \quad (4.23)$$

with $k_1, k_2 > 0$. From the boundary condition

$$\psi(0) = 0 \quad (4.24)$$

follows

$$C = -C_2, \quad (4.25)$$

So define $C := C$, then the approach applies

$$\psi(x) = C (\exp(ik_1 x) - \exp(ik_2 x)). \quad (4.26)$$

From the boundary condition

$$\psi(L) = 0 \quad (4.27)$$

follows

$$\exp(ik_1 L) = \exp(ik_2 L). \quad (4.28)$$

In general, the two solution components $\exp(ik_1 x)$ and $\exp(ik_2 x)$ are allowed to be linearly independent, therefore the following applies

$$k_1 L = k_2 L + 2n\pi \quad (4.29)$$

with $n \in \mathbb{Z}$, so

$$k_1 - k_2 = \frac{2n\pi}{L}. \quad (4.30)$$

So set

$$k_1 = n_1 \frac{\pi}{L}, \quad k_2 = n_2 \frac{\pi}{L} \quad (4.31)$$

with $n_1 - n_2 \in \mathbb{Z}$ even. The case $k_1 = k_2$ must be excluded, otherwise the wave function disappears. The normalization condition applies

$$\begin{aligned} 1 &\stackrel{!}{=} \int_0^L |\psi(x)|^2 dx = |C|^2 \int_0^L 2 - \exp(i(k_1 - k_2)x) - \exp(i(k_2 - k_1)x) dx \\ &\Leftrightarrow |C|^2 2L \Leftrightarrow |C| = \frac{1}{\sqrt{2L}}. \end{aligned} \quad (4.32)$$

The overall solution for the wave function is therefore even under the assumption $C > 0$ with $n_1, n_2 \in \mathbb{Z}, n_1 \neq n_2$ and $n_1 - n_2$

$$\psi(x) = \frac{1}{\sqrt{2L}} \left[\exp\left(in_1 \frac{\pi}{L} x\right) - \exp\left(in_2 \frac{\pi}{L} x\right) \right]. \quad (4.33)$$

For the energy eigenvalues E_{n_1, n_2} follows

$$E_{n_1, n_2} = \frac{\hbar^2}{2m} \frac{\pi^2}{L^2} (n_1^2 + n_2^2). \quad (4.34)$$

The energy $E = 0$ is not possible because n_1 and n_2 cannot be zero at the same time. This is different in classical mechanics.

4.3 potential level

The potential is given

$$V(x) = \begin{cases} V_0, & 0 \leq x \leq L, \\ 0, & \text{sonst} \end{cases} \quad (4.35)$$

with $V_0, L > 0$. If a classical particle with an energy $0 < E < V_0$ is in the range $x < 0$, it can never reach the range $x > L$. In quantum mechanics this is different; this is called the *tunnel effect* because, to put it bluntly, the particle digs a tunnel through the potential barrier.

This will also be discussed here, but for the simpler case $L \rightarrow \infty$. From now on, an index 1 stands for the range $x < 0$, while an index 2 stands from now on for the range $x \geq 0$. The potential $V(x)$ is given by

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases} \quad (4.36)$$

with $V_0 > 0$. Two different stationary Schrödinger equations apply in the two areas 1 and 2

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_1(x) = E \psi_1(x), \quad (4.37)$$

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_2(x) = (E - V_0) \psi_2(x) \quad (4.38)$$

for the two wave functions $\psi_1(x), \psi_2(x), E < V_0$ be the energy of the particle. For $\psi_1(x)$ one makes an approach

$$\psi_1(x) = C \exp(ikx) + C_2 \exp(-ikx) \quad (4.39)$$

with $k > 0$. The first term corresponds to the part of the wave arriving to the right, while the second term corresponds to the reflection. This time C, C_2 are not normalization constants, since one cannot normalize on unbounded sets. For $\psi_2(x)$ one makes an approach

$$\psi_2(x) = C_3 \exp(-\lambda x) \quad (4.40)$$

with $C_3, \lambda > 0$.

The stationary Schrödinger equation applies to ψ , so the second derivative of ψ has the same continuity properties as the potential V . In this case the second derivative is discontinuous, but ψ is still continuously differentiable. This results in the following two connection conditions:

$$C + C_2 = C_3, \quad (4.41)$$

$$ikC - ikC_2 = -\lambda C_3 \quad (4.42)$$

Substituting the first equation into the second one gives

$$\begin{aligned} ikC - ikC_2 &= -\lambda C - \lambda C_2 \Leftrightarrow C_2(\lambda - ik) = -C(\lambda + ik) \\ \Leftrightarrow C_2 &= -\frac{\lambda + ik}{\lambda - ik} = -\exp(2\varphi) \end{aligned} \quad (4.43)$$

with

$$\varphi = \arctan\left(\frac{k}{\lambda}\right). \quad (4.44)$$

This follows

$$C_3 = C - \exp(2\varphi). \quad (4.45)$$

k is obtained from the Schrödinger equation for region 1:

$$\frac{\hbar^2 k^2}{2m} = E \Rightarrow k = \frac{1}{\hbar} \sqrt{2mE} \quad (4.46)$$

λ is obtained from the Schrödinger equation for area 2:

$$-\frac{\hbar^2}{2m} \lambda^2 = E - V_0 \Rightarrow \lambda = \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \quad (4.47)$$

The solutions are summarized again:

$$\psi_1(x) = C \exp\left(\frac{i}{\hbar} \sqrt{2mE}x\right) - \exp\left(2\varphi - \frac{i}{\hbar} \sqrt{2mE}x\right), \quad (4.48)$$

$$\psi_2(x) = (C - \exp(2\varphi)) \exp\left(-\frac{1}{\hbar} \sqrt{2m(V_0 - E)}x\right). \quad (4.49)$$

C is not determined by the Schrödinger equation, but by a normalization that is not possible here. In the case $L < \infty$ one can calculate transmission and reflection coefficients of the probability current density at the potential threshold.

The result of this section and sections 4.1 and 4.2 can be stated:

- In the case $E > V_0 = \text{const.}$ there is a continuous energy spectrum.
- In the case $E < V_0 = \text{const.}$ the particle can propagate into this area in the form of an exponential decay.
- If the motion of the particle is limited, a discrete energy spectrum exists.

4.4 Product wave functions

Let a one-dimensional potential $V_x(x)$ be given with an associated Hamiltonian

$$\hat{H}_x = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_x(x), \quad (4.50)$$

the solutions $(\psi_{n_x}(x), E_{n_x})$ of the eigenvalue problem

$$\hat{H}_x \psi_{n_x}(x) = E_{n_x} \psi_{n_x}(x) \quad (4.51)$$

are known. Now expand the problem to three dimensions, so

$$V(x, y, z) = V_x(x) + V_y(y) + V_z(z), \quad (4.52)$$

where, analogous to the x component, the solutions of the Schrödinger equation belonging to $V_y(y)$ and $V_z(z)$ are also known. However, it does not have to be $V_x = V_y$. The Hamiltonian $\hat{H}$ of the three-dimensional system becomes.

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z \quad (4.53)$$

Now do a product approach for the solution $\psi(x, y, z)$

$$\psi(x, y, z) = \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z), \quad (4.54)$$

then applies

$$\begin{aligned} \hat{H}\psi(x, y, z) &= (\hat{H}_x + \hat{H}_y + \hat{H}_z) \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z) \\ &= (E_{n_x} + E_{n_y} + E_{n_z}) \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z). \end{aligned} \quad (4.55)$$

The solutions constructed in this way $\psi(x, y, z)$ form the complete solution set of

$$\hat{H}\psi(x, y, z) = E\psi(x, y, z). \quad (4.56)$$

With this knowledge, one can easily solve, for example, the Schrödinger equation for a particle in a three-dimensional harmonic oscillator or in a three-dimensional potential well if the one-dimensional solutions are known.

4.5 Harmonic oscillator

The Hamiltonian $\hat{H}$ of the harmonic oscillator is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2, \quad (4.57)$$

So the stationary Schrödinger equation is

$$-\frac{\hbar^2}{2m} \psi'' + \frac{1}{2} m \omega^2 x^2 \psi = E\psi. \quad (4.58)$$

This eigenvalue problem needs to be solved. You can write this as

$$\psi'' - \frac{x^2}{b^4} \psi = -\frac{2mE}{\hbar^2} \psi \quad (4.59)$$

with $b := \sqrt{\frac{\hbar}{m\omega}}$. Define $u := \frac{x}{b}$, then are

$$\frac{d}{dx} = \frac{du}{dx} \frac{d}{du} = \frac{1}{b} \frac{d}{du}, \quad \frac{d^2}{dx^2} = \frac{1}{b^2} \frac{d^2}{du^2}. \quad (4.60)$$

The stationary SG will start with the replacement

$$\psi(x) \rightarrow \psi(u) \quad (4.61)$$

to

$$\psi'' - u^2 \psi = -\frac{2E}{\hbar\omega} \psi. \quad (4.62)$$

In infinity this becomes

$$\psi'' - u^2 \psi \approx 0. \quad (4.63)$$

This is the approach

$$f(u) = \exp\left(-\frac{u^2}{2\sigma^2}\right) \quad (4.64)$$

made with $\sigma > 0$. This results in twice derived

$$\frac{d^2}{du^2} \exp\left(-\frac{u^2}{2\sigma^2}\right) = \frac{d}{du} \left(-\frac{u}{\sigma^2} \exp\left(-\frac{u^2}{2\sigma^2}\right)\right) \approx \frac{u^2}{\sigma^4} \exp\left(-\frac{u^2}{2\sigma^2}\right) \quad (4.65)$$

for large u . If you put this in, you get

$$\frac{u^2}{\sigma^4} - u^2 \stackrel{!}{=} 0 \Rightarrow \sigma = 1. \quad (4.66)$$

One does the approach for ψ

$$\psi(u) = P(u) \exp\left(-\frac{u^2}{2}\right). \quad (4.67)$$

The second derivative is given by

$$\frac{d^2 \psi}{du^2} = \frac{d}{du} \left[P' \exp\left(-\frac{u^2}{2}\right) - uP \exp\left(-\frac{u^2}{2}\right) \right] = \exp\left(-\frac{u^2}{2}\right) [P'' - 2uP' - P + u^2 P]. \quad (4.68)$$

Eq. (4.62) becomes with $\tilde{E} = \frac{2E}{\hbar\omega}$

$$P'' - 2uP' - P = -\tilde{E}P \Leftrightarrow P'' - 2uP' + P(\tilde{E} - 1) = 0. \quad (4.69)$$

For $P(u)$ a power series approach is used

$$P(u) = \sum_{i=0}^{\infty} a_i u^i \quad (4.70)$$

made. This results in

$$P'(u) = \sum_{i=0}^{\infty} i a_i u^{i-1} \quad (4.71)$$

and

$$P''(u) = \sum_{i=0}^{\infty} (i-1) i a_i u^{i-2} = \sum_{i=0}^{\infty} (i+2)(i+1) a_{i+2} u^i. \quad (4.72)$$

Putting this into Eq. (4.69), you get

$$\sum_{i=0}^{\infty} (i+2)(i+1)a_{i+2}u^i - 2 \sum_{i=0}^{\infty} ia_iu^i + (\tilde{E}-1) \sum_{i=0}^{\infty} a_iu^i = 0. \quad (4.73)$$

For this to apply to all $y \in \mathbb{R}$, the individual coefficients must disappear:

$$(i+2)(i+1)a_{i+2} - 2ia_i + (\tilde{E}-1)a_i = 0, \quad (4.74)$$

So you get the recursion formula for a_i

$$a_{i+2} = a_i \frac{2i - \tilde{E} + 1}{(i+2)(i+1)}. \quad (4.75)$$

Since the geometric series $\sum_{n=1}^{\infty} n^{-1}$ diverges, $\sum_{i=0}^{\infty} a_iu^i$ also diverges. Therefore there must be an $n \in \mathbb{N}$ with

$$2n - \tilde{E} + 1 = 0 \Leftrightarrow \frac{2E}{\hbar\omega} = 1 + 2n \Leftrightarrow E = E_n = \hbar\omega \left(n + \frac{1}{2} \right). \quad (4.76)$$

These are the energy eigenvalues of the oscillator. n defines a state. The states are therefore quantized, their energies are equidistant with the distance $\hbar\omega$ and the ground state energy $E_0 > 0$ is positive.

If you rewrite the recursion formula, you get

$$a_i = a_{i+2} \frac{(i+2)(i+1)}{2(i-n)}, \quad (4.77)$$

The polynomials $P_n(u)$ are determined by a_n and $a_{n+1} = 0$, they are called *Hermite polynomials* $H_n(u)$, see section C.3.

The normalization condition applies

$$\int_{-\infty}^{\infty} |\psi(y)|^2 dy = \int_{-\infty}^{\infty} c_n^2 \exp\left(-\frac{y^2}{b^2}\right) H_n^2\left(\frac{y}{b}\right) dy = \int_{-\infty}^{\infty} c_n^2 b \exp(-u^2) H_n^2(u) du = 1, \quad (4.78)$$

so with Eq. (C.124)

$$c_n^2 b = \frac{1}{\sqrt{\pi} 2^n n!}. \quad (4.79)$$

So the eigenstates of the harmonic oscillator are

$$\psi_n(u) = c_n H_n(u) \exp\left(-\frac{u^2}{2}\right) \quad (4.80)$$

with

$$b = \sqrt{\frac{\hbar}{m\omega}}, \quad c_n = \frac{1}{\sqrt{b\sqrt{\pi} 2^n n!}}, \quad u = \frac{x}{b}. \quad (4.81)$$

Finally, two important relationships are noted:

$$u\psi_n(u) \stackrel{\text{Glg. (C.123)}}{=} n \frac{\mathbf{I}}{\sqrt{2n}} \psi_{n-1}(u) + \frac{\mathbf{I}}{2} \sqrt{n+1} \psi_{n+1}(u) = \sqrt{\frac{n}{2}} \psi_{n-1}(u) + \sqrt{\frac{n+1}{2}} \psi_{n+1}(u), \quad (4.82)$$

$$\begin{aligned} \frac{d\psi_n}{du}(u) &\stackrel{\text{Glg. (C.122)}}{=} 2n \frac{\mathbf{I}}{\sqrt{2n}} \psi_{n-1}(u) - u\psi_n(u) = \sqrt{2n} \psi_{n-1}(u) - u\psi_n(u) \\ &= \sqrt{2n} \psi_{n-1}(u) - \sqrt{\frac{n}{2}} \psi_{n-1}(u) - \sqrt{\frac{n+1}{2}} \psi_{n+1}(u) = \sqrt{n} \left(\sqrt{2} - \frac{\mathbf{I}}{\sqrt{2}} \right) \psi_{n-1}(u) - \sqrt{\frac{n+1}{2}} \psi_{n+1}(u) \\ &= \sqrt{n} \left(\frac{2}{\sqrt{2}} - \frac{\mathbf{I}}{\sqrt{2}} \right) \psi_{n-1}(u) - \sqrt{\frac{n+1}{2}} \psi_{n+1}(u) = \sqrt{\frac{n}{2}} \psi_{n-1}(u) - \sqrt{\frac{n+1}{2}} \psi_{n+1}(u) \end{aligned} \quad (4.83)$$

4.6 Hilbert space and operators

A particle is described in QM by its generally time-dependent wave function $\psi(t) : \mathbb{R}^3 \rightarrow \mathbb{C}$. This wave function is also referred to as the *state* of the particle.

4.6.1 Hilbert space

The set of all continuously differentiable functions $\mathbb{R}^3 \rightarrow \mathbb{C}$ is called *Hilbert space* H in QM. The dimension of H is infinite. One can specify an infinite number of different bases $(f_1, f_2, \dots)$ with $f_i \in H$ for all $i \in \mathbb{N}$ with $i \geq \mathbf{1}$ of H . Usually you choose orthonormal bases, i.e. bases with

$$\langle f_i | f_j \rangle = \delta_{i,j} \quad (4.84)$$

for all $i, j \in \mathbb{N}$ with $i, j \geq \mathbf{1}$. One can thus write for a state $\psi(\mathbf{r}, t)$

$$\psi(\mathbf{r}, t) = \sum_{i=1}^{\infty} a_i(t) f_i(\mathbf{r}). \quad (4.85)$$

For which a_i holds, let $k \in \mathbb{N}$ with $k \geq \mathbf{1}$,

$$\langle f_k | \psi \rangle = \int_{\mathbb{R}^3} f_k^*(\mathbf{r}) \left(\sum_{i=1}^{\infty} a_i f_i(\mathbf{r}) \right) d^3r = \sum_{i=1}^{\infty} a_i \int_{\mathbb{R}^3} f_k^*(\mathbf{r}) f_i(\mathbf{r}) d^3r = \sum_{i=1}^{\infty} a_i \delta_{ki} = a_k, \quad (4.86)$$

so

$$a_i = \langle f_i | \psi \rangle. \quad (4.87)$$

If the order of the f_i is chosen appropriately, $\lim_{i \rightarrow \infty} a_i = \mathbf{o}$, so in practice the above sum can be broken off somewhere depending on the desired precision. The vector (a_i) determines the state $\psi(\mathbf{r})$ of a particle. You can transform to another basis $(\tilde{f}_i)$, the transformation results from

$$\psi(\mathbf{r}, t) = \sum_{i=1}^{\infty} a_i(t) f_i(\mathbf{r}) = \sum_{i=1}^{\infty} \tilde{a}_i(t) \tilde{f}_i(\mathbf{r}). \quad (4.88)$$

In this case, the state $\psi(\mathbf{r}, t)$ is determined by $(\tilde{a}_i(t))$. An example of such a transformation is the Fourier transform.

If you have solved the Schrödinger equation for a system and found a quantization of the states, you can define a state $\psi(\mathbf{r})$ by $N \geq \mathbf{1}$ quantum numbers $n_1, \dots, n_N$, $\psi(\mathbf{r}, t) = \psi(n_1, \dots, n_N, \mathbf{r}, t)$. So there are infinitely many ways to determine a state of a particle. If you don't want to commit to such a possibility, just write

$$|\psi\rangle. \quad (4.89)$$

These can be, for example, spectral coefficients a_i $|\psi\rangle = (a_i)$ or a quantum number n as in the one-dimensional harmonic oscillator, $|\psi\rangle = |n\rangle$. This notation is also known as *Dirac notation*. If you need two quantum numbers n, m to define a state, you write $|\psi\rangle = |n, m\rangle$. You define

$$\langle \psi | := |\psi\rangle^*. \quad (4.90)$$

This means: If $|\psi\rangle = \psi(\mathbf{r}, t)$ applies to the state $|\psi\rangle$ in spatial space, then $\langle \psi | \text{applies} = \psi^*(\mathbf{r}, t)$. Derived from the English word *bracket* (bracket), $|\psi\rangle$ is also called a *Ket state* or simply Ket, and $\langle \psi |$ is called a *Bra state* or simply Bra.

An operator $\hat{O}$ turns a state into a new state (see also section A.8), so it is a mapping in Hilbert space. You write

$$|\chi\rangle = \hat{O}|\psi\rangle \quad (4.91)$$

for the state $|\chi\rangle$, which arises when the operator $\hat{O}$ acts on the state $|\psi\rangle$. If $\hat{O}$ is linear (all operators used in QM are linear), then $\hat{O}$ is a matrix if one expands the states with respect to some orthonormal basis of H . This matrix has an infinite number of rows and columns, unless you use only a finite number of base elements. The operator adjoint to $\hat{O}$ is called $\hat{O}^+$ and is defined by the relation

$$\langle \psi | \hat{O} \chi \rangle = \langle \hat{O}^+ \psi | \chi \rangle, \quad (4.92)$$

which should hold for all $\psi, \chi \in H$. This sets $\hat{O}^+$. In linear algebra, a matrix A over $\mathbb{C}$ is called *unitary*, if

$$A^+ = A^{-1} \quad (4.93)$$

applies. Here A^{-1} is the *inverse matrix* for A , i.e

$$A^{-1}A = \mathbf{1} \quad (4.94)$$

and A^+ is the *adjoint matrix*

$$A^+ = (A^*)^T. \quad (4.95)$$

You write for a state

$$|\psi\rangle = \sum_{i=1}^{\infty} a_i |\psi_i\rangle, \quad (4.96)$$

so applies

$$\begin{aligned} \mathbf{1} &= \langle \psi | \psi \rangle = \left\langle \sum_{i=1}^{\infty} a_i^* f_i^*(\mathbf{r}) \left| \sum_{j=1}^{\infty} a_j f_j(\mathbf{r}) \right. \right\rangle \\ &= \int_{\mathbb{R}^3} \left(\sum_{i=1}^{\infty} a_i^* f_i^*(\mathbf{r}) \right) \left(\sum_{j=1}^{\infty} a_j f_j(\mathbf{r}) \right) d^3r = \sum_{i,j=1}^{\infty} \int_{\mathbb{R}^3} a_i^* f_i^*(\mathbf{r}) a_j f_j(\mathbf{r}) d^3r \\ &= \sum_{i,j=1}^{\infty} a_i^* a_j \delta_{i,j} = \sum_{i=1}^{\infty} |a_i|^2. \end{aligned} \quad (4.97)$$

The probability density in spatial space is given by $\rho = \psi \psi^* = \sum_{i,j=1}^{\infty} a_i^* a_j f_i^*(\mathbf{r}) f_j(\mathbf{r})$. The probability P_i of encountering the particle in a state f_i is given by

$$P_i = |\langle f_i | \psi \rangle|^2 = |a_i|^2. \quad (4.98)$$

If every state i is accompanied by an energy E_i , then the expected value of the energy $\langle E \rangle$ is given by

$$\langle E \rangle = \sum_{i=1}^{\infty} P_i E_i = \sum_{i=1}^{\infty} |\langle f_i | \psi \rangle|^2 E_i. \quad (4.99)$$

If the equation $\hat{O}|f_i\rangle = o_i|f_i\rangle$ applies to an operator $\hat{O}$, then the expected value $\langle o \rangle$ of size o is given by

$$\begin{aligned} \langle o \rangle &= \sum_{i=1}^{\infty} P_i o_i = \sum_{i=1}^{\infty} |\langle f_i | \psi \rangle|^2 o_i = \sum_{i=1}^{\infty} \langle \psi | f_i \rangle o_i \langle f_i | \psi \rangle = \sum_{i=1}^{\infty} \langle \psi | o_i f_i \rangle a_i \\ &= \sum_{i=1}^{\infty} \int_{\mathbb{R}^3} \psi^* o_i a_i f_i d^3 r = \int_{\mathbb{R}^3} \psi^* \sum_{i=1}^{\infty} o_i a_i f_i d^3 r = \int_{\mathbb{R}^3} \psi^* \sum_{i=1}^{\infty} \hat{O} a_i f_i d^3 r \\ &= \int_{\mathbb{R}^3} \psi^* \hat{O} \sum_{i=1}^{\infty} a_i f_i d^3 r = \int_{\mathbb{R}^3} \psi^* \hat{O} \psi d^3 r. \end{aligned} \quad (4.100)$$

In general, the expected value $\langle \hat{O} \rangle$ of the operator $\hat{O}$ in the state $|\psi\rangle$ is given by

$$\langle \hat{O} \rangle = \int_{\mathbb{R}^3} \psi^* \hat{O} \psi d^3 r = \langle \psi | \hat{O} | \psi \rangle. \quad (4.101)$$

Now develop $\hat{O}$ as a matrix with respect to the base (f_i) and write $O_{i,j}$ for the entry in the j -th column of the i -th row. As the initial state you choose $|\psi\rangle = f_j$, so the system is definitely in the j -th state. You write

$$|\chi\rangle := \hat{O}|\psi\rangle = \sum_{i=1}^{\infty} b_i f_i(\mathbf{r}) \quad (4.102)$$

for the state $|\chi\rangle$ of the system under the action of the operator $\hat{O}$. Let $k \in \mathbb{N}$ with $k \geq 1$, then is

$$b_k = \sum_{l=1}^{\infty} O_{k,l} \langle f_l | \psi \rangle = \sum_{l=1}^{\infty} O_{k,l} \delta_{l,j} = O_{k,j}. \quad (4.103)$$

$|b_k|^2$ is the probability of finding the system in state f_k after the operator acts, $|O_{k,j}|^2$ is therefore the probability that the system changes from state j to state k under the effect of the operator $\hat{O}$. If $O_{k,j} = 0$, then the system cannot transition from state j to state k under the action of the operator $\hat{O}$, you get a *forbidden transition*. So you can write

$$O_{i,j} = \langle f_i | \hat{O} | f_j \rangle. \quad (4.104)$$

This is a computationally evaluable formula to determine the matrix elements $O_{i,j}$ of the operator $\hat{O}$ with respect to the base (f_k) .

Now it is shown that every linear operator $\hat{O}$ has at least one eigenvalue $\lambda \in \mathbb{C}$. With $x \in \mathbb{C}$ and $|\psi\rangle \in H$ the eigenvalue problem is

$$\hat{O}|\psi\rangle = x|\psi\rangle. \quad (4.105)$$

Now choose an orthonormal basis $(|\psi_1\rangle, \dots)$ of H and expand $\hat{O}$ and $|\psi\rangle$ with respect to this basis, then the problem becomes

$$O\mathbf{a} = x\mathbf{a} \quad (4.106)$$

with $\mathbf{a} = (a_1, \dots)^T$ and $|\psi\rangle = \sum_{i=1}^{\infty} a_i |\psi_i\rangle$. The existence of an eigenvalue $\lambda \in \mathbb{C}$ is equivalent to that the characteristic polynomial

$$p(x) := \det(O - x) \quad (4.107)$$

has at least one complex zero. Since $p(x)$ breaks down into linear factors over $\mathbb{C}$ according to the main theorem of algebra, this is the case.

4.6.2 Hermitian operators

An operator $\hat{O}$ is called *Hermitian* if it holds

$$\langle \hat{O}f|g \rangle = \langle f|\hat{O}g \rangle, \quad (4.108)$$

so advertised

$$\int_{\mathbb{R}^3} (\hat{O}f)^* g d^3r = \int_{\mathbb{R}^3} f^* (\hat{O}g) d^3r. \quad (4.109)$$

Hermitian operators are therefore self-adjoint,

$$\hat{O}^+ = \hat{O}. \quad (4.110)$$

Now it is shown that the eigenvalues of Hermitian operators are real. So let a Hermitian operator $\hat{O}$ be given and $|\psi\rangle \in H, a \in \mathbb{C}$ with $\hat{O}|\psi\rangle = a|\psi\rangle$. Then applies

$$a^* \langle \psi|\psi \rangle = \langle \hat{O}\psi|\psi \rangle = \langle \psi|\hat{O}\psi \rangle = a \langle \psi|\psi \rangle, \quad (4.111)$$

therefore $a^* = a$ and therefore $a \in \mathbb{R}$. Furthermore, the expected values of Hermite operators are also real:

$$\begin{aligned} \langle \psi|\hat{O}|\psi \rangle^* &= \left(\int_{\mathbb{R}^3} \psi^* \hat{O}\psi d^3r \right)^* = \int_{\mathbb{R}^3} \psi (\hat{O}\psi)^* d^3r \\ &= \int_{\mathbb{R}^3} (\hat{O}\psi)^* \psi d^3r = \langle \hat{O}\psi|\psi \rangle = \langle \psi|\hat{O}|\psi \rangle \end{aligned} \quad (4.112)$$

Measured variables are always real. Hermite operators are therefore suitable for determining measured variables.

Now it is shown that the eigenvectors of Hermitian operators are orthogonal to different eigenvalues. So let a Hermitian operator $\hat{O}$ be given and $|\psi\rangle, |\chi\rangle \in H, a, \beta \in \mathbb{R}$ with $a \neq \beta$ and

$$\hat{O}|\psi\rangle = a|\psi\rangle, \quad \hat{O}|\chi\rangle = \beta|\chi\rangle. \quad (4.113)$$

Then applies

$$\beta \langle \psi|\chi \rangle = \langle \psi|\hat{O}\chi \rangle = \langle \hat{O}\psi|\chi \rangle = a \langle \psi|\chi \rangle, \quad (4.114)$$

so is

$$\langle \psi|\chi \rangle = 0. \quad (4.115)$$

Of course, eigenvectors to degenerate eigenvalues do not have to be orthonormal per se. However, the Gram-Schmidt orthonormalization method can be applied to them.

Now some operators will be examined for hermitism. It applies

$$\int \left(-\frac{d}{dx} \varphi \right)^* \psi dx = \int -\frac{d}{dx} \varphi^* \psi dx = \int \varphi^* \frac{d}{dx} \psi dx, \quad (4.116)$$

so is

$$\left(\frac{d}{dx}\right)^+ = -\frac{d}{dx}. \quad (4.117)$$

Partial derivatives are therefore not Hermitian. However, the x-component of the momentum operator $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ is Hermitian and so are the other components. It applies

$$\int \left((-1)^n \frac{d^n}{dx^n} \varphi\right)^* \psi dx = (-1)^n \int \frac{d^n}{dx^n} \varphi^* \psi dx = (-1)^n (-1)^n \int \varphi^* \frac{d^n \psi}{dx^n} dx, \quad (4.118)$$

so is

$$\left(\frac{d^n}{dx^n}\right)^+ = (-1)^n \frac{d^n}{dx^n}. \quad (4.119)$$

Because of

$$\begin{aligned} \int (\Delta \varphi)^* \psi d^3 r &= \int \left(\sum_{i=1}^3 \frac{d^2}{dx_i^2} \varphi\right)^* \psi d^3 r = \sum_{i=1}^3 \int \left(\frac{d^2 \varphi}{dx_i^2}\right)^* \psi d^3 r \\ &= \sum_{i=1}^3 \int \varphi^* \left(\frac{d^2 \psi}{dx_i^2}\right) d^3 r = \int \varphi^* \Delta \psi d^3 r \end{aligned} \quad (4.120)$$

is $\Delta^+ = \Delta$. The Laplace operator is therefore Hermitian. Because of

$$\begin{aligned} \int \left(\left(-1 - x \frac{d}{dx}\right) \varphi\right)^* \psi dx &= - \int \varphi^* \psi dx - \int \left(x \frac{d}{dx} \varphi\right)^* \psi dx \\ &= - \int \varphi^* \psi dx + \int \varphi^* \left(\psi + x \frac{d}{dx} \psi\right) dx = \int \varphi^* x \frac{d}{dx} \psi dx \end{aligned} \quad (4.121)$$

is

$$\left(x \frac{d}{dx}\right)^+ = -1 - x \frac{d}{dx}. \quad (4.122)$$

The *Annihilation operator* $\hat{a}$ is defined by

$$\hat{a} := \frac{1}{\sqrt{2}} \left(x + \frac{\partial}{\partial x}\right). \quad (4.123)$$

It applies

$$\int \left(\frac{1}{\sqrt{2}} \left(x - \frac{\partial}{\partial x}\right) \varphi\right)^* \psi dx = \int \frac{1}{\sqrt{2}} \varphi^* x \psi + \frac{1}{\sqrt{2}} \varphi^* \frac{\partial \psi}{\partial x} dx = \int \varphi^* \frac{1}{\sqrt{2}} \left(x + \frac{\partial}{\partial x}\right) \psi dx, \quad (4.124)$$

That means

$$\hat{a}^+ = \frac{1}{\sqrt{2}} \left(x - \frac{\partial}{\partial x}\right), \quad (4.125)$$

this is called the *creation operator*. For the *particle number operator* $\hat{N}$ applies

$$\hat{N} := \frac{1}{2} \left(x^2 - \frac{\partial^2}{\partial x^2}\right). \quad (4.126)$$

This applies

$$\begin{aligned}
\int \left(\frac{1}{2} \left(x^2 - \frac{\partial^2}{\partial x^2} \right) \varphi \right)^* \psi dx &= \int \frac{1}{2} x^2 \varphi^* \psi - \frac{1}{2} \frac{\partial^2}{\partial x^2} \varphi^* \psi dx \\
&= \int \varphi^* \frac{1}{2} \left(x^2 - \frac{\partial^2}{\partial x^2} \right) \psi dx = \int \varphi^* \hat{N} \psi dx,
\end{aligned} \tag{4.127}$$

so is

$$\hat{N}^+ = \hat{N}. \tag{4.128}$$

The particle number operator is therefore Hermitian.

At this point some general statements about Hermite operators are made. Let $\hat{A}, \hat{B}$ be two linear Hermitian operators. Then $a\hat{A} + \beta\hat{B}$ with $a, \beta \in \mathbb{R}$ is also Hermitian. Let $f, g \in H$. Then applies

$$\langle f | (a\hat{A} + \beta\hat{B}) g \rangle = \langle f | a\hat{A}g \rangle + \langle f | \beta\hat{B}g \rangle = \langle a\hat{A}f | g \rangle + \langle \beta\hat{B}f | g \rangle = \langle (a\hat{A} + \beta\hat{B}) f | g \rangle. \tag{4.129}$$

This also applies in this case

$$\langle f | \hat{A}\hat{B}g \rangle = \langle \hat{A}f | \hat{B}g \rangle = \langle \hat{B}\hat{A}f | g \rangle, \tag{4.130}$$

so

$$(\hat{A}\hat{B})^+ = \hat{B}\hat{A}. \tag{4.131}$$

If $\hat{A}$ and $\hat{B}$ commute, then the consecutive execution $\hat{A}\hat{B}$ is also Hermitian. Furthermore, the following applies with $n \in \mathbb{N}$

$$(\hat{A}^n)^+ = \hat{A}^n. \tag{4.132}$$

Thus, the momentum operator $\hat{\mathbf{p}} = \sum_{j=1}^3 \hat{p}_j \mathbf{e}_j$ as a linear combination of Hermitian operators is Hermitean. Furthermore, all potentials $\hat{v}_h$ are Hermitian since they are real and contain no differential operators. Furthermore, the Hamilton operator is

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hat{v}_h \tag{4.133}$$

Hermitian

4.6.3 Commuting operators

The *commutator* $[\hat{A}, \hat{B}]$ of two operators $\hat{A}, \hat{B}$ is defined by

$$[\hat{A}, \hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{4.134}$$

Let $|\psi\rangle$ be a state. If the commutator of a constant operator $\hat{A}$ disappears with the Hamiltonian $\hat{H}$

$$[\hat{H}, \hat{A}] = 0, \tag{4.135}$$

then $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$ is a conserved quantity:

$$\frac{\partial}{\partial t} \langle \hat{A} \rangle = \frac{\partial}{\partial t} \langle \psi | \hat{A} | \psi \rangle = \left\langle \frac{\partial}{\partial t} \psi \middle| \hat{A} \middle| \psi \right\rangle + \left\langle \psi \middle| \frac{\partial}{\partial t} \hat{A} \middle| \psi \right\rangle + \left\langle \psi \middle| \hat{A} \middle| \frac{\partial}{\partial t} \psi \right\rangle \tag{4.136}$$

Since $\hat{A}$ is assumed to be constant, the SG follows

$$\frac{\partial}{\partial t} \langle \hat{A} \rangle = -\frac{\mathbf{i}}{\hbar} \langle \hat{H} \psi | \hat{A} | \psi \rangle + \frac{\mathbf{i}}{\hbar} \langle \psi | \hat{A} | \hat{H} \psi \rangle = -\frac{\mathbf{i}}{\hbar} \langle \hat{H} \psi | \hat{A} | \psi \rangle + \frac{\mathbf{i}}{\hbar} \langle \psi | \hat{H} \hat{A} \psi \rangle = 0, \quad (4.137)$$

since $\hat{H}$ is Hermitian. If $[\hat{A}, \hat{B}] = 0$ for Hermitian operators $\hat{A}, \hat{B}$, simultaneous eigenfunctions of the two operators can be found. This can be made clear as follows: First of all:

$$\hat{B}\hat{A}|\psi\rangle = \hat{B}a|\psi\rangle \Leftrightarrow \hat{A}(\hat{B}|\psi\rangle) = a(\hat{B}|\psi\rangle), \quad (4.138)$$

so $\hat{B}|\psi\rangle$ is an eigenvector from $\hat{A}$ to the eigenvalue a . If a is not degenerate, then the corresponding eigenspace is one-dimensional and therefore there exists a $b \in \mathbb{C}$ with $\hat{B}|\psi\rangle = b|\psi\rangle$.

However, if a as an eigenvalue of $\hat{A}$ is degenerate n -fold, with $n \in \mathbb{N}$, $n \geq 2$, this means that the associated eigenspace is spanned by n basis vectors $|\psi_1\rangle, \dots, |\psi_n\rangle$, which can be assumed to be orthonormal, i.e

$$\langle \psi_i | \psi_j \rangle = \delta_{i,j}. \quad (4.139)$$

Because of Eq. (4.138) exist $k_i \in \mathbb{C}$ for $1 \leq i \leq n$ with

$$\hat{B}|\psi\rangle = \sum_{i=1}^n k_i |\psi_i\rangle. \quad (4.140)$$

Since $\hat{B}$ is Hermitian, the matrix $(B_{i,j}) := \langle \psi_i | \hat{B} | \psi_j \rangle$ can be converted into diagonal form by a unitary transformation U

$$B' = U^T B U = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix} \quad (4.141)$$

with not necessarily different eigenvalues $\lambda_1, \dots, \lambda_n \in \mathbb{C}$. The transformed basis elements $|\psi'_i\rangle := U|e_i\rangle$ are also eigenfunctions of $\hat{A}$ as superpositions of the $|\psi_i\rangle$. Thus, n simultaneous eigenfunctions of the two operators $\hat{A}, \hat{B}$ have been found.

4.6.4 Ladder operators

The *ladder operators* (also: creation and destruction operators) $\hat{a}^+$ and $\hat{a}$ are defined by

$$\hat{a}^+ := \frac{\mathbf{i}}{\sqrt{2}} \left(u - \frac{\partial}{\partial u} \right). \quad (4.142)$$

and

$$\hat{a} := \frac{\mathbf{i}}{\sqrt{2}} \left(u + \frac{\partial}{\partial u} \right) \quad (4.143)$$

For the states $\psi_n(u)$ of the harmonic oscillator, the equations (4.82) and (4.83) apply

$$\hat{a}\psi_n(u) = \sqrt{n}\psi_{n-1}(u) \quad (4.144)$$

and

$$\hat{a}^+\psi_n(u) = \sqrt{n+1}\psi_{n+1}(u). \quad (4.145)$$

This is where ladder operators get their name. You can still create any state $\psi_n(u)$ from the ground state $\psi_0(u)$:

$$(\hat{a}^+)^n \psi_o(u) = \sqrt{n!} \psi_n(u) \Leftrightarrow \psi_n(u) = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n \psi_o(u) \quad (4.146)$$

It should apply

$$\hat{a} \psi_o(u) \stackrel{!}{=} 0. \quad (4.147)$$

This means

$$\left(u + \frac{\partial}{\partial u}\right) \psi_o(u) \propto \left(u + \frac{\partial}{\partial u}\right) \exp\left(-\frac{u^2}{2}\right) = (u - u) \exp\left(-\frac{u^2}{2}\right) = 0, \quad (4.148)$$

So the required statement is correct. It holds for $f, g : \mathbb{R} \rightarrow \mathbb{R}$ continuously-differentiable

$$\begin{aligned} \langle f | \hat{a} g \rangle &= \int_{-\infty}^{\infty} f^* \hat{a} g du = \int_{-\infty}^{\infty} f^* \frac{1}{\sqrt{2}} \left(u + \frac{\partial}{\partial u}\right) g du \\ &= \int_{-\infty}^{\infty} g \frac{1}{\sqrt{2}} \left(u - \frac{\partial}{\partial u}\right) f^* du = \langle \hat{a}^+ f | g \rangle \end{aligned} \quad (4.149)$$

The ladder operators are therefore adjoint in pairs, as was already taken into account in the notation $\hat{a}, \hat{a}^+$. For the operator

$$\hat{N} := \hat{a}^+ \hat{a} \quad (4.150)$$

applies

$$\hat{N} \psi_n(u) = \hat{a}^+ \sqrt{n} \psi_{n-1}(u) = n \psi_n(u). \quad (4.151)$$

$\hat{N}$ is called the *particle number operator*. For the commutator $[\hat{a}, \hat{a}^+]$ of the two operators applies

$$\begin{aligned} [\hat{a}, \hat{a}^+] \psi_n(u) &= (\hat{a} \hat{a}^+ - \hat{a}^+ \hat{a}) \psi_n(u) = \hat{a} \sqrt{n+1} \psi_{n+1}(u) - \hat{a}^+ \sqrt{n} \psi_{n-1}(u) \\ &= (n+1) \psi_n(u) - n \psi_n(u) = \psi_n(u). \end{aligned} \quad (4.152)$$

So it's general

$$[\hat{a}, \hat{a}^+] = \hat{1}. \quad (4.153)$$

For the x-component $\hat{x}$ of the location operator $\hat{\mathbf{r}}$ applies

$$\hat{a} + \hat{a}^+ = \sqrt{2} u = \frac{\sqrt{2} x}{b} \Leftrightarrow \hat{x} = \frac{b}{\sqrt{2}} (\hat{a} + \hat{a}^+). \quad (4.154)$$

For the x-component $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ of the momentum operator $\hat{\mathbf{p}}$ applies

$$\hat{a} - \hat{a}^+ = \sqrt{2} \frac{\partial}{\partial u} = \sqrt{2} b \frac{\partial}{\partial x} = i b \frac{\sqrt{2}}{\hbar} \hat{p}_x \Leftrightarrow \hat{p}_x = -i \frac{\hbar}{b \sqrt{2}} (\hat{a} - \hat{a}^+). \quad (4.155)$$

For the Hamiltonian $\hat{H}$ of the harmonic oscillator applies

$$\begin{aligned} \hat{H} &= \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m \omega^2 x^2 = -\frac{1}{2m} \frac{\hbar^2}{b^2} (\hat{a}^2 + (\hat{a}^+)^2 - \hat{a} \hat{a}^+ - \hat{a}^+ \hat{a}) + \frac{1}{4} m \omega^2 b^2 (\hat{a}^2 + (\hat{a}^+)^2 + \hat{a} \hat{a}^+ + \hat{a}^+ \hat{a}) \\ &= \frac{\hbar \omega}{4} (2 \hat{a} \hat{a}^+ + 2 \hat{a}^+ \hat{a}) = \frac{\hbar \omega}{2} (2 \hat{N} + 1). \end{aligned} \quad (4.156)$$

4.7 Uncertainty principle

Let $\hat{A}, \hat{B}$ be two operators and be a particle in the state $|\psi\rangle$. Define the variances $\langle (\Delta\hat{A})^2 \rangle, \langle (\Delta\hat{B})^2 \rangle$ of the operators $\hat{A}, \hat{B}$ in the state $|\psi\rangle$ by

$$\langle (\Delta\hat{A})^2 \rangle := \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle \quad (4.157)$$

and analogously for $\langle (\Delta\hat{B})^2 \rangle$. It still applies

$$\begin{aligned} \langle (\Delta\hat{A})^2 \rangle &= \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \hat{A}^2 + \langle \hat{A} \rangle^2 - 2\hat{A} \langle \hat{A} \rangle \rangle \\ &= \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2. \end{aligned} \quad (4.158)$$

Now assume that $\hat{A}$ and $\hat{B}$ are Hermitian. The expected values $\langle \hat{A} \rangle, \langle \hat{B} \rangle$ of $\hat{A}$ and $\hat{B}$ are then real. Define the function $F: \mathbb{R} \rightarrow \mathbb{R}$ by

$$\begin{aligned} F(x) &:= \int_{\mathbb{R}^3} \left| \left[x(\hat{A} - \langle \hat{A} \rangle) - i(\hat{B} - \langle \hat{B} \rangle) \right] \psi \right|^2 d^3r \\ &= \int_{\mathbb{R}^3} \left(\left[x(\hat{A} - \langle \hat{A} \rangle) - i(\hat{B} - \langle \hat{B} \rangle) \right] \psi \right)^* \left[x(\hat{A} - \langle \hat{A} \rangle) - i(\hat{B} - \langle \hat{B} \rangle) \right] \psi d^3r \\ &= \int_{\mathbb{R}^3} \psi^* \left[x(\hat{A} - \langle \hat{A} \rangle) + i(\hat{B} - \langle \hat{B} \rangle) \right] \left[x(\hat{A} - \langle \hat{A} \rangle) - i(\hat{B} - \langle \hat{B} \rangle) \right] \psi d^3r. \end{aligned} \quad (4.159)$$

With

$$\begin{aligned} &xi \left[(\hat{B} - \langle \hat{B} \rangle) (\hat{A} - \langle \hat{A} \rangle) - (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) \right] \\ &= xi \left[\hat{B}\hat{A} - \hat{B}\langle \hat{A} \rangle - \langle \hat{B} \rangle \hat{A} + \langle \hat{B} \rangle \langle \hat{A} \rangle - \hat{A}\hat{B} + \hat{A}\langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle \right] \\ &= -xi [\hat{A}, \hat{B}] \end{aligned} \quad (4.160)$$

follows

$$\begin{aligned} F(x) &= \int_{\mathbb{R}^3} \psi^* \left[x^2 (\hat{A} - \langle \hat{A} \rangle)^2 + (\hat{B} - \langle \hat{B} \rangle)^2 - xi [\hat{A}, \hat{B}] \right] \psi d^3r \\ &= x^2 \langle (\Delta\hat{A})^2 \rangle + \langle (\Delta\hat{B})^2 \rangle - x \langle i [\hat{A}, \hat{B}] \rangle \geq 0. \end{aligned} \quad (4.161)$$

Let $f, g \in H$. Then applies

$$\begin{aligned} \langle i[A, B]fg \rangle &= \langle i(\hat{A}\hat{B} - \hat{B}\hat{A})fg \rangle = \langle i\hat{A}\hat{B}f - i\hat{B}\hat{A}fg \rangle \\ &= \langle i\hat{A}\hat{B}fg \rangle - \langle i\hat{B}\hat{A}fg \rangle = -\langle \hat{B}fi\hat{A}g \rangle + \langle \hat{A}fi\hat{B}g \rangle = \langle f|i\hat{A}\hat{B}g \rangle - \langle f|i\hat{B}\hat{A}g \rangle \\ &= \langle f|i(\hat{A}\hat{B} - \hat{B}\hat{A})g \rangle = \langle f|i[\hat{A}, \hat{B}]g \rangle. \end{aligned} \quad (4.162)$$

So $i[\hat{A}, \hat{B}]$ is Hermitian and $\langle i[\hat{A}, \hat{B}] \rangle$ is real. $F(x)$ is an upwardly opened parabola with exactly one minimum x_0 . This is obtained by setting the derivative to zero

$$0 = 2x_0 \langle (\Delta\hat{A})^2 \rangle - \langle i[\hat{A}, \hat{B}] \rangle \Leftrightarrow x_0 = \frac{\langle i[\hat{A}, \hat{B}] \rangle}{2 \langle (\Delta\hat{A})^2 \rangle}. \quad (4.163)$$

Putting this into Eq. (4.161), you get

$$\frac{\mathfrak{r}}{4} \frac{\langle i [\hat{A}, \hat{B}] \rangle^2}{\langle (\Delta \hat{A})^2 \rangle} + \langle (\Delta \hat{B})^2 \rangle - \frac{\langle i [\hat{A}, \hat{B}] \rangle^2}{2 \langle (\Delta \hat{A})^2 \rangle} \geq 0 \Leftrightarrow \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq \frac{\mathfrak{r}}{4} \langle i [\hat{A}, \hat{B}] \rangle^2. \quad (4.164)$$

This can also be written as

$$\langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq \frac{\mathfrak{r}}{4} \left| \langle [\hat{A}, \hat{B}] \rangle \right|^2. \quad (4.165)$$

From this it can be concluded that in general the expected values of non-commuting operators cannot be determined with any precision at the same time. The eigenvalues of Hermitian operators are the measured variables of quantum mechanics. Let a bound state be given that can be specified by $N \geq \mathfrak{r}$ quantum numbers. A set of Hermitian operators $\hat{A}_1, \dots, \hat{A}_N$ is called *complete observables* if the $\hat{A}_i$ commute in pairs with $\mathfrak{r} \leq i \leq N$. With this requirement, the quantum numbers can be measured simultaneously.

4.8 H atom

The matter on Earth is structured into atoms, which consist of a positively charged nucleus made of protons and neutrons with the atomic number $Z \in \mathbb{N}$ with $Z \geq \mathfrak{r}$, as well as an electron shell. Z is also called the atomic number, all atoms with the same atomic number are combined into a *chemical element*. The *mass number* $N \in \mathbb{N}$, $N \geq Z \geq \mathfrak{r}$ corresponds to the number of protons and neutrons in the nucleus. Protons are simply positively charged (in units of elementary charge e), neutrons are neutral. Atoms with the same atomic number but different mass numbers are called *isotopes*. Since the electrons are also simply negatively charged, a neutral atom consists of as many protons as electrons. If electrons are missing or additional ones are present, this is an *ion*, the atom has been *ionized*. Each element receives a symbol, e.g. B. A , one writes ${}_Z^N A$ if A has the atomic number Z and isotopes of mass number N are meant. Atomic numbers up to 92 occur in nature; elements with higher atomic numbers can be produced in nuclear reactors. For atmospheric physics, the exact structure of the nucleus is irrelevant; it is assumed to be a positively charged point mass.

The hydrogen atom (element symbol H) is the simplest atom; it consists of a proton as a nucleus and an electron in the shell. It is examined here. The concept of reduced mass is known from Sect. 2.1. This can also be applied quantum mechanically. To do this, we start from the classic case and set up the Lagrange function of the two-particle system:

$$L(\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \mathbf{r}_1, \mathbf{r}_2) = \frac{m_1}{2} \dot{\mathbf{r}}_1^2 + \frac{m_2}{2} \dot{\mathbf{r}}_2^2 - V(\mathbf{r}_2 - \mathbf{r}_1) \quad (4.166)$$

It makes sense to assume that the potential only depends on the relative vector. If you do the definitions

$$\mathbf{r} := \mathbf{r}_2 - \mathbf{r}_1, \quad \mathbf{R} := \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}, \quad (4.167)$$

$$M := m_1 + m_2, \quad \mu := \frac{m_1 m_2}{m_1 + m_2} \quad (4.168)$$

one, you can calculate

$$\begin{aligned} \frac{M}{2} \dot{\mathbf{R}}^2 + \frac{\mu}{2} \dot{\mathbf{r}}^2 &= \frac{\mathfrak{r}}{2M} (m_1^2 \dot{\mathbf{r}}_1^2 + m_2^2 \dot{\mathbf{r}}_2^2 + 2m_1 m_2 \dot{\mathbf{r}}_1 \cdot \dot{\mathbf{r}}_2) + \frac{m_1 m_2}{2(m_1 + m_2)} (\dot{\mathbf{r}}_1^2 + \dot{\mathbf{r}}_2^2 - 2\dot{\mathbf{r}}_1 \cdot \dot{\mathbf{r}}_2) \\ &= \frac{\mathfrak{r}}{2} m_1 \dot{\mathbf{r}}_1^2 + \frac{\mathfrak{r}}{2} m_2 \dot{\mathbf{r}}_2^2. \end{aligned} \quad (4.169)$$

Thus, an alternative Lagrange function is:

$$L(\dot{\mathbf{R}}, \dot{\mathbf{r}}, \mathbf{r}) = \frac{M}{2} \dot{\mathbf{R}}^2 + \frac{\mu}{2} \dot{\mathbf{r}}^2 - V(\mathbf{r}). \quad (4.170)$$

For the canonical impulses follows

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} = \mu \dot{\mathbf{r}}, \quad \mathbf{P} = \frac{\partial L}{\partial \dot{\mathbf{R}}} = M \dot{\mathbf{R}}. \quad (4.171)$$

For the Hamilton function follows

$$H(\mathbf{P}, \mathbf{p}, \mathbf{r}) = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2\mu} + V(\mathbf{r}). \quad (4.172)$$

The replacement rules for operators are used to write

$$\mathbf{P} \rightarrow \hat{\mathbf{P}} = -i\hbar \frac{\partial}{\partial \mathbf{R}}, \quad (4.173)$$

$$\mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \frac{\partial}{\partial \mathbf{r}}. \quad (4.174)$$

This is how we get the Hamilton operator

$$\hat{H}' = -\frac{\hbar^2}{2m} \Delta_{\mathbf{R}} - \frac{\hbar^2}{2\mu} \Delta_{\mathbf{r}} + V(\mathbf{r}). \quad (4.175)$$

It can be applied to a wave function $\psi = \psi(\mathbf{R}, \mathbf{r})$:

$$\hat{H}' \psi(\mathbf{R}, \mathbf{r}) = E \psi(\mathbf{R}, \mathbf{r}). \quad (4.176)$$

$\hat{H}'$ does not explicitly depend on $\mathbf{R}$, so

$$[\hat{H}', \hat{\mathbf{P}}] = 0. \quad (4.177)$$

According to section 4.6.3 $\hat{H}'$ and $\hat{\mathbf{P}}$ therefore have the same eigenfunctions. One therefore looks for solutions that are eigenfunctions of $\hat{\mathbf{P}}$:

$$\hat{\mathbf{P}} \psi(\mathbf{R}, \mathbf{r}) = \hbar \mathbf{K} \psi(\mathbf{R}, \mathbf{r}). \quad (4.178)$$

It follows

$$\psi(\mathbf{R}, \mathbf{r}) = \exp(i\mathbf{K} \cdot \mathbf{R}) \varphi(\mathbf{r}). \quad (4.179)$$

This is what you put into the stationary SG:

$$\left(-\frac{\hbar^2}{2M} \Delta_{\mathbf{R}} - \frac{\hbar^2}{2\mu} \Delta_{\mathbf{r}} + V(\mathbf{r}) - E \right) \exp(i\mathbf{K} \cdot \mathbf{R}) \varphi(\mathbf{r}) = 0 \quad (4.180)$$

With the definitions

$$\Delta := \Delta_{\mathbf{r}}, \quad \varepsilon := E - \frac{\hbar^2 K^2}{2M} \quad (4.181)$$

this will be too

$$\left(-\frac{\hbar^2}{2\mu} \Delta + V(\mathbf{r}) - \varepsilon \right) \varphi(\mathbf{r}) = 0. \quad (4.182)$$

With the Hamilton operator

$$\hat{H} := -\frac{\hbar^2}{2\mu} \Delta + V(\mathbf{r}) \quad (4.183)$$

you get

$$\hat{H} \varphi(\mathbf{r}) = \varepsilon \varphi(\mathbf{r}). \quad (4.184)$$

The center of mass movement leads to a modulation of the wave function with $e^{i\mathbf{K}\cdot\mathbf{R}}$ and a contribution to the kinetic energy of $\hbar^2 K^2 / 2m$. This has been decoupled here. So you can go through the transition

$$m_e \rightarrow \mu \quad (4.185)$$

achieve greater accuracy in the hydrogen eigenstates. Now these eigenfunctions should be determined. The Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad (4.186)$$

must be solved for a potential $V = V(r)$ that only depends on the distance:

$$-\frac{\hbar^2}{2m}\Delta\psi + V(r)\psi = E\psi, \quad (4.187)$$

here m is the mass of the particle under consideration. The solution is to make a product batch of the form

$$\psi(r, \theta, \varphi) = R(r) G(\theta, \varphi). \quad (4.188)$$

One can write Δ for the Laplace operator

$$\Delta = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Delta_{\theta, \varphi} \quad (4.189)$$

with a portion $\Delta_{\theta, \varphi}$, which only contains partial angle derivatives (see equation (B.94)). If you put this with Eq. (4.188) into the Schrödinger equation, you first get

$$\begin{aligned} & -G(\theta, \varphi) \frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) R(r) - R(r) \frac{\hbar^2}{2m} \frac{1}{r^2} \Delta_{\theta, \varphi} G(\theta, \varphi) \\ & + V(r) R(r) G(\theta, \varphi) = ER(r) G(\theta, \varphi). \end{aligned} \quad (4.190)$$

One knows that ψ is not zero outside of zero sets, so one can separate

$$-\frac{1}{R(r)} \frac{\hbar^2}{2m} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) R(r) + r^2 V(r) - Er^2 = \frac{1}{G(\theta, \varphi)} \frac{\hbar^2}{2m} \Delta_{\theta, \varphi} G(\theta, \varphi). \quad (4.191)$$

Both sides are therefore equal to a separation constant, which should be denoted by $-\frac{\hbar^2 l(l+1)}{2m}$ with $l \in \mathbb{N}$. The solutions therefore get an index l . First you solve the angle component. The DGL for this is:

$$\Delta_{\theta, \varphi} G_l(\theta, \varphi) = -l(l+1) G_l(\theta, \varphi). \quad (4.192)$$

This is determined by the spherical surface functions $Y_{l,m}(\theta, \varphi)$ Eq. (C.155) is fulfilled, see Eq. (C.166), where $|m| \leq l$ applies. The normalization condition is:

$$\int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} |G_l|^2 \sin(\theta) d\theta d\varphi \stackrel{!}{=} 1. \quad (4.193)$$

This is also fulfilled by the spherical surface functions $Y_{l,m}(\theta, \varphi)$. For the radial part one obtains

$$\begin{aligned} & -\frac{\hbar^2}{2m} [r^2 R_l''(r) + 2r R_l'(r)] + r^2 V(r) R_l(r) - Er^2 R_l(r) = -\frac{\hbar^2 l(l+1)}{2m} R_l(r) \\ \Leftrightarrow & \left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - E \right] R_l(r) = 0. \end{aligned} \quad (4.194)$$

Define $U_l(r) := R_l(r) r$, then $R_l(r) = \frac{U_l(r)}{r}$ and thus

$$\begin{aligned}
\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr}\right) \frac{U_l(r)}{r} &= \frac{d}{dr} \left(-\frac{U_l(r)}{r^2} + \frac{\frac{dU_l(r)}{dr}}{r} \right) + \frac{2}{r} \left(\frac{\frac{dU_l(r)}{dr}}{r} - \frac{1}{r^2} U_l(r) \right) \\
&= \frac{2}{r^3} U_l(r) - \frac{\frac{dU_l(r)}{dr}}{r^2} + \frac{\frac{d^2 U_l(r)}{dr^2}}{r} - \frac{\frac{dU_l(r)}{dr}}{r^2} + \frac{2}{r^2} \frac{dU_l(r)}{dr} - \frac{2}{r^3} U_l(r),
\end{aligned} \tag{4.195}$$

so is

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr}\right) R_l(r) = \frac{1}{r} \frac{d^2}{dr^2} U_l(r). \tag{4.196}$$

The $U_l(r)$ therefore satisfy the differential equation

$$\begin{aligned}
&\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - E \right] U_l(r) = 0 \\
&\Leftrightarrow \left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{2mV(r)}{\hbar^2} - \frac{2mE}{\hbar^2} \right] U_l(r) = 0.
\end{aligned} \tag{4.197}$$

Eq. (4.197) is the *radial Schrödinger equation*. Now the Coulomb potential is used for $V(r)$

$$V(r) = -\frac{Ze^2}{r}. \tag{4.198}$$

This generally assumes that there are Z protons in the nucleus and only one electron in the shell. Eq. (4.197) becomes

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2mZe^2}{\hbar^2 r} - \frac{2mE}{\hbar^2} \right] U_l(r) = 0. \tag{4.199}$$

At this point the drilling radius a_B is defined by

$$a_B := \frac{\hbar^2}{e^2 m_e}, \tag{4.200}$$

and continue to define $u := \frac{r}{a_B}$. Then applies

$$\frac{d^2}{dr^2} = \frac{d}{dr} \left(\frac{du}{dr} \frac{d}{du} \right) = \frac{d}{dr} \left(\frac{1}{a_B} \frac{d}{du} \right) = \frac{1}{a_B^2} \frac{d^2}{du^2}. \tag{4.201}$$

With the replacement

$$U_l(r) \rightarrow U_l(u) \tag{4.202}$$

and the definitions

$$E_{\text{at}} := \frac{\hbar^2}{m_e a_B^2}, \quad \varepsilon := \frac{E}{E_{\text{at}}} \tag{4.203}$$

becomes Eq. (4.199) to

$$\left[-\frac{d^2}{du^2} + \frac{l(l+1)}{u^2} - \frac{2Z}{u} - 2\varepsilon \right] U_l(u) = 0. \tag{4.204}$$

For large u applies

$$-\frac{d^2}{du^2} U_l(u) - 2\varepsilon U_l(u) \approx 0. \tag{4.205}$$

You make an approach

$$U_l(u) = \exp(-\lambda u) \quad (4.206)$$

with $\lambda \in \mathbb{R}$, $\lambda > 0$.
This results

$$\lambda^2 = -2\varepsilon. \quad (4.207)$$

For small r holds

$$\frac{d^2 U_l(u)}{du^2} \approx l(l+1) \frac{U_l(u)}{u^2}. \quad (4.208)$$

There is an approach here

$$U_l(u) = u^k \quad (4.209)$$

with $k \in \mathbb{N}$, $k \geq 2$. It follows

$$k(k-1) = l(l+1), \quad (4.210)$$

so

$$k = l+1. \quad (4.211)$$

Now set a function $P_l(u)$ with

$$U_l(u) = P_l(u) u^{l+1} \exp(-\lambda u) \quad (4.212)$$

to. Then apply

$$U'_l = P'_l u^{l+1} \exp(-\lambda u) + (l+1) \frac{U_l}{u} - \lambda U_l = P'_l u^{l+1} \exp(-\lambda u) + U_l \left(\frac{l+1}{u} - \lambda \right), \quad (4.213)$$

$$\begin{aligned} U''_l &= P''_l u^{l+1} \exp(-\lambda u) + (l+1) P'_l u^l \exp(-\lambda u) \\ &\quad - \lambda P'_l u^{l+1} \exp(-\lambda u) + U'_l \left(\frac{l+1}{u} - \lambda \right) - \frac{l+1}{u^2} U_l = P''_l u^{l+1} \exp(-\lambda u) \\ &\quad + (l+1) P'_l u^l \exp(-\lambda u) - \lambda P'_l u^{l+1} \exp(-\lambda u) \\ &\quad + \left(\frac{l+1}{u} - \lambda \right) \left[P'_l u^{l+1} \exp(-\lambda u) + U_l \left(\frac{l+1}{u} - \lambda \right) \right] - \frac{l+1}{u^2} U_l \\ &= P''_l u^{l+1} \exp(-\lambda u) + P'_l u^l \exp(-\lambda u) 2(l+1) - 2\lambda P'_l u^{l+1} \exp(-\lambda u) \\ &\quad + \lambda^2 P_l u^{l+1} \exp(-\lambda u) - 2\lambda(l+1) P_l u^l \exp(-\lambda u) + l(l+1) P_l u^{l-1} \exp(-\lambda u) \\ &= \exp(-\lambda u) u^{l+1} \left[P''_l + \frac{2(l+1)P'_l}{u} - 2\lambda P'_l + \lambda^2 P_l - 2\lambda \frac{l+1}{u} P_l + l \frac{l+1}{u^2} P_l \right]. \end{aligned} \quad (4.214)$$

Putting this into Eq. (4.204), you get

$$\begin{aligned} & - \exp(-\lambda u) u^{l+1} \left[P''_l + \frac{2(l+1)P'_l}{u} - 2\lambda P'_l + \lambda^2 P_l - 2\lambda \frac{l+1}{u} P_l + l \frac{l+1}{u^2} P_l \right] \\ & + l \frac{l+1}{u^2} P_l \exp(-\lambda u) u^{l+1} - 2Z \exp(-\lambda u) u^l P_l - 2\varepsilon \exp(-\lambda u) u^{l+1} P_l = 0 \\ & \Leftrightarrow -u^{l+1} P''_l - u^l 2(l+1) P'_l + 2\lambda P'_l u^{l+1} - \lambda^2 P_l u^{l+1} + 2\lambda(l+1) u^l P_l - 2Z u^l P_l - 2\varepsilon u^{l+1} P_l = 0 \\ & \Leftrightarrow u P''_l + 2(l+1) P'_l - 2\lambda P'_l u + \lambda^2 P_l u - 2\lambda(l+1) P_l + 2Z P_l + 2\varepsilon u P_l = 0 \\ & \Leftrightarrow u P''_l + (2l+2-2\lambda u) P'_l + (\lambda^2 u - 2\lambda(l+1) + 2Z + 2\varepsilon u) P_l = 0 \\ & \Leftrightarrow u P''_l + (2l+2-2\lambda u) P'_l + (-2\lambda(l+1) + 2Z) P_l = 0, \end{aligned} \quad (4.215)$$

the last step follows because $\mathcal{L}^2 = -2\varepsilon$, Eq. (4.207). This is divided by $2\mathcal{L}$:

$$\frac{1}{2\mathcal{L}}uP_l'' + \left(\frac{l+1}{\mathcal{L}} - u\right)P_l' + \left(\frac{Z}{\mathcal{L}} - l - 1\right)P_l = 0 \quad (4.216)$$

Define

$$x := 2\mathcal{L}u, \quad (4.217)$$

then are

$$u = \frac{x}{2\mathcal{L}}, \quad \frac{d}{du} = 2\mathcal{L}\frac{d}{dx}, \quad \frac{d^2}{du^2} = 4\mathcal{L}^2\frac{d^2}{dx^2}. \quad (4.218)$$

You replace it

$$P_l(u) \rightarrow P_l(x), \quad (4.219)$$

you get

$$\begin{aligned} xP_l'' + \left(\frac{l+1}{\mathcal{L}} - \frac{x}{2\mathcal{L}}\right)2\mathcal{L}P_l' + \left(\frac{Z}{\mathcal{L}} - l - 1\right)P_l &= 0 \\ \Leftrightarrow xP_l'' + (2l+2-x)P_l' + \left(\frac{Z}{\mathcal{L}} - l - 1\right)P_l &= 0. \end{aligned} \quad (4.220)$$

This is the *Laguerre's differential equation*. In section C.4 it is shown that the in Eq. (C.134) defined *Laguerre polynomials* $L_{n_r, 2l+1}(x)$ satisfy this equation, here $n_r \in \mathbb{N}$. Define $n := \frac{Z}{\mathcal{L}} \in \mathbb{N}$, n is the *principal quantum number*. applies to it

$$n = n_r + l + 1, \quad (4.221)$$

from this it follows $l < n$. It therefore applies to the energy eigenvalues with Eq. (4.207)

$$\varepsilon = -\frac{\mathcal{L}^2}{2} = -\frac{Z^2}{2n^2}, \quad (4.222)$$

so $n \geq 1$. It follows in original units

$$E_n = -\frac{Z^2}{2n^2}E_{\text{at}} = -\frac{Z^2\hbar^2}{2n^2m_e a_B^2}. \quad (4.223)$$

This therefore applies to the radial functions

$$\begin{aligned} R_{n_r, l}(r) &= C_{n_r, l} \frac{U_{n_r, l}(r)}{r} = C_{n_r, l} \frac{1}{r} L_{n_r, 2l+1}\left(\frac{2Zr}{na_B}\right) \left(\frac{2Zr}{na_B}\right)^{l+1} \exp\left(-\frac{Zr}{na_B}\right) \\ &= C_{n_r, l} \frac{2Z}{na_B} \left(\frac{2Zr}{na_B}\right)^l L_{n_r, 2l+1}\left(\frac{2Zr}{na_B}\right) \exp\left(-\frac{Zr}{na_B}\right) \end{aligned} \quad (4.224)$$

with a normalization constant $C_{n_r, l} \in \mathbb{R}$ that now needs to be determined. The probability $P(r)$ of encountering the particle at a distance of at most r from the origin is given by

$$P(r) = \int_0^r \int_0^{2\pi} \int_0^\pi |\psi_{n, l, m}(r', \theta, \varphi)|^2 r'^2 \sin(\theta) d\theta d\varphi dr' = \int_0^r |R_{n_r, l}(r')|^2 r'^2 dr', \quad (4.225)$$

so the radial probability density $\rho_{n_r, l}(r)$ is given by

$$\varrho_{n_r,l}(r) = \frac{dP}{dr} = R_{n_r,l}(r)^2 r^2. \quad (4.226)$$

The normalization condition is therefore:

$$\int_0^\infty R_{n_r,l}(r)^2 r^2 dr \stackrel{!}{=} 1. \quad (4.227)$$

You bet

$$\int_0^\infty U_{n_r,l}(r)^2 dr \stackrel{!}{=} \frac{1}{C_{n_r,l}^2} \quad (4.228)$$

and rescales the integral with $y = \frac{Zr}{na_B}$:

$$\begin{aligned} \int_0^\infty U_{n_r,l}(r)^2 dr &= \int_0^\infty y^{2l+2} L_{n_r,2l+1}(y)^2 \exp(-y) \frac{na_B}{2Z} dy \\ &= \frac{na_B}{2Z} \int_0^\infty y^{2l+2} L_{n_r,2l+1}(y)^2 \exp(-y) dy. \end{aligned} \quad (4.229)$$

For the remaining integral, Eq. (C.143)

$$\int_0^\infty y^{2l+2} L_{n_r,2l+1}(y)^2 \exp(-y) dy = \frac{(n_r + 2l + 1)!}{n_r!} (2n_r + 2l + 2) = 2n \frac{(n+l)!}{n_r!}. \quad (4.230)$$

It follows

$$C_{n_r,l} = \sqrt{\frac{Z}{a_B} \frac{1}{n}} \sqrt{\frac{n_r!}{(n+l)!}}. \quad (4.231)$$

The normalized radial functions are:

$$R_{n,l}(r) = \sqrt{\frac{Z^3}{a_B^3}} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \frac{2}{n^2} \left(\frac{Zr}{na_B}\right)^l L_{n-l-1,2l+1}\left(\frac{Zr}{na_B}\right) \exp\left(-\frac{Zr}{na_B}\right). \quad (4.232)$$

The hydrogen eigenfunctions are ultimately $\psi_{n,l,m}(r, \theta, \varphi)$

$$\begin{aligned} \psi_{n,l,m}(r, \theta, \varphi) &= R_{n,l}(r) Y_{l,m}(\theta, \varphi) \\ &= \sqrt{\frac{Z^3}{a_B^3} \frac{2}{n^2}} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \left(\frac{Zr}{na_B}\right)^l L_{n-l-1,2l+1}\left(\frac{Zr}{na_B}\right) \exp\left(-\frac{Zr}{na_B}\right) Y_{l,m}(\theta, \varphi). \end{aligned} \quad (4.233)$$

The probability densities $|\psi_{n,l,m}|^2$ are also referred to as *orbitals*. According to the so-called *angular momentum quantum number* l , it is named as given in Tab. 4.1. Different eigenfunctions with the same eigenvalue are called *degenerate*. From the conditions $n \in \mathbb{N}$, $l < n$ and $|m| \leq l$ one can determine the multiplicity N of the degeneracy for a given principal quantum number n (the energy depends only on the principal quantum number n):

$$N = \sum_{l=0}^{n-1} \sum_{m=-l}^l 1 = \sum_{l=0}^{n-1} (2l+1) = \sum_{l=1}^n (2l-1) = n(n+1) - n = n^2. \quad (4.234)$$

The Gaussian molecular formula Eq. (A.6) is used. The hydrogen eigenfunctions for the energy eigenvalue E_n are therefore n^2 -fold degenerate. If the spin is taken into account and relativistic corrections are not taken into

l	Bezeichnung
0	s
1	p
2	d
3	f

Table 4.1: Designation of the hydrogen eigenfunctions depending on the angular momentum quantum number l . For higher l it continues alphabetically.

account, the degree of degeneracy doubles.

4.9 Angular momentum

The angular momentum $\mathbf{L}$ of a point mass with the momentum $\mathbf{p} = (p_1, p_2, p_3)^T$ at the location $\mathbf{r} = (x_1, x_2, x_3)^T$ is given in classical mechanics by

$$\mathbf{L} := \mathbf{r} \times \mathbf{p} = \sum_{j,k,l=1}^3 \varepsilon_{j,k,l} x_j p_k \mathbf{e}_l \quad (4.235)$$

defined. Replace the Cartesian position components in this equation with the corresponding operators

$$x_j \rightarrow \hat{x}_j \quad (4.236)$$

as well as the Cartesian momentum components through the momentum operators

$$p_k \rightarrow \hat{p}_k, \quad (4.237)$$

one obtains the *angular momentum operator*

$$\hat{\mathbf{L}} := \hbar \sum_{j,k,l=1}^3 -i \varepsilon_{j,k,l} \hat{x}_j \frac{\partial}{\partial x_k} \mathbf{e}_l. \quad (4.238)$$

The location representation is written out in Cartesian coordinates

$$\hat{L}_x = \frac{\hbar}{i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right), \quad (4.239)$$

$$\hat{L}_y = \frac{\hbar}{i} \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right), \quad (4.240)$$

$$\hat{L}_z = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right). \quad (4.241)$$

The momentum operator $\hat{\mathbf{p}}$ is Hermitian just like the position operator $\hat{\mathbf{r}}$. Since $\hat{p}_j$ is swapped with $\hat{x}_k$ for $x \neq k$, according to Sect. 4.6.2 is also the sequential execution $\hat{p}_j \hat{x}_k = \hat{x}_k \hat{p}_j$ Hermitian. Thus the angular momentum operators are Hermitian. You define

$$\hat{L}_{\pm} := \hat{L}_x \pm i \hat{L}_y. \quad (4.242)$$

As a shorthand notation, one uses a generalized angular momentum operator

$$\hat{\mathbf{J}} := -i \hat{\mathbf{r}} \times \nabla \quad (4.243)$$

a. Now some commutator relations of the angular momentum operators will be derived. It applies in the representation of the location

$$\hat{J}_l = -i \sum_{j,k=1}^3 \varepsilon_{j,k,l} x_j \frac{\partial}{\partial x_k}. \quad (4.244)$$

This means that the commutator has two components of the angular momentum operator

$$\begin{aligned} [\hat{J}_j, \hat{J}_k] &= \hat{J}_j \hat{J}_k - \hat{J}_k \hat{J}_j = \left(-i \sum_{l,m=1}^3 \varepsilon_{l,m,j} x_l \frac{\partial}{\partial x_m} \right) \left(-i \sum_{l,m=1}^3 \varepsilon_{l,m,k} x_l \frac{\partial}{\partial x_m} \right) \\ &\quad - \left(-i \sum_{l,m=1}^3 \varepsilon_{l,m,k} x_l \frac{\partial}{\partial x_m} \right) \left(-i \sum_{l,m=1}^3 \varepsilon_{l,m,j} x_l \frac{\partial}{\partial x_m} \right) \\ &= - \left(\sum_{l,m=1}^3 \varepsilon_{l,m,j} x_l \frac{\partial}{\partial x_m} \right) \left(\sum_{l,m=1}^3 \varepsilon_{l,m,k} x_l \frac{\partial}{\partial x_m} \right) + \left(\sum_{l,m=1}^3 \varepsilon_{l,m,k} x_l \frac{\partial}{\partial x_m} \right) \left(\sum_{l,m=1}^3 \varepsilon_{l,m,j} x_l \frac{\partial}{\partial x_m} \right) \\ &= - \sum_{l,m,n,o=1}^3 \varepsilon_{l,m,j} \varepsilon_{n,o,k} x_l \frac{\partial}{\partial x_m} x_n \frac{\partial}{\partial x_o} + \sum_{l,m,n,o=1}^3 \varepsilon_{l,m,k} \varepsilon_{n,o,j} x_l \frac{\partial}{\partial x_m} x_n \frac{\partial}{\partial x_o} \\ &= - \sum_{l,m,n,o=1}^3 \varepsilon_{l,m,j} \varepsilon_{n,o,k} x_l x_n \frac{\partial^2}{\partial x_o \partial x_m} + \sum_{l,m,n,o=1}^3 \varepsilon_{l,m,k} \varepsilon_{n,o,j} x_l x_n \frac{\partial^2}{\partial x_o \partial x_m} \\ &\quad - \sum_{l,m,n,o=1}^3 \varepsilon_{l,m,j} \varepsilon_{n,o,k} x_l \delta_{n,m} \frac{\partial}{\partial x_o} + \sum_{l,m,n,o=1}^3 \varepsilon_{l,m,k} \varepsilon_{n,o,j} x_l \delta_{mn} \frac{\partial}{\partial x_o} \\ &= \sum_{l,m,n,o=1}^3 x_l x_n (\varepsilon_{l,m,k} \varepsilon_{n,o,j} - \varepsilon_{l,m,j} \varepsilon_{n,o,k}) \frac{\partial^2}{\partial x_o \partial x_m} - \sum_{l,n,o=1}^3 \varepsilon_{l,n,j} \varepsilon_{n,o,k} x_l \frac{\partial}{\partial x_o} + \sum_{l,n,o=1}^3 \varepsilon_{l,n,k} \varepsilon_{n,o,j} x_l \frac{\partial}{\partial x_o} \\ &= \sum_{l,n,o=1}^3 x_l \frac{\partial}{\partial x_o} (\varepsilon_{l,n,k} \varepsilon_{n,o,j} - \varepsilon_{l,n,j} \varepsilon_{n,o,k}) = \sum_{n=1}^3 \sum_{l,o=1}^3 (\varepsilon_{l,n,k} \varepsilon_{n,o,j} - \varepsilon_{l,n,j} \varepsilon_{n,o,k}) x_l \frac{\partial}{\partial x_o} \\ &= \sum_{n=1}^3 \sum_{l,o=1}^3 \varepsilon_{j,k,n} \varepsilon_{l,o,n} x_l \frac{\partial}{\partial x_o} = \sum_{n=1}^3 \varepsilon_{j,k,n} \sum_{l,o=1}^3 \varepsilon_{l,o,n} x_l \frac{\partial}{\partial x_o} = \sum_{n=1}^3 \varepsilon_{j,k,n} \frac{1}{-i} \hat{J}_n = i \sum_{n=1}^3 \varepsilon_{j,k,n} \hat{J}_n. \end{aligned} \quad (4.245)$$

Eq. (A.22) is used. This means in particular

$$[\hat{J}_1, \hat{J}_2] = i\hat{J}_3, \quad [\hat{J}_2, \hat{J}_3] = i\hat{J}_1, \quad [\hat{J}_3, \hat{J}_1] = i\hat{J}_2. \quad (4.246)$$

Thus is

$$[\hat{J}_3, \hat{J}_\pm] = [\hat{J}_3, \hat{J}_1 \pm i\hat{J}_2] = [\hat{J}_3, \hat{J}_1] \pm [\hat{J}_3, i\hat{J}_2] = i\hat{J}_2 \pm i(-i\hat{J}_1) = \pm\hat{J}_1 + i\hat{J}_2 = \pm\hat{J}_\pm. \quad (4.247)$$

Still apply

$$\begin{aligned} \hat{J}_\pm \hat{J}_\mp &= (\hat{J}_1 \pm i\hat{J}_2) (\hat{J}_1 \mp i\hat{J}_2) = \hat{J}_1^2 + \hat{J}_2^2 \mp i\hat{J}_1 \hat{J}_2 \pm i\hat{J}_2 \hat{J}_1 \\ &= \hat{J}^2 - \hat{J}_3^2 \mp i[\hat{J}_1, \hat{J}_2] = \hat{J}^2 - \hat{J}_3^2 \mp i \quad (4.248) \end{aligned}$$

and

$$\begin{aligned}
[\hat{\mathbf{J}}^2, \hat{J}_1] &= [\hat{J}_2^2 + \hat{J}_3^2, \hat{J}_1] = \hat{J}_2 \hat{J}_2 \hat{J}_1 - \hat{J}_1 \hat{J}_2 \hat{J}_2 + \hat{J}_3 \hat{J}_3 \hat{J}_1 - \hat{J}_1 \hat{J}_3 \hat{J}_3 \\
&= \hat{J}_2 \hat{J}_2 \hat{J}_1 - \hat{J}_1 \hat{J}_2 \hat{J}_2 + \hat{J}_2 \hat{J}_1 \hat{J}_2 - \hat{J}_2 \hat{J}_1 \hat{J}_2 + \hat{J}_3 \hat{J}_3 \hat{J}_1 - \hat{J}_1 \hat{J}_3 \hat{J}_3 + \hat{J}_3 \hat{J}_1 \hat{J}_3 - \hat{J}_3 \hat{J}_1 \hat{J}_3 \\
&= \hat{J}_2 [\hat{J}_2, \hat{J}_1] + [\hat{J}_2, \hat{J}_1] \hat{J}_2 + \hat{J}_3 [\hat{J}_3, \hat{J}_1] + [\hat{J}_3, \hat{J}_1] \hat{J}_3 \\
&= -i\hat{J}_2 \hat{J}_3 - i\hat{J}_3 \hat{J}_2 + i\hat{J}_3 \hat{J}_2 + i\hat{J}_2 \hat{J}_3 = 0,
\end{aligned} \tag{4.249}$$

analogously for $\hat{J}_2$ and $\hat{J}_3$ and thus also

$$[\hat{\mathbf{J}}^2, \hat{J}_\pm] = 0. \tag{4.250}$$

To deal with the angular momentum in the H atom, the angular momentum operators should now be transformed into spherical coordinates. For this purpose, in addition to Eq. (B.91) the representation

$$\nabla = \mathbf{e}_r \frac{\partial}{\partial r} + \mathbf{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_\varphi \frac{1}{r \sin(\theta)} \frac{\partial}{\partial \varphi}. \tag{4.251}$$

of the gradient. The well-known relations still apply

$$\mathbf{e}_r \times \mathbf{e}_\theta = \mathbf{e}_\varphi \tag{4.252}$$

as well as

$$\mathbf{e}_r \times \mathbf{e}_\varphi = -\mathbf{e}_\theta. \tag{4.253}$$

This follows in the location representation

$$\hat{\mathbf{J}} = -i\mathbf{r} \times \nabla = -i\mathbf{r} \times \left(\mathbf{e}_r \frac{\partial}{\partial r} + \mathbf{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_\varphi \frac{1}{r \sin(\theta)} \frac{\partial}{\partial \varphi} \right) = -i\mathbf{e}_\varphi \frac{\partial}{\partial \theta} + i\mathbf{e}_\theta \frac{1}{\sin(\theta)} \frac{\partial}{\partial \varphi}. \tag{4.254}$$

Due to the equations (B.74) - (B.76) apply

$$\hat{J}_x = -i \left(-\sin(\varphi) \frac{\partial}{\partial \theta} - \cos(\varphi) \cot(\theta) \frac{\partial}{\partial \varphi} \right), \tag{4.255}$$

$$\hat{J}_y = -i \left(\cos(\varphi) \frac{\partial}{\partial \theta} - \sin(\varphi) \cot(\theta) \frac{\partial}{\partial \varphi} \right), \tag{4.256}$$

$$\hat{J}_z = -i \frac{\partial}{\partial \varphi}. \tag{4.257}$$

Still applies

$$\begin{aligned}
\hat{\mathbf{J}}^2 &= \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \\
&= -\sin^2(\varphi) \frac{\partial^2}{\partial \theta^2} - \cos^2(\varphi) \cot^2(\theta) \frac{\partial^2}{\partial \varphi^2} - \cos^2(\varphi) \frac{\partial^2}{\partial \theta^2} - \sin^2(\varphi) \cot^2(\theta) \frac{\partial^2}{\partial \varphi^2} - \frac{\partial^2}{\partial \varphi^2} - \cot(\theta) \frac{\partial}{\partial \theta} \\
&= - \left(\frac{\partial^2}{\partial \theta^2} + \cot^2(\theta) \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial \varphi^2} + \cot(\theta) \frac{\partial}{\partial \theta} \right) = - \left(\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \varphi^2} \right).
\end{aligned} \tag{4.258}$$

This corresponds to Eq. (B.96) of the statement

$$\hat{\mathbf{J}}^2 = -\Delta_{\theta, \varphi}. \tag{4.259}$$

Let $|n, l, m\rangle$ be the state of an electron in the hydrogen atom with quantum numbers n , l and m . Due to the location representation of $|n, l, m\rangle$ Eq. (4.233), the definition of the spherical area functions Eq. (C.155), the representation of the z-components of the angular momentum operator Eq. (4.257), the equation just derived.

(4.259) and the property Eq. (C.166) of the spherical harmonic functions, the following two statements apply:

$$\hat{L}^2 |n, l, m\rangle = \hbar^2 l(l+1) |n, l, m\rangle, \quad (4.260)$$

$$\hat{L}_z |n, l, m\rangle = m\hbar |n, l, m\rangle \quad (4.261)$$

From this follow:

- The total torque L in state $|n, l, m\rangle$ is $\hbar\sqrt{l(l+1)}$. Therefore l is called angular momentum quantum number.
- The z-component of the angular momentum L_z in the state $|n, l, m\rangle$ is $L_z = m\hbar$. m is called *magnetic quantum number*.
- $\hat{L}^2$, $\hat{L}_z$ and $\hat{H}$ commute in pairs. Therefore, L^2 and L_z are conserved quantities and since the hydrogen eigenstates depend on three quantum numbers, these three operators in the hydrogen atom are complete observables regardless of spin.

You can still find

$$\begin{aligned} \hat{J}_\pm &= \hat{J}_x \pm i\hat{J}_y = -i \left(-\sin(\varphi) \frac{\partial}{\partial \theta} - \cos(\varphi) \cot(\theta) \frac{\partial}{\partial \varphi} \right) \pm \left(\cos(\varphi) \frac{\partial}{\partial \theta} - \sin(\varphi) \cot(\theta) \frac{\partial}{\partial \varphi} \right) \\ &= (\cos(\varphi) \mp i\sin(\varphi)) \cot(\theta) \frac{\partial}{\partial \varphi} + (\pm \cos(\varphi) + i\sin(\varphi)) \frac{\partial}{\partial \theta} \\ &= ie^{\pm i\varphi} \cot(\theta) \frac{\partial}{\partial \varphi} \pm e^{\pm i\varphi} \frac{\partial}{\partial \theta} = \exp(\pm i\varphi) \left(i\cot(\theta) \frac{\partial}{\partial \varphi} \pm \frac{\partial}{\partial \theta} \right). \end{aligned} \quad (4.262)$$

Now the generalized angular momentum operator $\hat{\mathcal{J}}$ becomes Eq. (4.243) is treated a little further. It and its components were identified as Hermitian, so $\hat{\mathcal{J}}^2$ is also Hermitian as a successive execution of Hermitian commutative operators according to section 4.6.2. It still applies

$$\hat{\mathcal{J}}_+^+ = \hat{\mathcal{J}}_-, \quad \hat{\mathcal{J}}_-^+ = \hat{\mathcal{J}}_+. \quad (4.263)$$

Among the four operators $\hat{\mathcal{J}}^2, \hat{\mathcal{J}}_x, \hat{\mathcal{J}}_y, \hat{\mathcal{J}}_z$ one can use Eq. (4.245) and Eq. (4.249) find two that commute, namely $\hat{\mathcal{J}}^2$ and another, for this $\hat{\mathcal{J}}_z$ is chosen. According to section 4.6.3, these have the same eigenfunctions, so you can write

$$\hat{\mathcal{J}}^2 |\mathcal{J}, m\rangle = \mathcal{J} |\mathcal{J}, m\rangle, \quad \hat{\mathcal{J}}_z |\mathcal{J}, m\rangle = m |\mathcal{J}, m\rangle \quad (4.264)$$

with real eigenvalues $\mathcal{J}, m \in \mathbb{R}$. Now look at the conditions

$$\hat{\mathcal{J}}_+ |\mathcal{J}, m\rangle \quad (4.265)$$

and

$$\hat{\mathcal{J}}_- |\mathcal{J}, m\rangle \quad (4.266)$$

to. Since $\hat{\mathcal{J}}^2$ commutes with $\hat{\mathcal{J}}_\pm$, we have

$$\hat{\mathcal{J}}^2 \hat{\mathcal{J}}_\pm |\mathcal{J}, m\rangle = \hat{\mathcal{J}}_\pm \hat{\mathcal{J}}^2 |\mathcal{J}, m\rangle = \mathcal{J} \hat{\mathcal{J}}_\pm |\mathcal{J}, m\rangle. \quad (4.267)$$

With Eq. (4.247) follows

$$\hat{\mathcal{J}}_z \hat{\mathcal{J}}_\pm - \hat{\mathcal{J}}_\pm \hat{\mathcal{J}}_z = \pm \hat{\mathcal{J}}_\pm \Leftrightarrow \hat{\mathcal{J}}_z \hat{\mathcal{J}}_\pm = \hat{\mathcal{J}}_\pm \hat{\mathcal{J}}_z \pm \hat{\mathcal{J}}_\pm \quad (4.268)$$

and thus

$$\hat{\mathcal{J}}_z \hat{\mathcal{J}}_\pm |\mathcal{J}, m\rangle = (\hat{\mathcal{J}}_\pm \hat{\mathcal{J}}_z \pm \hat{\mathcal{J}}_\pm) |\mathcal{J}, m\rangle = \hat{\mathcal{J}}_\pm (\hat{\mathcal{J}}_z \pm 1) |\mathcal{J}, m\rangle = (m \pm 1) \hat{\mathcal{J}}_\pm |\mathcal{J}, m\rangle. \quad (4.269)$$

So it applies

$$\hat{J}_{\pm} |\mathcal{J}, m\rangle = c_{\pm} |\mathcal{J}, m \pm 1\rangle. \quad (4.270)$$

with $c_{\pm} \in \mathbb{R}$. Therefore, $\hat{J}_+$ is called *ascend operator* and $\hat{J}_-$ *descend operator*. You now have to calculate the normalization constants $c_{\pm}$. This is done by normalization

$$\langle \mathcal{J}, m | \mathcal{J}, m \rangle \stackrel{!}{=} 1 \quad (4.271)$$

of the conditions, you can simply demand this. So you get

$$c_{\pm}^2 = \langle \mathcal{J}, m \pm 1 | c_{\pm} c_{\pm} | \mathcal{J}, m \pm 1 \rangle = \langle \hat{J}_{\pm} \mathcal{J}, m | \hat{J}_{\pm} | \mathcal{J}, m \rangle = \langle \mathcal{J}, m | \hat{J}_{\mp} \hat{J}_{\pm} | \mathcal{J}, m \rangle. \quad (4.272)$$

Here you can see Eq. Insert (4.248) and get $c_{\pm} > 0$ with the requirement

$$\begin{aligned} c_{\pm}^2 &= \langle \mathcal{J}, m | \hat{J}^2 - \hat{J}_z^2 \mp \hat{J}_z | \mathcal{J}, m \rangle = \mathcal{J} - m^2 \mp m \\ \Leftrightarrow c_{\pm} &= \sqrt{\mathcal{J} - m^2 \mp m} = \sqrt{\mathcal{J} - m(m \pm 1)}. \end{aligned} \quad (4.273)$$

Now we have to derive a condition for $\mathcal{J}$ and m . For a Hermitian operator $\hat{A}$ holds

$$\langle f | \hat{A}^2 f \rangle = \langle \hat{A} f | \hat{A} f \rangle \geq 0. \quad (4.274)$$

It follows

$$0 \leq \langle \mathcal{J}, m | \hat{J}_x^2 | \mathcal{J}, m \rangle + \langle \mathcal{J}, m | \hat{J}_y^2 | \mathcal{J}, m \rangle = \langle \mathcal{J}, m | \hat{J}^2 - \hat{J}_z^2 | \mathcal{J}, m \rangle = \mathcal{J} - m^2. \quad (4.275)$$

Consequently applies

$$\mathcal{J} \geq m^2 \geq 0. \quad (4.276)$$

From a state $|\mathcal{J}, m\rangle$ one obtains the states $|\mathcal{J}, m \pm 1\rangle$, $|\mathcal{J}, m \pm 2\rangle$ and so on by applying the ascending and descending operators. However, this has to stop somewhere because of (4.276), so the normalization Eq. (4.273) at a maximum $m_{\max}$ and at a minimum $m_{\min}$ disappear:

$$\hat{J}_+ |\mathcal{J}, m_{\max}\rangle = 0 \Rightarrow c_+ = 0 \Rightarrow \mathcal{J} = m_{\max}(m_{\max} + 1), \quad (4.277)$$

$$\hat{J}_- |\mathcal{J}, m_{\min}\rangle = 0 \Rightarrow c_- = 0 \Rightarrow \mathcal{J} = m_{\min}(m_{\min} - 1) \quad (4.278)$$

$$\Rightarrow (m_{\max} + m_{\min})(m_{\max} - m_{\min} + 1) = 0 \quad (4.279)$$

Because $m_{\max} \geq m_{\min}$ the second bracket is not equal to zero, so the first bracket is equal to zero:

$$m_{\max} = -m_{\min} =: j \quad (4.280)$$

It applies

$$\mathcal{J} = j(j + 1). \quad (4.281)$$

The ascending operator therefore leads from $-j$ to j in integer steps. So $2j$ is an integer, therefore j is an integer or half integer. Now there is a name change

$$|\mathcal{J}, m\rangle = |j(j + 1), m\rangle \rightarrow |j, m\rangle \quad (4.282)$$

a. These states are normalized and, as eigenstates of Hermitian operators, they are orthogonal to different eigenvalues:

$$\langle j', m' | j, m \rangle = \delta_{j,j'} \delta_{m,m'}. \quad (4.283)$$

If j is an integer, the spatial representation of the solution is given by the spherical area functions Eq. (C.155). This describes, for example, the orbital torque of particles in the central force field, see section 4.8. The case that j is half-integer is important for particles with half-integer spin. Particles with half-integer spin are called *Fermions*, while particles with integer spin are called *Bosons*. Examples of fermions are electrons, protons and neutrons, photons are bosons.

From now on we assume half-integer spin, namely $j = \frac{1}{2}$. In this case, the states $|j, m\rangle$ are denoted by $|ss_z\rangle = |\frac{1}{2}, s_z\rangle$. You define

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} := \left| \frac{1}{2}, \frac{1}{2} \right\rangle, \quad (4.284)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} := \left| \frac{1}{2}, -\frac{1}{2} \right\rangle. \quad (4.285)$$

Eq. (4.284) is given as *spin-up state* and Eq. (4.285) is called *spin-down state*. We have $\hat{J}_z \left| \frac{1}{2}, m \right\rangle = m \left| \frac{1}{2}, m \right\rangle$, so follows in matrix notation

$$J_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, \quad J_z \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{1}{2} \end{pmatrix}, \quad (4.286)$$

what is fulfilled for

$$J_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.287)$$

For the normalization constant $c_{\pm}$ from Eq. (4.273) apply with $\lambda = j(j+1) = \frac{1}{2} \cdot \frac{3}{2} = \frac{3}{4}$

$$c_+ = \sqrt{\frac{3}{4} + \frac{1}{2} \left(-\frac{1}{2} + 1 \right)} = 1, \quad (4.288)$$

$$c_- = \sqrt{\frac{3}{4} - \frac{1}{2} \left(\frac{1}{2} - 1 \right)} = 1. \quad (4.289)$$

Therefore, because of $\hat{J}_+ \left| \frac{1}{2}, \frac{1}{2} \right\rangle = 0$ and $\hat{J}_+ \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \left| \frac{1}{2}, \frac{1}{2} \right\rangle$ also applies

$$J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (4.290)$$

Because $\hat{J}_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \left| \frac{1}{2}, -\frac{1}{2} \right\rangle$ and $\hat{J}_- \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = 0$ holds

$$J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (4.291)$$

Therefore apply

$$J_x = \frac{1}{2} (J_+ + J_-) = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (4.292)$$

$$J_y = -i \frac{1}{2} (J_+ - J_-) = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (4.293)$$

The matrices appearing here

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (4.294)$$

are also called *Pauli matrices* or spin matrices.

4.10 Spin

The question arises as to whether the half-integer states have any physical relevance at all or are just purely mathematical phenomena. In fact, these states describe the intrinsic torque of the elementary particles, namely the *spin*. Experimentally, you can only change the direction, but not the amount, of spin, which is a particle property, just like charge and mass. It is not linked to a rotating mass distribution, so no angular momentum in the pure sense.

Now the Schrödinger equation should be generalized to a particle with mass m , charge q and spin $1/2$. If you have now been given a particle with charge q and spin $1/2$, a simple wave function $\mathbb{R}^3 \rightarrow \mathbb{C}$ is no longer sufficient to describe the state of this particle. The probability density no longer only depends on the location, but also on the spin state. However, one can write for the state of such a particle using the definitions Equations (4.284) and (4.285)

$$|\psi(\mathbf{r}, t)\rangle = \varphi_+(\mathbf{r}, t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \varphi_-(\mathbf{r}, t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (4.295)$$

with location- and time-dependent components $\varphi_+(\mathbf{r}, t)$ and $\varphi_-(\mathbf{r}, t)$. Such a wave function is called *Spinor*. This state is of course normalized:

$$\langle \psi | \psi \rangle = \int_{\mathbb{R}^3} (|\varphi_+(\mathbf{r})|^2 + |\varphi_-(\mathbf{r})|^2) d^3r \quad (4.296)$$

You can use Eq. (3.23)

$$\hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - \frac{q}{c} \hat{\mathbf{A}}, \quad (4.297)$$

replace to take into account the energy of a particle in the electromagnetic field. Furthermore, the potential energy term must be expanded. A magnetic moment $\boldsymbol{\mu}$ has potential energy in a B field $\mathbf{B}$

$$E_{\text{pot}} = -\boldsymbol{\mu} \cdot \mathbf{B}. \quad (4.298)$$

Since an elementary particle only knows one distinct direction in its rest system, namely that of the spin, the magnetic moment must be parallel to the spin. The spin is replaced by the *spin operator*

$$\mathbf{s} \rightarrow \hat{\mathbf{s}}. \quad (4.299)$$

For particles with spin $1/2$ this can be written using the operators $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ defined by the Pauli matrices as

$$\hat{\mathbf{s}} = \frac{\hbar}{2} \hat{\boldsymbol{\sigma}} = \frac{\hbar}{2} \boldsymbol{\sigma}. \quad (4.300)$$

This was a vector

$$\boldsymbol{\sigma} = \sigma_x \mathbf{e}_x + \sigma_y \mathbf{e}_y + \sigma_z \mathbf{e}_z \in \mathbb{C}^{2 \times 2 \times 3} \quad (4.301)$$

introduced. If φ is the scalar potential of the electromagnetic field, then the desired Hamiltonian is

$$\hat{H} = \frac{1}{2m} \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A} \right)^2 + q\varphi - \hat{\boldsymbol{\mu}} \cdot \mathbf{B}. \quad (4.302)$$

For the magnetic moment applies

$$\boldsymbol{\mu} = g \frac{q}{2mc} \mathbf{s} \quad (4.303)$$

with a classically inferable factor g , which is called *Landé factor*. For the Pauli-Hamilton operator follows

$$\hat{H}_P = \frac{1}{2m} \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A} \right)^2 + q\varphi - g \frac{q\hbar}{4mc} \boldsymbol{\sigma} \cdot \mathbf{B}. \quad (4.304)$$

The *Pauli equation* is therefore:

$$\hat{H}_P |\psi(\mathbf{r}, t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(\mathbf{r}, t)\rangle. \quad (4.305)$$

for a spinor $|\psi(\mathbf{r}, t)\rangle$, see Eq. (4.295).

4.11 Perturbation theory

4.11.1 Time-independent case

Be an intrinsic value problem

$$\hat{H}_o \left| \psi^{(o)} \right\rangle = E^{(o)} \left| \psi^{(o)} \right\rangle \quad (4.306)$$

given a Hamiltonian $\hat{H}_o$, orthonormal and complete eigenfunctions $\left| \psi_n^{(o)} \right\rangle$ and associated eigenvalues $E_n^{(o)}$. Now replace the Hamiltonian $\hat{H}_o$ with a new Hamiltonian $\hat{H}$, which is given by

$$\hat{H} := \hat{H}_o + \hat{v}_h \quad (4.307)$$

with a disturbance potential $\hat{v}_h$. One wants solutions $\left| \psi \right\rangle$ of the eigenvalue equation

$$\hat{H} \left| \psi \right\rangle = E \left| \psi \right\rangle \quad (4.308)$$

find. To do this, you first set

$$\hat{H}(\lambda) := \hat{H}_o + \lambda \hat{v}_h \quad (4.309)$$

with $\lambda \in [0, 1]$. Now one develops the eigenstates $\left| \psi \right\rangle$ and eigenvalues E according to powers of λ :

$$E(\lambda) = \sum_{i=0}^{\infty} \lambda^{(i)} E^{(i)}, \quad \left| \psi(\lambda) \right\rangle = \sum_{i=0}^{\infty} \lambda^{(i)} \left| \psi^{(i)} \right\rangle \quad (4.310)$$

This is put into Eq. (4.308):

$$\hat{H}(\lambda) \left| \psi(\lambda) \right\rangle = E(\lambda) \left| \psi(\lambda) \right\rangle \quad (4.311)$$

$$\Rightarrow \left(\hat{H}_o + \lambda \hat{v}_h \right) \sum_{i=0}^{\infty} \lambda^{(i)} \left| \psi^{(i)} \right\rangle = \left(\sum_{i=0}^{\infty} \lambda^{(i)} E^{(i)} \right) \left(\sum_{i=0}^{\infty} \lambda^{(i)} \left| \psi^{(i)} \right\rangle \right) \quad (4.312)$$

You sort Eq. (4.312) now to powers of λ , for the m -th order then applies

$$\hat{H}_o \left| \psi^{(m)} \right\rangle + \hat{v}_h \left| \psi^{(m-1)} \right\rangle = \sum_{k=0}^m E^{(m-k)} \left| \psi^{(k)} \right\rangle. \quad (4.313)$$

There exist $C_{n,k}^{(1)} \in \mathbb{C}$ with

$$\left| \psi_n^{(1)} \right\rangle = \sum_{k=1}^{\infty} C_{n,k}^{(1)} \left| \psi_k^{(o)} \right\rangle. \quad (4.314)$$

If you apply the undisturbed Hamiltonian $\hat{H}_o$ to this, you get

$$\hat{H}_o \left| \psi_n^{(1)} \right\rangle = \sum_{k=1}^{\infty} C_{n,k}^{(1)} E_k^{(o)} \left| \psi_k^{(o)} \right\rangle. \quad (4.315)$$

If you put in Eq. (4.313) $m = 1$ and $\left| \psi \right\rangle = \left| \psi_n \right\rangle$ and multiply this from the left by $\left\langle \psi_n^{(o)} \right|$, you get

$$\left\langle \psi_n^{(o)} \right| \hat{H}_o \left| \psi_n^{(1)} \right\rangle + \left\langle \psi_n^{(o)} \right| \hat{v}_h \left| \psi_n^{(o)} \right\rangle = E_n^{(1)} + \left\langle \psi_n^{(o)} \right| E_n^{(o)} \left| \psi_n^{(1)} \right\rangle. \quad (4.316)$$

Also applies

$$\left\langle \psi_n^{(0)} \left| \hat{H}_0 \right| \psi_n^{(1)} \right\rangle = C_{n,n}^{(1)} E_n^{(0)} = \left\langle \psi_n^{(0)} \left| E_n^{(0)} \right| \psi_n^{(1)} \right\rangle. \quad (4.317)$$

The following applies to the first-order energy correction:

$$E_n^{(1)} = \left\langle \psi_n^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle. \quad (4.318)$$

Now the $\left| \psi_n^{(1)} \right\rangle$ are searched for, i.e. the $C_{n,k}^{(1)}$, $k \in \mathbb{N}$ with $k \neq n$. Multiply Eq. (4.313) with $m = \mathfrak{z}$ from the left with $\left\langle \psi_k^{(0)} \right|$. It emerges

$$\begin{aligned} \left\langle \psi_k^{(0)} \left| \hat{H}_0 \right| \psi_n^{(1)} \right\rangle + \left\langle \psi_k^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle &= \left\langle \psi_k^{(0)} \left| E_n^{(0)} \right| \psi_n^{(1)} \right\rangle \\ \Leftrightarrow C_{n,k}^{(1)} E_k^{(0)} + \left\langle \psi_k^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle &= E_n^{(0)} C_{n,k}^{(1)} \\ \Leftrightarrow C_{n,k}^{(1)} &= \frac{\left\langle \psi_k^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}}. \end{aligned} \quad (4.319)$$

This only works in the case of non-degenerate energy levels $E_n^{(0)}, E_k^{(0)}$. For the state $\left| \psi_n(\mathcal{L}) \right\rangle$ we now get

$$\left| \psi_n(\mathcal{L}) \right\rangle = \left| \psi_n^{(0)} \right\rangle + \mathcal{L} \sum_{\substack{m=1, \\ m \neq n}}^{\infty} \frac{\left\langle \psi_m^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_m^{(0)}} \left| \psi_m^{(0)} \right\rangle + C_{n,n}^{(1)} \left| \psi_n^{(0)} \right\rangle + \mathcal{O}(\mathcal{L}^2). \quad (4.320)$$

The norm of this is

$$\left\langle \psi_n(\mathcal{L}) \left| \psi_n(\mathcal{L}) \right\rangle = \mathbf{1} + C_{n,n}^{(1)*} + C_{n,n}^{(1)} + \mathcal{O}(\mathcal{L}^2) \quad (4.321)$$

So $C_{n,n}^{(1)} = ir$ with $r \in \mathbb{R}$. Therefore, the amplitude of $\left| \psi_n^{(0)} \right\rangle$ in $\left| \psi_n(\mathcal{L}) \right\rangle$ is given by

$$\mathbf{1} + i\mathcal{L}r = \exp(i\mathcal{L}r) + \mathcal{O}(\mathcal{L}^2). \quad (4.322)$$

The coefficient $C_{n,n}^{(1)}$ leads to a first order phase shift of $\left| \psi_n^{(0)} \right\rangle$, this phase shift can be absorbed in $\left| \psi_n^{(0)} \right\rangle$ and

$$C_{n,n}^{(1)} = \mathbf{0} \quad (4.323)$$

set. So you get first order in the case of non-degenerate energy levels

$$E_n = E_n^{(0)} + E_n^{(1)} = E_n^{(0)} + \left\langle \psi_n^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle, \quad (4.324)$$

$$\left| \psi_n \right\rangle = \left| \psi_n^{(0)} \right\rangle + \left| \psi_n^{(1)} \right\rangle = \left| \psi_n^{(0)} \right\rangle + \sum_{\substack{m=1, \\ m \neq n}}^{\infty} \frac{\left\langle \psi_m^{(0)} \left| \hat{v}_h \right| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_m^{(0)}} \left| \psi_m^{(0)} \right\rangle. \quad (4.325)$$

A necessary condition for meaningful applicability of first-order perturbation theory is that the admixtures of states are small.

You can already see the advantage of perturbation theory: While stationary problems in quantum mechanics are eigenvalue problems in which you have to determine the eigenvalue and eigenvector simultaneously, in perturbation theory you can calculate the energy corrections and the state corrections successively one after the other.

To calculate the second order, one inserts into Eq. (4.313) with $m = \mathfrak{z}$ first enter $\left| \psi \right\rangle = \left| \psi_n \right\rangle$ and multiply this from the left by $\left\langle \psi_n^{(0)} \right|$:

$$\left\langle \psi_n^{(0)} \left| \hat{H}_0 \right| \psi_n^{(2)} \right\rangle + \left\langle \psi_n^{(0)} \left| \hat{v}_h \right| \psi_n^{(1)} \right\rangle = E_n^{(2)} + \left\langle \psi_n^{(0)} \left| E_n^{(1)} \right| \psi_n^{(1)} \right\rangle + \left\langle \psi_n^{(0)} \left| E_n^{(0)} \right| \psi_n^{(2)} \right\rangle \quad (4.326)$$

For the $\left| \psi_n^{(2)} \right\rangle$ you now do the approach

$$\left| \psi_n^{(2)} \right\rangle = \sum_{m=1}^{\infty} C_{n,m}^{(2)} \left| \psi_m^{(0)} \right\rangle. \quad (4.327)$$

This follows

$$\left\langle \psi_n^{(0)} \left| \hat{H}_0 \sum_{m=1}^{\infty} C_{n,m}^{(2)} \left| \psi_m^{(0)} \right\rangle \right\rangle = \left\langle \psi_n^{(0)} \left| \sum_{m=1}^{\infty} C_{n,m}^{(2)} E_m^{(0)} \left| \psi_m^{(0)} \right\rangle \right\rangle = C_{n,n}^{(2)} E_n^{(0)}. \quad (4.328)$$

Still applies

$$\left\langle \psi_n^{(0)} \left| E_n^{(1)} \left| \psi_n^{(1)} \right\rangle \right\rangle = \left\langle \psi_n^{(0)} \left| E_n^{(1)} \sum_{m=1}^{\infty} C_{n,m}^{(1)} \left| \psi_m^{(0)} \right\rangle \right\rangle = E_n^{(1)} C_{n,n}^{(1)} = 0. \quad (4.329)$$

Thus follows

$$\begin{aligned} E_n^{(2)} &= \left\langle \psi_n^{(0)} \left| \hat{v}_h \left| \psi_n^{(1)} \right\rangle \right\rangle = \left\langle \psi_n^{(0)} \left| \hat{v}_h \sum_{m=1}^{\infty} C_{n,m}^{(1)} \left| \psi_m^{(0)} \right\rangle \right\rangle = \sum_{m=1}^{\infty} C_{n,m}^{(1)} \left\langle \psi_n^{(0)} \left| \hat{v}_h \left| \psi_m^{(0)} \right\rangle \right\rangle \\ &= \sum_{\substack{m=1, \\ m \neq n}}^{\infty} \frac{\left\langle \psi_m^{(0)} \left| \hat{v}_h \left| \psi_n^{(0)} \right\rangle \right\rangle \left\langle \psi_n^{(0)} \left| \hat{v}_h \left| \psi_m^{(0)} \right\rangle \right\rangle}{E_n^{(0)} - E_m^{(0)}} = \sum_{\substack{m=1, \\ m \neq n}}^{\infty} \frac{\left| \left\langle \psi_n^{(0)} \left| \hat{v}_h \left| \psi_m^{(0)} \right\rangle \right\rangle \right|^2}{E_n^{(0)} - E_m^{(0)}}. \end{aligned} \quad (4.330)$$

The coefficients $C_{m,n}^{(2)}$ are no longer calculated here, since one usually only goes up to the first order in the state and up to the second order in the energy. You can successively calculate further orders.

Now the case of degenerate energy eigenvalues is considered. So let $N \in \mathbb{N}$ with $N \geq 2$ and the first N undisturbed states $\left| \psi_1^{(0)} \right\rangle, \dots, \left| \psi_N^{(0)} \right\rangle$ are degenerate, i.e

$$\hat{H}_0 \left| \psi_m^{(0)} \right\rangle = E_0 \left| \psi_m^{(0)} \right\rangle \quad (4.331)$$

for $1 \leq m \leq N$. Formula (4.325) is not applicable. However, one can see that with small energy differences $E_n^{(0)} - E_m^{(0)}$ the admixture of the states is very strong. Even with a very weak perturbation $\lambda \rightarrow 0$ you have to assume that degenerate states are mixed in, so you do this approach

$$\left| \psi(\lambda) \right\rangle = \sum_{l=1}^N C_l \left| \psi_l^{(0)} \right\rangle + \lambda \sum_{m=N+1}^{\infty} C_m^{(1)} \left| \psi_m^{(0)} \right\rangle + \mathcal{O}(\lambda^2), \quad (4.332)$$

$$E(\lambda) = E_0 + \lambda E^{(1)} + \mathcal{O}(\lambda^2). \quad (4.333)$$

This is put into the Schrödinger equation Eq. (4.311) a:

$$\begin{aligned} &\sum_{l=1}^N C_l \hat{H}_0 \left| \psi_l^{(0)} \right\rangle + \sum_{l=1}^N C_l \lambda \hat{v}_h \left| \psi_l^{(0)} \right\rangle + \lambda \sum_{m=N+1}^{\infty} C_m^{(1)} \hat{H}_0 \left| \psi_m^{(0)} \right\rangle + \mathcal{O}(\lambda^2) \\ &= E_0 \sum_{l=1}^N C_l \left| \psi_l^{(0)} \right\rangle + \lambda E^{(1)} \sum_{l=1}^N C_l \left| \psi_l^{(0)} \right\rangle + \lambda E_0 \sum_{m=N+1}^{\infty} C_m^{(1)} \left| \psi_m^{(0)} \right\rangle + \mathcal{O}(\lambda^2) \end{aligned} \quad (4.334)$$

This is true to zero order. In the following only the first order is considered. The $\left| \psi_l^{(0)} \right\rangle, 1 \leq l \leq N$, are orthonormalized. Let $j \in \mathbb{N}$ with $1 \leq j \leq N$ given. By multiplying the first-order terms in Eq. (4.334) from the left with $\left\langle \psi_j^{(0)} \right|$ is obtained

$$\sum_{l=1}^N C_l \langle \psi_j^{(0)} | \hat{v}_h | \psi_l^{(0)} \rangle = E^{(1)} C_j. \quad (4.335)$$

The solution $(C, \dots, C_N, E^{(1)})$ gives the zero-order correction in the state and first-order correction in the energy. The equation applies to all $1 \leq l \leq N$, so you can also write this as a matrix

$$v_h \mathbf{C} = E^{(1)} \mathbf{C} \quad (4.336)$$

with the matrix elements

$$V_{j,l} := \langle \psi_j^{(0)} | \hat{v}_h | \psi_l^{(0)} \rangle \quad (4.337)$$

and the vector $\mathbf{C} := (C, \dots, C_N)^T$. Since $\hat{v}_h$ is Hermitian, the matrix v_h is also Hermitian. As a solution, one obtains N orthonormal eigenvectors $\mathbf{C}^k$ to the eigenvalues $E_k^{(1)}$. The associated N states are

$$|\psi_k\rangle = \sum_{l=1}^N C_l^{(k)} |\psi_l^{(0)}\rangle \quad (4.338)$$

with the respective energy

$$E_k = E_0 + E_k^{(1)}. \quad (4.339)$$

These conditions are orthonormal. Namely, let $k, m \in \mathbb{N}$ with $1 \leq k, m \leq N$ be given. Then applies

$$\langle \psi_k | \psi_m \rangle = \sum_{l=1}^{\infty} C_l^{(k)*} C_l^{(m)} = \langle \mathbf{C}^{(k)} | \mathbf{C}^{(m)} \rangle = \delta_{m,n}. \quad (4.340)$$

4.11.2 Spin-orbit coupling in the H atom

The *spin-orbit coupling* describes the effect of the interaction of the magnetic moment of the electron with the magnetic field of the nucleus; It is a relativistic effect because the nuclear motion arises from a coordinate transformation into the rest frame of the electron. This effect is treated here in the H atom in first order perturbation theory.

First of all, let us consider the definition of Bohr's radius a_B according to Eq. (4.200) reminds:

$$a_B = \frac{\hbar^2}{m_e e^2} \quad (4.341)$$

For the energy eigenvalues in the H atom, Eq. (4.223)

$$E_n = -\frac{Z^2}{2n^2} E_{\text{at}} \quad (4.342)$$

For E_{at} one can now do further calculations

$$E_{\text{at}} = \frac{\hbar^2}{m_e a_B^2} = \frac{1}{a_B} \frac{\hbar^2}{m_e a_B} = \frac{1}{a_B} \frac{\hbar^2}{m_e} \frac{m_e e^2}{\hbar^2} = \frac{e^2}{a_B}. \quad (4.343)$$

For a $(Z - 1)$ -fold ionized atom is the atomic energy scale

$$\varepsilon_{\text{at}} = Z^2 E_{\text{at}} = Z^2 \frac{e^2}{a_B} = Z^2 e^2 \frac{m_e e^2}{\hbar^2} = Z^2 e^4 \frac{m_e}{\hbar^2} \frac{1}{c^2} = m_e c^2 \left(\frac{Z e^2}{\hbar c} \right)^2 = m_e c^2 (Z \alpha)^2. \quad (4.344)$$

a is the *fine structure constant* for which applies

$$a := \frac{e^2}{\hbar c} \stackrel{\text{SI}}{=} \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137}. \quad (4.345)$$

The spin-orbit coupling does not arise from a possible magnetic core dipole. In a semi-classical view, the electron moves around the nucleus with an instantaneous speed $\mathbf{v}$. In the current rest frame of the electron, according to Eq. (3.105) a magnetic field

$$\mathbf{B}' = -\gamma \frac{\mathbf{v}}{c} \times \mathbf{E}, \quad (4.346)$$

which the electron feels. The function

$$\mathbf{u}(\mathbf{v}') := \frac{\mathbf{v}'}{\sqrt{1 - v'^2}} \quad (4.347)$$

with

$$\mathbf{v}' := \frac{\mathbf{v}}{c} \quad (4.348)$$

describes the strength of the relativistic effect. The linear Taylor expansion of this function is

$$\mathbf{u} = \mathbf{v}' + \mathcal{O}(v'^2), \quad (4.349)$$

so that one approaches here for the relativistic B field

$$\mathbf{B}' = -\frac{\mathbf{v}}{c} \times \mathbf{E} + \mathcal{O}\left(\left(\frac{\mathbf{v}}{c}\right)^2\right). \quad (4.350)$$

The higher order terms are no longer noted. With $g \approx 2$ the magnetic moment of the electron is given by Eq. (4.303)

$$\boldsymbol{\mu} = -\frac{e}{m_e c} \mathbf{s}. \quad (4.351)$$

This gives you energy

$$-\boldsymbol{\mu} \cdot \mathbf{B}' = \frac{e}{m_e c} \mathbf{s} \cdot \mathbf{B}' = -\frac{e}{m_e c^2} \mathbf{s} \cdot (\mathbf{v} \times \mathbf{E}). \quad (4.352)$$

For the E field, $\mathbf{E} = \frac{Zer}{r^3}$, with the definition $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ one obtains the spin-orbit interaction

$$V = -\boldsymbol{\mu} \cdot \mathbf{B}' = -\frac{e}{m_e c^2} \mathbf{s} \cdot (\mathbf{v} \times \mathbf{E}) = \frac{Ze^2}{m_e^2 c^2} \frac{\mathbf{l} \cdot \mathbf{s}}{r^3}. \quad (4.353)$$

A relativistic quantum mechanical observation of the accelerated electron using the *Dirac equation* results in an additional factor $1/2$ at this point. The perturbation operator we are looking for is:

$$\hat{v}_h = \frac{Ze^2}{2m_e^2 c^2} \frac{\hat{\mathbf{l}} \cdot \hat{\mathbf{s}}}{\hat{r}^3}. \quad (4.354)$$

Using the total torque operator

$$\hat{\mathbf{j}} := \hat{\mathbf{l}} + \hat{\mathbf{s}} \quad (4.355)$$

you can do this

$$\begin{aligned}
\hat{v}_h &= \frac{Ze^2}{4m_e^2 c^2} \frac{\hat{\mathbf{l}} \cdot \hat{\mathbf{s}}}{\hat{r}^3} = \frac{Ze^2}{4m_e^2 c^2} \frac{\hat{\mathbf{l}} \cdot \hat{\mathbf{s}} + \hat{\mathbf{s}}^2 - \hat{\mathbf{s}}^2}{\hat{r}^3} = \frac{Ze^2}{4m_e^2 c^2} \frac{(\hat{\mathbf{l}} + \hat{\mathbf{s}}) \cdot \hat{\mathbf{s}} - \hat{\mathbf{s}}^2}{\hat{r}^3} = \frac{Ze^2}{4m_e^2 c^2} \frac{(\hat{\mathbf{j}} + \hat{\mathbf{l}}) \cdot (\hat{\mathbf{j}} - \hat{\mathbf{l}}) - \hat{\mathbf{s}}^2}{\hat{r}^3} \\
&= \frac{Ze^2}{4m_e^2 c^2} \frac{\hat{\mathbf{j}}^2 - \hat{\mathbf{l}}^2 - \hat{\mathbf{s}}^2}{\hat{r}^3}
\end{aligned} \tag{4.356}$$

rewrite. In order to be able to continue working with this, the angular momentum eigenstates of the H atom are coupled

$$|n, l, m, s, s_z\rangle = |n, l\rangle |l, m, s, s_z\rangle = |n, l\rangle |j, l, s, m_j\rangle = |n, j, l, s, m_j\rangle. \tag{4.357}$$

Since the angular momentum eigenstates are orthogonal and $\hat{v}_h$ only acts on the radial coordinates, the energy splitting applies

$$\langle n, j, l, s, m_j | \hat{v}_h | n, j', l', s, m_j' \rangle = \Delta E \delta_{j,j'} \delta_{l,l'} \delta_{m_j, m_j'} \tag{4.358}$$

with

$$\Delta E = \frac{Ze^2 \hbar^2}{4m_e^2 c^2} \left\langle n, l \left| \frac{\mathbf{l}}{\hat{r}^3} \right| n, l \right\rangle [j(j+1) - l(l+1) - s(s+1)]. \tag{4.359}$$

It holds for $l \neq 0$

$$\begin{aligned}
\left\langle \frac{\mathbf{l}}{\hat{r}^3} \right\rangle &= \int_{\mathbb{R}^3} \frac{\mathbf{l}}{r^3} |\psi|^2 d^3 r = \int_{r=0}^{\infty} \int_0^{2\pi} \int_0^{\pi} \frac{\mathbf{l}}{r^3} |\psi|^2 r^2 \sin(\vartheta) d\vartheta d\varphi dr \\
&= \int_{r=0}^{\infty} \int_{\varphi=0}^{2\pi} \int_{\vartheta=0}^{\pi} \frac{\mathbf{l}}{r} R_{n,l}(r)^2 |Y_{l,m}(\vartheta, \varphi)|^2 \sin(\vartheta) d\vartheta d\varphi dr \\
&= \int_0^{\infty} \frac{\mathbf{l}}{r} R_{n,l}(r)^2 dr = \frac{4Z^3}{a_B^3 n^4} \frac{(n-l-1)!}{(n+l)!} \int_0^r \frac{\mathbf{l}}{r} \left(\frac{2Zr}{na_B} \right)^{2l} \left[L_{n-l-1, 2l+1} \left(\frac{2Zr}{na_B} \right) \right]^2 \exp\left(-\frac{2Zr}{na_B}\right) dr \\
&= \frac{4Z^3}{a_B^3 n^4} \frac{(n-l-1)!}{(n+l)!} \int_0^{\infty} r^{2l-1} [L_{n-l-1, 2l+1}(r)]^2 \exp(-r) dr.
\end{aligned}$$

You identify

$$m := n - l - 1 \geq 0 \Rightarrow n = m + l + 1, \tag{4.360}$$

$$k := 2l + 1 \geq 3. \tag{4.361}$$

This is where the transformations follow

$$n := m + 1 + \frac{1}{2}(k-1) = m + \frac{1}{2}(k+1), \tag{4.362}$$

$$l := \frac{1}{2}(k-1). \tag{4.363}$$

With Eq. (C.147) follows

$$\begin{aligned}
&\int_0^{\infty} r^{2l-1} [L_{n-l-1, 2l+1}(r)]^2 \exp(-r) dr = \int_0^{\infty} r^{k-2} [L_{m,k}(r)]^2 \exp(-r) dr \\
&= \frac{(m+k)!}{m!} \frac{2m+1+k}{(k-1)k(k+1)} = \frac{(m+k)!}{m!} \frac{2n}{(k-1)k(k+1)} = \frac{(n+l)!}{(n-l-1)!} \frac{n}{(2l+1)(l+1)} \\
&= \frac{(n+l)!}{(n-l-1)!} \frac{n}{4l(l+\frac{1}{2})(l+1)}.
\end{aligned} \tag{4.364}$$

Therefore applies

$$\left\langle \frac{\mathbf{I}}{\hat{r}^3} \right\rangle = \frac{Z^3}{a_B^3 n^3 l \left(l + \frac{1}{2} \right) (l + 1)} = \frac{Z^3 m_e^3 e^6}{\hbar^6 n^3 l \left(l + \frac{1}{2} \right) (l + 1)}. \quad (4.365)$$

For $l = 0$

$$\left\langle \frac{\mathbf{I}}{\hat{r}^3} \right\rangle \notin \mathbb{R}, \quad (4.366)$$

However, in this case the spin-orbit coupling is zero anyway because of $j = l = \frac{1}{2}$. So you get with

$$\frac{Ze^2 \hbar^2}{4 m_e^2 c^2} \frac{Z^3 m_e^3 e^6}{\hbar^6 n^3} = \frac{m_e Z^4 e^8}{4 \hbar^4 n^3 c^2} = \frac{m_e c^2}{4 n^3} \frac{Z^4 e^8}{\hbar^4 c^4} \quad (4.367)$$

as a summary

$$\Delta E = \begin{cases} 0, & l = 0, \\ \frac{m_e c^2 (Z\alpha)^4}{4 n^3} \frac{j(j+1) - l(l+1) - s(s+1)}{l(l + \frac{1}{2})(l+1)}, & l \neq 0. \end{cases} \quad (4.368)$$

Relativistic effects therefore have an influence on the own energies in the H atom and thus also on the spectrum.

4.11.3 Time-dependent case

Previously only time-constant perturbations $\hat{V}$ were considered, now a time dependence $\hat{V}(t)$ is allowed. Into the time-dependent Schrödinger equation

$$\hat{H}(t) |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \quad (4.369)$$

is now a perturbation operator

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t) \quad (4.370)$$

to use. The solutions $(|\psi_n^{(0)}\rangle, E_n)$ of the stationary problem

$$\hat{H}_0 |\psi_n^{(0)}\rangle = E_n |\psi_n^{(0)}\rangle \quad (4.371)$$

are known again. The $|\psi_n^{(0)}\rangle$ can be provided with a time-dependent part; one can write with a misuse of the term

$$|\psi_n^{(0)}\rangle = |\psi_n^{(0)}\rangle \exp\left(-i \frac{E_n}{\hbar} t\right). \quad (4.372)$$

This section does not go further than the first order. Now you set with $\lambda \in [0, 1]$

$$\hat{H}(\lambda, t) = \hat{H}_0 + \lambda \hat{v}_h(t), \quad (4.373)$$

$$|\psi(\lambda, t)\rangle = \sum_{m=1}^{\infty} C_m^{(0)} |\psi_m^{(0)}\rangle \exp\left(-i \frac{E_m}{\hbar} t\right) + \lambda \sum_{m=1}^{\infty} C_m^{(1)}(t) |\psi_m^{(0)}\rangle \exp\left(-i \frac{E_m}{\hbar} t\right) + \mathcal{O}(\lambda^2). \quad (4.374)$$

This gives you

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} |\psi(\lambda, t)\rangle &= \sum_{m=1}^{\infty} E_m C_m^{(0)} |\psi_m^{(0)}\rangle \exp\left(-i \frac{E_m}{\hbar} t\right) \\ &+ \lambda \sum_{m=1}^{\infty} \left(i\hbar \frac{\partial C_m^{(1)}}{\partial t} + C_m^{(1)} E_m \right) |\psi_m^{(0)}\rangle \exp\left(-i \frac{E_m}{\hbar} t\right) + \mathcal{O}(\lambda^2). \end{aligned} \quad (4.375)$$

Putting this into Eq. (4.369), you get

$$\begin{aligned} & \hat{H}_o \sum_{m=1}^{\infty} C_m^{(o)} \left| \psi_m^{(o)} \right\rangle \exp \left(-i \frac{E_m}{\hbar} t \right) + \lambda \hat{H}_o \sum_{m=1}^{\infty} C_m^{(1)}(t) \left| \psi_m^{(o)} \right\rangle \exp \left(-i \frac{E_m}{\hbar} t \right) \\ & + \lambda \hat{v}_h(t) \sum_{m=1}^{\infty} C_m^{(o)} \left| \psi_m^{(o)} \right\rangle \exp \left(-i \frac{E_m}{\hbar} t \right) + \mathcal{O}(\lambda^2) = \sum_{m=1}^{\infty} C_m^{(o)} E_m \left| \psi_m^{(o)} \right\rangle \exp \left(-i \frac{E_m}{\hbar} t \right) \\ & + \lambda \sum_{m=1}^{\infty} \left(i\hbar \frac{\partial C_m^{(1)}}{\partial t} + C_m^{(1)} E_m \right) \left| \psi_m^{(o)} \right\rangle \exp \left(-i \frac{E_m}{\hbar} t \right) + \mathcal{O}(\lambda^2). \end{aligned} \quad (4.376)$$

The zeroth order is trivially satisfied. Now let $k \in \mathbb{N}$ be given by $k \geq 1$ and multiply the terms of the first order from the left by $\langle \psi_k^{(o)} |$. You receive

$$\begin{aligned} & C_k^{(1)}(t) E_k \exp \left(-i \frac{E_k}{\hbar} t \right) + \sum_{m=1}^{\infty} C_m^{(o)} \langle \psi_k^{(o)} | \hat{v}_h(t) | \psi_m^{(o)} \rangle \exp \left(-i \frac{E_m}{\hbar} t \right) = \left(i\hbar \frac{\partial C_k^{(1)}}{\partial t} + C_k^{(1)} E_k \right) \exp \left(-i \frac{E_k}{\hbar} t \right) \\ & \Leftrightarrow \frac{\partial C_k^{(1)}}{\partial t} = -\frac{i}{\hbar} \sum_{m=1}^{\infty} C_m^{(o)} \langle \psi_k^{(o)} | \hat{v}_h(t) | \psi_m^{(o)} \rangle \exp \left(i \frac{E_k - E_m}{\hbar} t \right). \end{aligned} \quad (4.377)$$

So you get for the admixture of the states

$$C_k^{(1)}(t') = C_k^{(1)}(t_o) - \frac{i}{\hbar} \int_{t_o}^{t'} \sum_{m=1}^{\infty} C_m^{(o)} \langle \psi_k^{(o)} | \hat{v}_h(t) | \psi_m^{(o)} \rangle \exp \left(i \frac{E_k - E_m}{\hbar} t \right) dt. \quad (4.378)$$

If the system is in state n at time t_o , then we get:

$$\begin{aligned} C_n^{(o)} &= 1, \\ C_{m \neq n}^{(o)} &= 0 \end{aligned} \quad (4.379)$$

and thus

$$C_k^{(1)}(t') = -\frac{i}{\hbar} \int_{t_o}^{t'} \langle \psi_k^{(o)} | \hat{v}_h(t) | \psi_n^{(o)} \rangle \exp \left(i \frac{E_k - E_n}{\hbar} t \right) dt. \quad (4.380)$$

From this you can get the time-dependent solution

$$\left| \psi(t) \right\rangle \approx \left| \psi_n^{(o)} \right\rangle \exp \left(-i \frac{E_n}{\hbar} t \right) + \sum_{k=1}^{\infty} C_k^{(1)}(t) \left| \psi_k^{(o)} \right\rangle \exp \left(-i \frac{E_k}{\hbar} t \right) \quad (4.381)$$

construct. The probability of encountering the state $\left| \psi_m^{(o)} \right\rangle$ is given by

$$p_m(t) = \left| \delta_{mn} + C_m^{(1)}(t) \right|^2 \quad (4.382)$$

To understand the absorption and emission induced by electromagnetic waves, one needs knowledge of the effect of a periodic perturbation operator

$$\hat{V}(t) = \hat{V}_o \exp(-i\omega t) + \hat{V}_o^* \exp(i\omega t), \quad (4.383)$$

the addition of the adjoint term guarantees hermiticity and thus real measurements. Putting this into Eq. (4.380), follows

$$\begin{aligned} i\hbar C_k^{(1)}(t) &= \left\langle \psi_k^{(\circ)} \left| \hat{V}_\circ \right| \psi_n^{(\circ)} \right\rangle \int_\circ^{\text{exp}} (i(\omega_{k,n} - \omega) t') dt' \\ &\quad + \left\langle \psi_k^{(\circ)} \left| \hat{V}_\circ^\star \right| \psi_n^{(\circ)} \right\rangle \int_\circ^{\text{exp}} (i(\omega_{k,n} + \omega) t') dt'. \end{aligned} \quad (4.384)$$

$t_\circ = \circ$ were set and

$$\omega_{k,n} := \omega_k - \omega_n \quad (4.385)$$

defined. Define further

$$\Omega_\pm := \omega_{k,n} \pm \omega, \quad (4.386)$$

then is

$$\begin{aligned} \int_\circ^{\text{exp}} (i\Omega_\pm t') dt' &= \frac{\exp(i\Omega_\pm t) - \mathbf{1}}{i\Omega_\pm} \\ \Rightarrow \left| \int_\circ^{\text{exp}} (i\Omega_\pm t') dt' \right|^2 &= \left| \frac{\exp(i\Omega_\pm t) - \mathbf{1}}{i\Omega_\pm} \right|^2 = \frac{\mathbf{1}}{\Omega_\pm^2} [(\cos(\Omega_\pm t) - \mathbf{1})^2 + \sin^2(\Omega_\pm t)] \\ &= \frac{\mathbf{1}}{\Omega_\pm^2} [\cos^2(\Omega_\pm t) + \mathbf{1} - 2\cos(\Omega_\pm t) + \sin^2(\Omega_\pm t)] = \frac{2}{\Omega_\pm^2} [\mathbf{1} - \cos(\Omega_\pm t)] \\ &= \frac{2}{\Omega_\pm^2} \left[\mathbf{1} - \cos^2\left(\frac{\Omega_\pm t}{2}\right) + \sin^2\left(\frac{\Omega_\pm t}{2}\right) \right] = \frac{4\sin^2\left(\frac{\Omega_\pm t}{2}\right)}{\Omega_\pm^2}. \end{aligned} \quad (4.387)$$

This only makes a significant contribution when $\Omega_\pm$ is small, because $\Omega_+ = \Omega_- + 2\omega$ usually only contributes to one of the two integrals in Eq. (4.384) contributes to the result. With $\hat{V}_- := \hat{V}_\circ$ and $\hat{V}_+ := \hat{V}_\circ^\star$ you get

$$R_{n \rightarrow k} = \frac{|C_k^{(1)}(t)|^2}{=} \frac{\left| \left\langle \psi_k^{(\circ)} \left| \hat{V}_\pm \right| \psi_n^{(\circ)} \right\rangle \right|^2}{\hbar^2} \frac{4\sin^2\left(\frac{\Omega_\pm t}{2}\right)}{\Omega_\pm^2 t}. \quad (4.388)$$

Here, $R_{n \rightarrow k}$ is the probability that the system changes from state n to state k in the time interval $[\circ, t]$, divided by the time available for this. Define

$$f(\Omega) := \frac{4\sin^2\left(\frac{\Omega t}{2}\right)}{\Omega^2 t}, \quad (4.389)$$

then with Eq. (A.83)

$$\lim_{t \rightarrow \infty} f(\Omega) = 2\pi \delta(\Omega). \quad (4.390)$$

This can be used in the case $t \gg \mathbf{1}/\Omega$, it follows

$$R_{n \rightarrow k} = \frac{2\pi}{\hbar} \left| \left\langle \psi_k^{(\circ)} \left| \hat{V}_\pm \right| \psi_n^{(\circ)} \right\rangle \right|^2 \delta(E_k - E_n \pm \hbar\omega). \quad (4.391)$$

The minus sign must be used for $E_k > E_n$. In the case of a time-independent disturbance $\omega = \circ$ follows

$$R_{n \rightarrow k} = \frac{2\pi}{\hbar} \left| \left\langle \psi_k^{(\circ)} \left| \hat{V}_\pm \right| \psi_n^{(\circ)} \right\rangle \right|^2 \delta(E_k - E_n). \quad (4.392)$$

4.11.4 Transitions in the H atom

Take a vector potential of the form

$$\mathbf{A}(\mathbf{r}, t) = A_\circ \mathbf{e} \cos(\mathbf{k} \cdot \mathbf{r} - \omega t) \quad (4.393)$$

an with $\omega = ck$ and $\boldsymbol{\epsilon} \cdot \mathbf{k} = 0$, here $\boldsymbol{\epsilon}$ is the normalized polarization vector. Then follows

$$\mathbf{B} = \nabla \times \mathbf{A} \stackrel{\text{Glg. (B.48)}}{=} -A_0 \boldsymbol{\epsilon} \times \mathbf{k} \cos(\mathbf{k} \cdot \mathbf{r} - \omega t) = A_0 \mathbf{k} \times \boldsymbol{\epsilon} \cos(\mathbf{k} \cdot \mathbf{r} - \omega t). \quad (4.394)$$

This describes an electromagnetic wave. For the Hamilton operator follows

$$\hat{H} = \frac{1}{2m_e} \left(-i\hbar \nabla + \frac{e}{c} \mathbf{A} \right)^2 - \frac{e^2}{r} \stackrel{\text{Glg. (B.49)}}{=} \frac{\hat{\mathbf{p}}^2}{2m_e} - \frac{e^2}{r} + \frac{e}{m_e c} \hat{\mathbf{A}} \cdot \hat{\mathbf{p}} = \hat{H}_0 + \hat{v}_h(t) \quad (4.395)$$

with the perturbation operator

$$\hat{v}_h(t) = \frac{e}{m_e c} \hat{\mathbf{A}} \cdot \hat{\mathbf{p}}. \quad (4.396)$$

The quadratic terms in the vector product were neglected. With

$$\cos = \frac{\exp(+)+\exp(-)}{2} \quad (4.397)$$

you can write

$$\hat{V}(t) = \hat{V}_0 \exp(-i\omega t) + \hat{V}_0^\dagger \exp(i\omega t), \quad (4.398)$$

this was done

$$\hat{V}_0 = \frac{eA_0}{2m_e c} \exp(i\mathbf{k} \cdot \mathbf{r}) \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} \quad (4.399)$$

used. With the *long-wave approximation*

$$\exp(i\mathbf{k} \cdot \mathbf{r}) = 1 + i\mathbf{k} \cdot \mathbf{r} + \dots = 1 + \mathcal{O}(\langle r \rangle / \lambda) \approx 1 \quad (4.400)$$

you get

$$\hat{V}_0 \approx \frac{eA_0}{2m_e c} \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}. \quad (4.401)$$

This is justified here because one can calculate with $\langle r \rangle \sim a_B$

$$\frac{\langle r \rangle}{\lambda} \sim \frac{a_B}{\lambda} = \frac{a_B \omega}{2\pi c} = \frac{a_B \Delta E}{2\pi \hbar c} \sim \frac{a_B E_{\text{at}}}{20\pi \hbar c} = \frac{\hbar}{m_e a_B 20\pi c} = \frac{e^2}{20 \hbar \pi c} \rightarrow \frac{e^2}{4\pi \epsilon_0 20 \hbar \pi c} \sim 10^{-4}. \quad (4.402)$$

$\Delta E \sim \frac{E_{\text{at}}}{10}$ was used. With Eq. (4.392) is obtained

$$R_{a \rightarrow b} = \frac{\pi e^2 A_0^2}{2m_e^2 c^2 \hbar} |\langle b | \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} | a \rangle|^2 [\delta(E_b - E_a + \hbar\omega) + \delta(E_b - E_a - \hbar\omega)]. \quad (4.403)$$

So the transition rates are proportional to A_0^2 , which in turn is proportional to the energy density of the electromagnetic field. The transition rates are therefore proportional to the amount of the matrix element

$$M_{b,a} = \langle b | \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} | a \rangle. \quad (4.404)$$

This needs to be rephrased a bit. First you do the math

$$[\hat{H}_0, \hat{\mathbf{r}}] = \hat{H}_0 \hat{\mathbf{r}} - \hat{\mathbf{r}} \hat{H}_0 = -\frac{\hbar^2}{2m_e} \nabla \nabla \cdot \hat{\mathbf{r}} + \hat{\mathbf{r}} \frac{\hbar^2}{2m_e} \Delta. \quad (4.405)$$

It applies

$$\begin{aligned}\nabla \cdot (\mathbf{r}\psi) &= 3\psi + \mathbf{r} \cdot \nabla \psi \\ \Rightarrow \nabla^2 (\mathbf{r}\psi) &= 6\nabla \psi + \mathbf{r}\Delta \psi.\end{aligned}\tag{4.406}$$

Thus follows

$$\left[\hat{H}_0, \hat{\mathbf{r}}\right] = -\frac{\hbar^2}{2m_e} 6\nabla \psi = \frac{3\hbar}{im_e} \hat{\mathbf{p}} \Rightarrow \hat{\mathbf{p}} = \frac{im_e}{3\hbar} \left[\hat{H}_0, \hat{\mathbf{r}}\right].\tag{4.407}$$

So you can write

$$M_{b,a} = im_e \frac{E_b - E_a}{3\hbar} \langle b | \boldsymbol{\epsilon} \cdot \hat{\mathbf{r}} | a \rangle.\tag{4.408}$$

The eigenstates in the H atom are given by Eq. (4.233) is known, so it applies

$$M_{b,a} \propto \langle n, l, m | \boldsymbol{\epsilon} \cdot \hat{\mathbf{r}} | n, l, m \rangle.\tag{4.409}$$

Spin is omitted here. The radial component does not provide any selection rules for Δn , so here is just

$$M_{b,a} \propto \int Y_{l_b, m_b}^* \boldsymbol{\epsilon} \cdot \hat{\mathbf{r}} Y_{l_a, m_a} d\Omega.\tag{4.410}$$

relevant. You write

$$\boldsymbol{\epsilon} \cdot \mathbf{r} = r (\varepsilon_x \sin(\theta) \cos(\varphi) + \varepsilon_y \sin(\theta) \sin(\varphi) + \varepsilon_z \cos(\theta)).\tag{4.411}$$

From the equations (C.171) - (C.172) follows

$$\cos(\theta) Y_{l,m} = a Y_{l-1,m} + \beta Y_{l+1,m}, \quad \sin(\theta) Y_{l,m} = \gamma e^{-i\varphi} Y_{l-1,m+1} + \delta e^{-i\varphi} Y_{l+1,m+1}\tag{4.412}$$

with coefficients a, β, γ, δ that are not relevant here. So you have

$$\Delta l = l_b - l_a = \pm 1,\tag{4.413}$$

$$\Delta m = 0, \pm 1.\tag{4.414}$$

4.11.5 Relativistic corrections in the H atom

4.12 Multi-particle systems

Let $N \in \mathbb{N}$ with $N \geq 1$ and be given N particles with spin. The state of such a system is determined by a wave function

$$\psi = \psi(x_i)\tag{4.415}$$

described with $1 \leq i \leq N$ and $x_i = (\mathbf{r}_i, \sigma_i)$, where $\mathbf{r}_i$ denotes the location of the i -th particle and σ_i its spin. In the case of spin 1/2 particles, one can imagine such a function as $\mathbb{R}^N$ functions $\mathbb{R}^N \rightarrow \mathbb{C}$.¹ Now define for $i, j \in \mathbb{N}$ with $1 \leq i, j \leq N$ the *Permutation operator* $\hat{P}_{i,j}$ through

$$\hat{P}_{i,j} \psi(\dots, x_i, \dots, x_j, \dots) := \psi(\dots, x_j, \dots, x_i, \dots).\tag{4.416}$$

This operator swaps the arguments belonging to two particles. If there are N particles of the same type, the Hamiltonian $\hat{H}$ is invariant under permutation:

$$\hat{P}_{i,j} \hat{H} = \hat{H}.\tag{4.417}$$

¹It is easy to see that it is not possible to tabulate such a function for a realistic system.

From this it follows

$$[\hat{P}_{i,j}, \hat{H}] = 0, \quad (4.418)$$

and that means the existence of a $\lambda \in \mathbb{C}$ with

$$\hat{P}_{i,j}\psi(x_k) = \lambda\psi(x_k) \quad (4.419)$$

for eigenfunctions $\psi(x_k)$ of the Hamiltonian, which can depend on i, j , which has been neglected in the notation here. It follows anyway by using the same operator again

$$\lambda^2 = 1, \quad (4.420)$$

therefore $\lambda = \pm 1$. In the case $\lambda = -1$ one speaks of *antisymmetry*, in the case $\lambda = 1$ of *symmetry*. Particles with half-integer spin (fermions) have antisymmetric wave functions, while particles with integer spin (bosons) have symmetrical wave functions. This has far-reaching implications. Assume that an N-fermion system is in a state in which particles i and j occupy the same orbitals, i.e

$$\psi(\dots, x_i, \dots, x_j, \dots) = \psi(\dots, x_j, \dots, x_i, \dots) \quad (4.421)$$

applies. If you now apply $\hat{P}_{i,j}$ to this, it follows

$$-\psi(\dots, x_i, \dots, x_j, \dots) = \psi(\dots, x_i, \dots, x_j, \dots), \quad (4.422)$$

so $\psi = 0$, which is a contradiction to the normalization condition. Two fermions can only have the same wave function (occupy the same orbital) if they have a different spin. This is not the case with bosons. This repulsion of fermions is not due to a force, but rather to symmetry properties of their wave function, which is known as *Pauli principle*.

4.12.1 Molecular spectra

To calculate the interaction of radiation with matter present in the atmosphere, Planck's radiation law is not sufficient. You also need the spectra, i.e. the energy levels and transition probabilities of molecules under excitation by dipole radiation. An H₂O molecule consists of ten electrons, so you would need to store the state of the electron shell when each axis is discretized into ten intervals (which is unlikely to be enough).

$$N_{\text{points}} = (10^3 \cdot 2)^N = 2^N \cdot 10^{3N} \approx 10^{33} \quad (4.423)$$

Data points. These are two complex numbers each, so you need approx.

$$S = 16 \cdot 10^{33} \approx 10^{22} \text{ Terrabyte} \quad (4.424)$$

of storage space, which is currently an unrealistic amount. If you want to derive spectra theoretically, you have to think about approximation methods (this is almost always the case in QM). The most common procedures are:

- Perturbation theory
- Monte Carlo simulation (a statistical procedure)
- Density functional theory

4.12.2 Chemical reactions

Chemical reactions are material transformations. Let a mixture of $N \in \mathbb{N}$ components be given with $N \geq 1$ and let the particle densities be given by n_i with $1 \leq i \leq N$. For $1 \leq j, k \leq N$, define the number $U_{j,k}$ by the rate at which the substance k transforms into the substance j (dimension: particles per time and volume). Then $1 \leq i \leq N$

$$\frac{dn_i}{dt} = \sum_{j=1}^N U_{i,j} - U_{j,i}. \quad (4.425)$$

If this takes place in the atmosphere, the composition of the air changes and thus also the gas constant $R_d = \frac{R}{M_d}$. The matrix v depends on the thermodynamic variables, the radiation field and the existing material densities.

5 STATISTICAL PHYSICS

Statistical physics is about macroscopic systems. Classically, the state r of a system of N particles is represented by $2f$ real numbers

$$r = (q_1, \dots, q_f; p_1, \dots, p_f) \quad (5.1)$$

where f is the number of degrees of freedom, q_i is the generalized coordinates and p_i is the generalized momenta. Here $\mathcal{O}(f) = \mathcal{O}(N)$. Examples of such a system would be a crystal or 10^{23} gas particles in a box. These examples make it clear that the microscopic state of a macroscopic system is not relevant. The exact speed of one of the 10^{23} particles does not matter. The *microstate* is therefore not of interest.

A significant simplification of the statistics is obtained if one assumes a quantum mechanical system. This is because a stationary state in quantum mechanics can be determined by a finite number of discrete quantum numbers if the system is confined in a finite volume. A microstate r can then be defined by a finite number of natural numbers n_i ,

$$r = (n_i). \quad (5.2)$$

A *macrostate* M is defined by specifying the probabilities P_r for the microstates r ,

$$M := (P_r). \quad (5.3)$$

To do this, imagine a number N of identical systems, a so-called *ensemble*. This can be a mental concept to understand a single system, but it can also be N actually existing systems, such as N spin-containing particles. Let there be N_r systems in the microstate r . Then you can use the P_r

$$P_r := \lim_{N \rightarrow \infty} \frac{N_r}{N} \quad (5.4)$$

define. Now one can assume as limiting conditions that the system is closed, i.e. that the number of particles and energy are constant. In addition, there should be no symmetries from which further restrictive conservation laws would follow. In particular, conservation of momentum and angular momentum should not apply. The *density operator* of the ensemble is defined by

$$\hat{\rho}(t) := \frac{1}{N} \sum_{j=1}^N |j\rangle \langle j|. \quad (5.5)$$

Here j runs over all ensemble members and $|j\rangle$ is the state of the j -th system. The states $|j\rangle$ do not have to be orthogonal to each other, but they must be normalized, in particular several systems can be in the same state. Let $(|\psi_k\rangle)$ for $k \geq 1$ be an orthonormal basis of the Hilbert space from which the $|j\rangle$ states come. The probability P_l of encountering a randomly chosen ensemble member in the state $|\psi_l\rangle$ follows

$$P_l = \frac{N_l}{N} = \frac{1}{N} \sum_{j=1}^N |\langle \psi_l | j \rangle|^2 = \frac{1}{N} \sum_{j=1}^N \langle \psi_l | j \rangle \langle j | \psi_l \rangle = \langle \psi_l | \hat{\rho} | \psi_l \rangle. \quad (5.6)$$

Here, N_r was interpreted as the number of systems that are encountered in a quantum mechanical measurement in the state $|\psi_r\rangle$. The macrostate (P_r) can be determined from the density operator, which is why the density operator is also called *statistical operator*. It follows from this

$$\text{tr}(\hat{\rho}) = 1. \quad (5.7)$$

For an expectation value $\langle \hat{A} \rangle$ it follows that $\hat{A}$ is Hermitian

$$\begin{aligned}
\langle \hat{A} \rangle &= \frac{1}{N} \sum_{j=1}^N \langle j | \hat{A} | j \rangle = \frac{1}{N} \sum_{j=1}^N \sum_{k=1}^{\infty} \langle j | \psi_k \rangle \langle \psi_k | \hat{A} | j \rangle = \frac{1}{N} \sum_{j=1}^N \sum_{k=1}^{\infty} \langle \psi_k | \hat{A} | j \rangle \langle j | \psi_k \rangle \\
&= \sum_{k=1}^{\infty} \langle \psi_k | \frac{1}{N} \sum_{j=1}^N \hat{A} | j \rangle \langle j | \psi_k \rangle = \sum_{k=1}^{\infty} \langle \psi_k | \hat{A} \hat{\rho} | \psi_k \rangle = \text{tr}(\hat{A} \hat{\rho}).
\end{aligned} \tag{5.8}$$

Let $|\psi_l\rangle, |\psi_m\rangle$ be two states, then the following applies

$$\begin{aligned}
\langle \psi_l | \hat{\rho} | \psi_m \rangle &= \frac{1}{N} \langle \psi_l | \sum_{j=1}^N | j \rangle \langle j | \psi_m \rangle = \frac{1}{N} \sum_{j=1}^N \langle \psi_l | j \rangle \langle j | \psi_m \rangle = \frac{1}{N} \left(\sum_{j=1}^N \langle \psi_m | j \rangle \langle j | \psi_l \rangle \right)^* \\
&= \frac{1}{N} \left(\langle \psi_m | \sum_{j=1}^N | j \rangle \langle j | \psi_l \rangle \right)^* = \langle \psi_m | \hat{\rho} | \psi_l \rangle^* = \langle \hat{\rho} | \psi_l \rangle \langle \psi_m \rangle.
\end{aligned} \tag{5.9}$$

The density operator is therefore Hermitian. The last property of the density operator to be noted here is

$$\begin{aligned}
\text{tr}(\hat{\rho}^2) &= \langle \hat{\rho} \rangle = \frac{1}{N} \sum_{j=1}^N \langle j | \hat{\rho} | j \rangle = \frac{1}{N} \sum_{j=1}^N \langle j | \frac{1}{N} \sum_{j'=1}^N | j' \rangle \langle j' | j \rangle \\
&= \frac{1}{N^2} \sum_{j,j'=1}^N |\langle j | j' \rangle|^2 \leq \frac{1}{N^2} \sum_{j,j'=1}^N 1 = 1.
\end{aligned} \tag{5.10}$$

So it is $\text{tr}(\hat{\rho}^2) = 1$ if and only if all ensemble members are in the same state. This is called a *pure state*, otherwise it is called a *mixed state*.

The expected value of the Hamiltonian is the expected value of the energy or the energy E for short. So it applies

$$E = \text{tr}(\hat{H} \hat{\rho}). \tag{5.11}$$

With the time-dependent SG follows

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = \frac{1}{N} \sum_{i=1}^N \hat{H} | j \rangle \langle j | + | j \rangle i\hbar \frac{\partial}{\partial t} \langle j | \tag{5.12}$$

With

$$i\hbar \frac{\partial}{\partial t} \langle j | = i\hbar \frac{\partial}{\partial t} | j \rangle^+ = - \left(i\hbar \frac{\partial}{\partial t} | j \rangle \right)^+ = - (\hat{H} | j \rangle)^+ = - \langle j | \hat{H} \tag{5.13}$$

you get

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]. \tag{5.14}$$

This is the *von Neumann equation*.

Let a closed system be exposed to a constant perturbation operator $\hat{v}_h$, then Eq. (4.392) for the transition rate $R_{r,r'}$ between two microstates $|\psi_r\rangle, |\psi_{r'}\rangle$

$$R_{r,r'} = \frac{2\pi}{\hbar} |\langle \psi_r | \hat{v}_h | \psi_{r'} \rangle|^2 = R_{r',r}. \tag{5.15}$$

For the time derivative of the probabilities $P_r(t)$ follows

$$\frac{dP_r(t)}{dt} = - \sum_{r'} R_{r,r'} P_r + \sum_{r'} R_{r',r} P_{r'} \quad (5.16)$$

$$\Leftrightarrow \frac{dP_r(t)}{dt} = \sum_{r'} R_{r,r'} (P_{r'} - P_r). \quad (5.17)$$

Eq. (5.137) is called *master equation*. Define

$$H(t) := \sum_{r=1}^{\infty} P_r \ln(P_r). \quad (5.18)$$

Then applies

$$\begin{aligned} \frac{dH}{dt} &= \sum_r \left(\dot{P}_r \ln(P_r) + \dot{P}_r \right) = \frac{1}{2} \left[\sum_r \dot{P}_r \ln(eP_r) + \sum_{r'} \dot{P}_{r'} \ln(eP_{r'}) \right] \\ &= \frac{1}{2} \sum_{r,r'} R_{r,r'} (P_{r'} - P_r) [\ln(eP_r) - \ln(eP_{r'})] = \frac{1}{2} \sum_{r,r'} R_{r,r'} P_r \left(1 - \frac{P_{r'}}{P_r} \right) \ln \left(\frac{P_{r'}}{P_r} \right) \end{aligned} \quad (5.19)$$

$R_{r,r'} P_r \geq 0$ as well apply

$$(1 - x) \ln(x) \leq 0. \quad (5.20)$$

Therefore applies

$$\frac{dH}{dt} \leq 0. \quad (5.21)$$

Eq. (5.21) is called *H-theorem*. The *equilibrium state* is defined as the state with constant P_r , i.e. with $\dot{H} = 0$ or $H = \text{minimal}$. We further define the entropy S by

$$S := -k_B H \quad (5.22)$$

What can be said about entropy is:

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The entropy S is maximum in equilibrium. For non-equilibrium processes, $\frac{dS}{dt} > 0$, which means that one time direction is excellent. Such a process is therefore irreversible.

5.1 Microcanonical ensemble

According to Eq. (5.19) holds in equilibrium

$$P_r = P_{r'} \quad (5.23)$$

for all r, r' with $E_r = E_{r'}$. In a closed system, by definition, only states with $E_r = E$ can be achieved.

A closed system in equilibrium is equally likely in each of its accessible microstates.

You can now measure the energy E of the system, with an accuracy $\delta E \gg \Delta E_r$, where ΔE_r represents a typical distance between the energy levels of the system. The fact that an energy E was measured with the precision δE should be interpreted as meaning that the true energy E' of the system lies in the interval $[E - \delta E, E]$. There are therefore a number of states r whose energies E_r lie in this interval and are therefore compatible with the measurement. One defines the *microcanonical partition function* Ω by

$$\Omega(E, x) := \sum_{r: E - \delta E \leq E_r < E} 1. \quad (5.24)$$

Here x denotes all parameters other than the energy that define the system macroscopically, in particular the volume. Since all accessible microstates are equally probable,

$$P_r = \frac{1}{\Omega(E, x)} \cdot \begin{cases} 1, & E - \delta E \leq E_r < E, \\ 0, & \text{sonst} \end{cases} \quad (5.25)$$

In the microcanonical ensemble, to which the microcanonical partition function refers, all systems are closed and have the same energies and particle numbers. So these are very specific physical requirements. In this case the entropy follows

$$S(E, x) = -k_B \sum_{r=1}^{\infty} \frac{1}{\Omega(E, x)} \ln \left(\frac{1}{\Omega(E, x)} \right) = k_B \ln [\Omega(E, x)]. \quad (5.26)$$

The energy of a system can be written with reference to an orthonormal basis ($|\psi_k\rangle$) from eigenstates of the Hamiltonian

$$E = \sum_{k=1}^{\infty} P_k E_k(x). \quad (5.27)$$

For the change in energy follows in linear order

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$$\Leftrightarrow dE = \underbrace{E \sum_{k=1}^{\infty} dP_k}_{= \text{Wärme } dQ} + \underbrace{\sum_{k=1}^{\infty} P_k \frac{\partial E_k(x)}{\partial x} dx}_{= -\text{Arbeit} = -dW}. \quad (5.28)$$

Here, a partial derivative was simply noted for the derivative with respect to x , in general it is a sum of several partial derivatives, and $E_k = E$ was also used. *Heat* means a change in the occupation probabilities with constant external parameters x , *Work* means a change in the energy due to a change in the external parameters; these are conceptual definitions. A differential df is a shorthand notation for a linear Taylor expansion of f ignoring the error term. Since the energy E as a state variable does not depend on the process that led to the state, o. B. d. A. a *quasi-static process*¹ can be assumed:

$$dE = dQ_{\text{qs}} - dW_{\text{qs}} \quad (5.29)$$

In such a process a sequence of equilibrium states is passed through; one can imagine it as an infinitely slow process. Furthermore, for each external parameter x_i one defines a *generalized force* X_i by

$$X_i := - \sum_{k=1}^{\infty} P_k \frac{\partial E_k(x)}{\partial x_i}. \quad (5.30)$$

In equilibrium this becomes

$$X_i = - \frac{\partial E(x)}{\partial x_i}. \quad (5.31)$$

In the case of a quasi-static process, the following applies:

¹The word *quasi* can be translated as *almost*.

$$dW_{\text{qs}} = - \sum_i \frac{\partial E(x)}{\partial x_i} dx_i = \sum_i X_i dx_i. \quad (5.32)$$

The pressure p is the generalized force of the volume:

$$p(E, x) := - \sum_{k=1}^{\infty} P_k \frac{\partial E_k(x)}{\partial V} \quad (5.33)$$

In the case $x = V$, when the only external parameter is the volume, it follows

$$dE = dQ_{\text{qs}} - p dV \quad (5.34)$$

The *temperature* T is given by

$$\frac{1}{T} := \frac{\partial S(E, x)}{\partial E} \quad (5.35)$$

defined, you continue to lay

$$\beta := \frac{1}{k_B T} \quad (5.36)$$

as an abbreviation. Eq. (5.30) is unwieldy because it has to be averaged over an infinite number of quantum mechanical states. To derive an alternative formula, one starts from the microcanonical partition function

$$\Omega(E, x) = \Omega(E, x_1, x_i) = \sum_{r: E - \delta E \leq E_r < E} 1 \quad (5.37)$$

from, here x_i stands for all external parameters except x_1 , where x_1 is chosen arbitrarily. It applies

$$\frac{\partial \ln [\Omega(E, x)]}{\partial x_1} = \frac{\ln [\Omega(E, x_1 + dx_1, x_i)] - \ln [\Omega(E, x_1, x_i)]}{dx_1}. \quad (5.38)$$

Now you do the math

$$\Omega(E, x_1 + dx_1, x_i) = \sum_{r: E - \delta E \leq E_r(x_1 + dx_1, x_i) < E} 1 = \sum_{r: E - \delta E \leq E_r(x) + dE_r < E} 1 \quad (5.39)$$

with

$$dE_r = \frac{\partial E_r}{\partial x_1} dx_1. \quad (5.40)$$

One can

$$dE_r = \overline{dE_r} \quad (5.41)$$

set, whereby the averaging takes place over all microstates of the equilibrium state:

$$\Omega(E, x_1 + dx_1, x_i) = \sum_{r: E - \overline{dE_r} - \delta E \leq E_r(x) < E - \overline{dE_r}} 1 = \Omega(E - \overline{dE_r}, x) \quad (5.42)$$

Because of

$$X_i = -\frac{\overline{\partial E}}{\partial x_i} \quad (5.43)$$

is

$$\overline{dE_r} = -X_i x_i. \quad (5.44)$$

Therefore applies

$$\begin{aligned} \frac{\partial \ln [\Omega(E, x)]}{\partial x_i} &= -\frac{\ln [\Omega(E - \overline{dE_r}, x)] - \ln [\Omega(E, x)]}{\overline{dE_r}/X_i} = \frac{\partial \ln [\Omega(E, x)]}{\partial E} X_i = \beta X_i \\ \Rightarrow X_i &= T \frac{\partial S(E, x)}{\partial x_i}. \end{aligned} \quad (5.45)$$

For printing follows

$$p = T \frac{\partial S(E, x)}{\partial V} \quad (5.46)$$

For the change in entropy applies

$$dS = \frac{\partial S(E, x)}{\partial E} dE + \sum_i \frac{\partial S(E, x)}{\partial x_i} dx_i = \frac{dE}{T} + \sum_i \frac{X_i}{T} dx_i \quad (5.47)$$

$$\Leftrightarrow dS = \frac{1}{T} (dQ - dW + dW_{\text{qs}}) = \frac{dQ_{\text{qs}}}{T} \quad (5.48)$$

If two systems A, B with the microcanonical partition sums $\Omega_A(E_A, x_A)$ and $\Omega_B(E_B, x_B)$ are in equilibrium, then the energy E of the entire system applies

$$E = E_A + E_B. \quad (5.49)$$

For the partition function $\Omega(E, x)$ of the entire system follows

$$\Omega(E, x) = \Omega_A(E_A, x_A) \Omega_B(E_B, x_B). \quad (5.50)$$

The partition sums of the subsystems must be multiplied because all combinations of microstates can occur. For the entropy S of the entire system follows

$$S(E, x) = k_B \ln [\Omega_A(E_A, x_A)] + k_B \ln [\Omega_B(E_B, x_B)] = S_A(E_A, x_A) + S_B(E - E_A, x_B). \quad (5.51)$$

So the entropy is additive. At equilibrium it is maximum:

$$\frac{\partial S}{\partial E_A} = 0 \Rightarrow \frac{\partial S_A}{\partial E_A} + \frac{\partial S_B}{\partial E_A} = \frac{\partial S_A}{\partial E_A} - \frac{\partial S_B}{\partial E_B} = 0 \Rightarrow T_A = T_B \quad (5.52)$$

If the systems A, B are also in x_i -exchange, one obtains the condition under the assumption $x_i = x_{i,A} + x_{i,B}$

$$\nabla S = 0 \Rightarrow \frac{\partial S}{\partial x_{i,A}} = 0 \Rightarrow \frac{\partial S_A}{\partial x_{i,A}} + \frac{\partial S_B}{\partial x_{i,A}} = \frac{\partial S_A}{\partial x_{i,A}} - \frac{\partial S_B}{\partial x_{i,B}} = 0. \quad (5.53)$$

From this, under the assumption $T_A = T_B$, the equality of the generalized forces follows

$$X_{i,A} = X_{i,B}. \quad (5.54)$$

An equation of the form

$$p = p(T, V, N) \quad (5.55)$$

is called *thermal equation of state*, while equations of the form

$$E = E(T, V, N) \quad (5.56)$$

can be referred to as *caloric equation of state*. At this point we refer to the notation usual in thermodynamics

$$\frac{\partial f(x, y, z)}{\partial x} = \left(\frac{\partial f}{\partial x} \right)_{y, z} \quad (5.57)$$

for partial derivatives. The *heat capacity* of a substance is defined by

$$C^{(p)} := \left(\frac{dQ_{\text{qs}}}{dT} \right)_p \quad (5.58)$$

or

$$C^{(V)} := \left(\frac{dQ_{\text{qs}}}{dT} \right)_V, \quad (5.59)$$

depending on whether the pressure or the volume is kept constant during the process. With Eq. (5.48) follows

$$C^{(p)} = T \left(\frac{\partial S}{\partial T} \right)_p, \quad (5.60)$$

$$C^{(V)} = T \left(\frac{\partial S}{\partial T} \right)_V. \quad (5.61)$$

The *specific heat capacity* of a system with mass m is defined by

$$c^{(p)} := \frac{1}{m} C^{(p)} \quad (5.62)$$

and analogously for $c^{(V)}$.

5.2 Canonical and grand canonical ensemble

The *canonical ensemble* consists of systems A that are in heat exchange with large surrounding systems B , so-called *bath systems*. However, there is no particle or xi exchange. The entire system consisting of A and B is complete so that the microcanonical ensemble can be used. Then applies to the total energy

$$E = E_A + E_B = \text{const.} \quad (5.63)$$

For the microcanonical partition sums Ω of the entire system applies

$$\Omega = \Omega(E, x). \quad (5.64)$$

The entire system is equally likely to be found in each of its accessible microstates. The number of states $n(E_A)$ with a fixed energy E_A of the system A is given by

$$n(E_A) = \Omega_A(E_A, x_A) \Omega_B(E_B, x_B), \quad (5.65)$$

where Ω_A is the microcanonical partition function of system A and Ω_B is that of system B . The probability of encountering a state r with an energy $E_r = E_A$ in the system A is the probability

$$P(E_A) = \frac{n_A}{\Omega(E, x)} = \frac{\Omega_A(E_A, x_A) \Omega_B(E_B, x_B)}{\Omega(E, x)}, \quad (5.66)$$

to find the system A at an energy E_A , divided by the number of these equally probable states:

$$P_r = \frac{P(E_A)}{\Omega_A(E_A, x_A)} = \frac{\Omega_B(E - E_A, x - x_A)}{\Omega(E, x)} \quad (5.67)$$

$E_B = E - E_A$ and $x_B = x - x_A$ were used. Because of $E_B \gg E_A$ you can expand the counter according to E_A around $E_A = 0$:

$$\ln [\Omega_B(E - E_A, x - x_A)] = \ln [\Omega_B(E, x - x_A)] - \beta E_A + \mathcal{O}(E_A^2) \quad (5.68)$$

There is

$$\beta = \frac{1}{k_B T_K} \quad (5.69)$$

with the temperature of the heat bath, which is equal to the temperature T of the entire system, since this is in equilibrium (see equation (5.223)). Neglecting the higher order terms:

$$P_r = \frac{\Omega_B(E, x - x_A)}{\Omega(E, x)} e^{-\beta E_r} = \frac{1}{Z} e^{-\beta E_r}. \quad (5.70)$$

$Z = \frac{\Omega(E, x - x_A)}{\Omega_B(E, x)}$ is the canonical partition function, which acts as a normalization constant and represents

$$\sum_r P_r = 1 \quad (5.71)$$

secure:

$$Z = \sum_r e^{-\beta E_r} \quad (5.72)$$

In the *grand canonical ensemble*, not only heat but also particle exchange is possible with the system B . Then additionally applies

$$N = N_A + N_B = \text{const.} \quad (5.73)$$

for the particle number. For the number of states $n(E_A, N_A)$ in which the system A has the energy E_A and the particle number N_A , applies

$$n(E_A, N_A) = \Omega_A(E_A, N_A, x_A) \Omega_B(E_B, N_B, x_B). \quad (5.74)$$

The probability $P(E_A, N_A)$ of finding a state r with the energy $E_r = E_A$ and the particle number $N_r = N_A$ in the system A is given by the probability

$$P(E_A, N_A) = \frac{n(E_A, N_A)}{\Omega(E, x)} = \frac{\Omega_A(E_A, N_A, x_A) \Omega_B(E_B, N_B, x_B)}{\Omega(E, x)}, \quad (5.75)$$

to find the system A with an energy E_A and particle number N_A , divided by the number of these equally probable states:

$$P_r = \frac{P(E_A, N_A)}{\Omega_A(E_A, N_A, x_A)} = \frac{\Omega_B(E - E_A, N - N_A, x_B)}{\Omega(E, x)} \quad (5.76)$$

$E_B = E - E_A$, $N_B = N - N_A$ and $x_B = x - x_A$ were used. Because of $E_B \gg E_A$ and $N_B \gg N_A$ you can develop the counter again:

$$\begin{aligned} \ln [\Omega_B(E - E_A, N - N_A, x - x_A)] &= \ln [\Omega_B(E, N, x - x_A)] - \beta E_A - \frac{1}{k_B} \frac{\partial S}{\partial N} N_A \\ &+ \mathcal{O}(E_A^2, N_A^2, E_A N_A). \end{aligned} \quad (5.77)$$

The negative generalized force of the particle number is defined by the *chemical potential*

$$\mu := -\frac{\partial E}{\partial N} = -T \frac{\partial S(E, N, x)}{\partial N}. \quad (5.78)$$

Neglecting the higher order terms, we therefore have:

$$P_r = \frac{\Omega_B(E, N, x - x_A)}{\Omega(E, x)} e^{-\beta(E_r - \mu N_r)} = \frac{1}{Y} e^{-\beta(E_r - \mu N_r)} \quad (5.79)$$

$Y = \frac{\Omega(E, x)}{\Omega_B(E, N, x - x_A)}$ is the grand canonical partition function, which acts as a normalization constant and represents

$$\sum_r P_r = 1 \quad (5.80)$$

secure:

$$Y = \sum_r e^{-\beta(E_r - \mu N_r)} \quad (5.81)$$

Now the first law should be generalized to the case $dN \neq 0$. With the equations (5.29) and (5.32) follows

$$dE = dQ_{\text{qs}} - dW_{\text{qs}} = dQ_{\text{qs}} - \sum_i X_i dx_i = dQ_{\text{qs}} - \frac{\partial E}{\partial V} dV - \frac{\partial E}{\partial N} dN = dQ_{\text{qs}} - p dV + \mu dN. \quad (5.82)$$

5.2.1 Thermodynamic potentials

A *thermodynamic potential* is a state variable from which all state variables can be determined by partial differentiation. In this section, only the volume V and the particle number N are considered as external parameters. In addition to the energy, the following thermodynamic potentials are defined:

$$F := E - ST (\text{freie Energie}) \quad (5.83)$$

$$H := E + pV (\text{Enthalpie}) \quad (5.84)$$

$$G := E - ST + pV (\text{Gibbs-Potential, freie Enthalpie}) \quad (5.85)$$

$$J := E - ST - \mu N (\text{großkanonisches Potential}) \quad (5.86)$$

For the differentials it follows that $dE = dQ - p dV + \mu dN$

$$dF = -S dT - p dV + \mu dN, \quad (5.87)$$

$$dH = T dS + V dp + \mu dN, \quad (5.88)$$

$$dG = -S dT + V dp + \mu dN, \quad (5.89)$$

$$dJ = -S dT - p dV - N d\mu. \quad (5.90)$$

The following statements can be seen from this:

$$\left(\frac{\partial E}{\partial S}\right)_{V,N} = T, \quad \left(\frac{\partial E}{\partial V}\right)_{S,N} = -p, \quad \left(\frac{\partial E}{\partial N}\right)_{S,V} = \mu \quad (5.91)$$

$$(5.92)$$

$$\left(\frac{\partial F}{\partial T}\right)_{V,N} = -S, \quad \left(\frac{\partial F}{\partial V}\right)_{T,N} = -p, \quad \left(\frac{\partial F}{\partial N}\right)_{T,V} = \mu \quad (5.93)$$

$$\left(\frac{\partial H}{\partial S}\right)_{p,N} = T, \quad \left(\frac{\partial H}{\partial p}\right)_{S,N} = V, \quad \left(\frac{\partial H}{\partial N}\right)_{S,p} = \mu \quad (5.94)$$

$$\left(\frac{\partial G}{\partial T}\right)_{p,N} = -S, \quad \left(\frac{\partial G}{\partial p}\right)_{T,N} = V, \quad \left(\frac{\partial G}{\partial N}\right)_{T,p} = \mu \quad (5.95)$$

$$\left(\frac{\partial J}{\partial T}\right)_{V,\mu} = -S, \quad \left(\frac{\partial J}{\partial V}\right)_{T,\mu} = -p, \quad \left(\frac{\partial J}{\partial \mu}\right)_{T,V} = -N \quad (5.96)$$

These are three statements each for the partial derivatives of E , F , H , G and J . By applying the equality of the second partial derivatives, 15 non-trivial thermodynamic relations can be derived, which are called *Maxwell relations*:

$$\left(\frac{\partial^2 E}{\partial V \partial S}\right)_N = \left(\frac{\partial^2 E}{\partial S \partial V}\right)_N \Rightarrow \left(\frac{\partial T}{\partial V}\right)_{S,N} = -\left(\frac{\partial p}{\partial S}\right)_{V,N} \quad (5.97)$$

$$\left(\frac{\partial^2 E}{\partial N \partial S}\right)_V = \left(\frac{\partial^2 E}{\partial S \partial N}\right)_V \Rightarrow \left(\frac{\partial T}{\partial N}\right)_{S,V} = \left(\frac{\partial \mu}{\partial S}\right)_{N,V} \quad (5.98)$$

$$\left(\frac{\partial^2 E}{\partial N \partial V}\right)_S = \left(\frac{\partial^2 E}{\partial V \partial N}\right)_S \Rightarrow -\left(\frac{\partial p}{\partial N}\right)_{V,S} = \left(\frac{\partial \mu}{\partial V}\right)_{N,S} \quad (5.99)$$

$$\left(\frac{\partial^2 F}{\partial V \partial T}\right)_N = \left(\frac{\partial^2 F}{\partial T \partial V}\right)_N \Rightarrow \left(\frac{\partial S}{\partial V}\right)_{T,N} = \left(\frac{\partial p}{\partial T}\right)_{V,N} \quad (5.100)$$

$$\left(\frac{\partial^2 F}{\partial N \partial T}\right)_V = \left(\frac{\partial^2 F}{\partial T \partial N}\right)_V \Rightarrow -\left(\frac{\partial S}{\partial N}\right)_{T,V} = \left(\frac{\partial \mu}{\partial T}\right)_{N,V} \quad (5.101)$$

$$\left(\frac{\partial^2 F}{\partial N \partial V}\right)_T = \left(\frac{\partial^2 F}{\partial V \partial N}\right)_T \Rightarrow -\left(\frac{\partial p}{\partial N}\right)_{V,T} = \left(\frac{\partial \mu}{\partial V}\right)_{N,T} \quad (5.102)$$

$$\left(\frac{\partial^2 H}{\partial p \partial S}\right)_N = \left(\frac{\partial^2 H}{\partial S \partial p}\right)_N \Rightarrow \left(\frac{\partial T}{\partial p}\right)_{S,N} = \left(\frac{\partial V}{\partial S}\right)_{p,N} \quad (5.103)$$

$$\left(\frac{\partial^2 H}{\partial N \partial S}\right)_p = \left(\frac{\partial^2 H}{\partial S \partial N}\right)_p \Rightarrow \left(\frac{\partial T}{\partial N}\right)_{S,p} = \left(\frac{\partial \mu}{\partial S}\right)_{N,p} \quad (5.104)$$

$$\left(\frac{\partial^2 H}{\partial N \partial p}\right)_S = \left(\frac{\partial^2 H}{\partial p \partial N}\right)_S \Rightarrow \frac{V}{N} = \left(\frac{\partial V}{\partial N}\right)_{p,S} = \left(\frac{\partial \mu}{\partial p}\right)_{N,S} \quad (5.105)$$

$$\left(\frac{\partial^2 G}{\partial p \partial T}\right)_N = \left(\frac{\partial^2 G}{\partial T \partial p}\right)_N \Rightarrow -\left(\frac{\partial S}{\partial p}\right)_{T,N} = \left(\frac{\partial V}{\partial T}\right)_{p,N} \quad (5.106)$$

$$\left(\frac{\partial^2 G}{\partial N \partial T}\right)_p = \left(\frac{\partial^2 G}{\partial T \partial N}\right)_p \Rightarrow -\frac{S}{N} = -\left(\frac{\partial S}{\partial N}\right)_{T,p} = \left(\frac{\partial \mu}{\partial T}\right)_{N,p} \quad (5.107)$$

$$\left(\frac{\partial^2 G}{\partial N \partial p}\right)_T = \left(\frac{\partial^2 G}{\partial p \partial N}\right)_T \Rightarrow \left(\frac{\partial V}{\partial N}\right)_{p,T} = \left(\frac{\partial \mu}{\partial p}\right)_{N,T} \quad (5.108)$$

$$\left(\frac{\partial^2 J}{\partial T \partial V}\right)_\mu = \left(\frac{\partial^2 J}{\partial V \partial T}\right)_\mu \Rightarrow \left(\frac{\partial p}{\partial T}\right)_{\mu,V} = \left(\frac{\partial S}{\partial V}\right)_{\mu,T} \quad (5.109)$$

$$\left(\frac{\partial^2 J}{\partial T \partial \mu}\right)_V = \left(\frac{\partial^2 J}{\partial \mu \partial T}\right)_V \Rightarrow \left(\frac{\partial N}{\partial T}\right)_{\mu,V} = \left(\frac{\partial S}{\partial \mu}\right)_{T,V} \quad (5.110)$$

$$\left(\frac{\partial^2 J}{\partial V \partial \mu}\right)_T = \left(\frac{\partial^2 J}{\partial \mu \partial V}\right)_T \Rightarrow \left(\frac{\partial N}{\partial V}\right)_{\mu,T} = \left(\frac{\partial p}{\partial \mu}\right)_{T,V} \quad (5.111)$$

If you know the microscopic structure of a system, you can determine the entropy, the microcanonical partition function or the grand canonical partition function, depending on the physical requirements. The question is how one can determine macroscopic quantities such as compressibilities or heat capacities from the partition sums. To do this, one must be able to express one of the thermodynamic potentials in terms of the partition function of the system. First, the canonical ensemble is considered. In this case (T, V, N) or alternatively (β, V, N) are fixed. It applies

$$d \ln [Z(\beta, V, N)] = \frac{\partial \ln(Z)}{\partial \beta} d\beta + \frac{\partial \ln(Z)}{\partial V} dV + \frac{\partial \ln(Z)}{\partial N} dN. \quad (5.112)$$

Now the partial derivatives of the partition function Eq. (5.72) calculated:

$$\frac{\partial \ln(Z)}{\partial \beta} = -\frac{1}{Z} \sum_r E_r \exp(-\beta E_r) = -E \quad (5.113)$$

$$\frac{\partial \ln(Z)}{\partial V} = -\frac{\beta}{Z} \sum_r \frac{\partial E_r(V, N)}{\partial V} \exp(-\beta E_r) = -\beta \overline{\frac{\partial E_r}{\partial V}} = \beta p \quad (5.114)$$

$$\frac{\partial \ln(Z)}{\partial N} = -\frac{\beta}{Z} \sum_r \frac{\partial E_r(V, N)}{\partial N} \exp(-\beta E_r) = -\beta \overline{\frac{\partial E_r}{\partial N}} = -\beta \mu \quad (5.115)$$

It therefore applies

$$\begin{aligned} d \ln(Z(\beta, V, N)) &= -E d\beta + \beta p dV - \beta \mu dN \\ \Rightarrow d(\ln(Z) + \beta E) &= \beta(dE + p dV - \mu dN) = \frac{1}{k_B} \left(\frac{dE}{T} + \frac{p}{T} dV - \frac{\mu}{T} dN \right) \end{aligned} \quad (5.116)$$

By comparing with Eq. (5.47) is obtained

$$k_B d[\ln(Z) + \beta E] = dS \Rightarrow S = k_B [\ln(Z) + \beta E] + C. \quad (5.117)$$

The constant C results in zero, which will not be shown here, so it follows

$$F = E - TS = -k_B T \ln(Z(T, V, \mu)). \quad (5.118)$$

In the grand canonical ensemble (T, V, μ) are fixed, the differential is obtained

$$d \ln[Y(\beta, V, \mu)] = \frac{\partial \ln(Y)}{\partial \beta} d\beta + \frac{\partial \ln(Y)}{\partial V} dV + \frac{\partial \ln(Y)}{\partial \mu} d\mu. \quad (5.119)$$

The partial derivatives are calculated using the partition function Eq. (5.81)

$$\frac{\partial \ln(Y)}{\partial \beta} = -\frac{1}{Y} \sum_r (E_r - \mu N_r) \exp(-\beta(E_r - \mu N_r)) = -E + \mu N, \quad (5.120)$$

$$\frac{\partial \ln(Y)}{\partial V} = -\frac{\beta}{Y} \sum_r \frac{\partial E_r(V, N)}{\partial V} \exp(-\beta(E_r - \mu N_r)) = -\beta \frac{\overline{\partial E_r}}{\partial V} = \beta p, \quad (5.121)$$

$$\frac{\partial \ln(Y)}{\partial \mu} = \frac{\beta}{Y} \sum_r N_r \exp(-\beta(E_r - \mu N_r)) = \beta \overline{N_r} = \beta N. \quad (5.122)$$

It is thus

$$\begin{aligned} d \ln[Y(\beta, V, \mu)] &= (-E + \mu N) d\beta + \beta p dV + \beta N d\mu \\ \Leftrightarrow d[\ln(Y) + \beta E - \beta \mu N] &= \beta (dE + p dV - \mu dN) = \frac{dS}{k_B}. \end{aligned} \quad (5.123)$$

This applies

$$S = k_B [\ln(Y) + \beta E - \beta \mu N] \Leftrightarrow k_B T \ln(Y) = TS - E + \mu N. \quad (5.124)$$

A possible constant here is also zero. By comparing with Eq. (5.86) follows

$$J = -k_B T \ln(Y(T, V, \mu)). \quad (5.125)$$

The equations (5.118) and (5.125) provide a connection between microscopic statistics and macroscopic thermodynamics.

For the complete differential $d\mu$ of the chemical potential $\mu = \mu(T, p)$ holds

$$d\mu = \left(\frac{\partial \mu}{\partial T}\right)_p dT + \left(\frac{\partial \mu}{\partial p}\right)_T dp \stackrel{\text{Glg.en (5.101), (5.108)}}{=} -\left(\frac{\partial S}{\partial N}\right)_{T,V} dT + \left(\frac{\partial V}{\partial N}\right)_{p,T} dp. \quad (5.126)$$

With

$$\left(\frac{\partial S}{\partial N}\right)_{T,V} = \frac{S}{N} =: s, \quad \left(\frac{\partial V}{\partial N}\right)_{p,T} = \frac{V}{N} =: v \quad (5.127)$$

follows

$$d\mu = -s dT + v dp, \quad (5.128)$$

which is called *Gibbs-Duhem relation*.

5.3 Ideal gas

An *ideal gas* is a gas in which the particles do not interact with each other. The Hamiltonian of an ideal gas made of N particles is

$$\hat{H} = \sum_{i=1}^N -\frac{\hbar^2}{2m} \Delta_i + V(\mathbf{r}_i) = \sum_{i=1}^N \hat{H}_i, \quad (5.129)$$

it is a superposition of one-particle Hamiltonians

$$\hat{H}_i = -\frac{\hbar^2}{2m}\Delta_i + V(\mathbf{r}_i). \quad (5.130)$$

$V(\mathbf{r}_i)$ ist das bekannte Wandpotential

$$V(\mathbf{r}_i) = \begin{cases} 0, & \mathbf{r}_i \in V, \\ \infty, & \text{sonst,} \end{cases} \quad (5.131)$$

where V is the volume to which the particles are confined. Here $V = L^3$ is a cube with edge length L . This corresponds to a 3D potential well, see section 4.2. The one-particle solution is

$$\psi(\mathbf{r}_i) \propto \sin(k_{3i-2}x) \sin(k_{3i-1}y) \sin(k_{3i}z). \quad (5.132)$$

The boundary condition applies here for $k_{3i-2}, k_{3i-1}, k_{3i}$

$$\frac{Lp_i}{\hbar} = k_i L = n_i \pi \quad (5.133)$$

with $n_i \in \mathbb{N}$ with $n \geq 1$. $p_i = \hbar k_i$ is the momentum. The particles do not penetrate the wall, so they have no potential energy. This therefore applies to the total energy of the system

$$E = \frac{1}{2m} \sum_{i=1}^{3N} p_i^2. \quad (5.134)$$

To determine the microcanonical state sum of the ideal gas, one assumes $\delta E = E$:

$$\Omega(E, V, N) = \sum_{E_r < E} 1 = \underbrace{\sum_{n_1=1,2,\dots} \dots \sum_{n_{3N}=1,2,\dots}}_{E_r < E} 1 \approx \frac{1}{2^{3N}} \underbrace{\int \dots \int}_{E_r < E} dn_1 \dots dn_{3N}. \quad (5.135)$$

Because $\bar{n}_i \gg 1$, the sums were replaced by integrals in the last step. The factor $1/2^{3N}$ arises from the inclusion of negative values in the integration (there are $3N$ coordinate axes that must be halved). Eq. (5.133) is implied

$$dn_i = \frac{L}{\hbar\pi} dp_i. \quad (5.136)$$

It follows

$$\Omega(E, V, N) = \left(\frac{L}{2\hbar\pi}\right)^{3N} \underbrace{\int \dots \int}_{\sum p_i^2 < 2mE} dp_1 \dots dp_{3N} = \frac{V^N}{(2\hbar\pi)^{3N}} \underbrace{\int \dots \int}_{\sum p_i^2 < 2mE} dp_1 \dots dp_{3N}. \quad (5.137)$$

The remaining $3N$ -dimensional integral is the volume of a $3N$ -dimensional sphere of radius $\sqrt{2mE}$, so Eq. (B.143) can be used:

$$\begin{aligned} \Omega(E, V, N) &= \frac{V^N}{(2\hbar\pi)^{3N}} \frac{\pi^{3N/2}}{\Gamma\left(\frac{3N}{2} + 1\right)} \sqrt{2mE}^{3N} \stackrel{\text{Glg. (A.111)}}{=} \frac{V^N}{(2\pi\hbar)^{3N}} \frac{\pi^{3N/2}}{(3N/2)!} (2m)^{3N/2} E^{3N/2} \\ &= \frac{V^N}{(2\pi\hbar)^{3N}} \frac{1}{(3N/2)!} (2m\pi)^{3N/2} E^{3N/2} = \left[\frac{2\pi m}{(2\pi\hbar)^2}\right]^{3N/2} \frac{E^{3N/2}}{(3N/2)!} V^N \end{aligned} \quad (5.138)$$

Using the Stirling formula Eq. (A.117) is obtained

$$\begin{aligned}
\Omega(E, V, N) &= \left[\frac{2\pi m}{(2\pi\hbar)^2} \right]^{3N/2} E^{3N/2} V^N \frac{1}{(3N/2)!} \approx \sqrt{\frac{1}{2\pi}} \left[\frac{2\pi m}{(2\pi\hbar)^2} \right]^{3N/2} e^{3N/2} \left(\frac{2}{3N} \right)^{\frac{3N}{2} + \frac{1}{2}} E^{3N/2} V^N \\
&= \frac{1}{\sqrt{3N\pi}} \left[\frac{2\pi me}{(2\pi\hbar)^2} \right]^{3N/2} \left(\frac{2}{3N} \right)^{\frac{3N}{2}} E^{3N/2} V^N = \frac{1}{\sqrt{3\pi N}} \left[\frac{4\pi me}{3(2\pi\hbar)^2} \right]^{3N/2} V^N \left(\frac{E}{N} \right)^{3N/2}. \quad (5.139)
\end{aligned}$$

This result is not yet correct; an important modification still needs to be made. The N particles are quantum mechanically indistinguishable, which means that swapping two particles changes nothing. So $N!$ states are the same, which is why one

$$\Omega \rightarrow \frac{\Omega}{N!} \quad (5.140)$$

needs to be replaced. From this it follows, again using the Stirling formula,

$$\begin{aligned}
\Omega(E, V, N) &= \frac{1}{\sqrt{6\pi^2}} \frac{1}{N} \left[\frac{4\pi me^{5/3}}{3(2\pi\hbar)^2} \right]^{3N/2} \left(\frac{V}{N} \right)^N \left(\frac{E}{N} \right)^{3N/2} \\
&= \frac{1}{\sqrt{6\pi^2}} \frac{1}{N} \left[\frac{me^{5/3}}{3\pi\hbar^2} \right]^{3N/2} \left(\frac{V}{N} \right)^N \left(\frac{E}{N} \right)^{3N/2}. \quad (5.141)
\end{aligned}$$

For the entropy follows

$$\begin{aligned}
\frac{S(E, V, N)}{k_B} &= \frac{1}{2} \ln \left(\frac{1}{6\pi^2} \right) - \ln(N) + \frac{3N}{2} \ln(c) + N \ln \left(\frac{V}{N} \right) + \frac{3N}{2} \ln \left(\frac{E}{N} \right) \\
&\approx \frac{3N}{2} \ln(c) + N \ln \left(\frac{V}{N} \right) + \frac{3N}{2} \ln \left(\frac{E}{N} \right) - \ln(N) \\
&\approx \frac{3N}{2} \ln(c) + N \ln \left(\frac{V}{N} \right) + \frac{3N}{2} \ln \left(\frac{E}{N} \right)
\end{aligned}$$

$$\Leftrightarrow S(E, V, N) = k_B N \left[\frac{3}{2} \ln(c) + \ln \left(\frac{V}{N} \right) + \frac{3}{2} \ln \left(\frac{E}{N} \right) \right] \quad (5.142)$$

with

$$c := \frac{me^{5/3}}{3\pi\hbar^2}. \quad (5.143)$$

Eq. (5.142) is also called *Sackur-tetrode equation*. One obtains the *caloric equation of state of ideal gases*

$$\frac{1}{k_B T} = \frac{\partial \ln(\Omega(E, V, N))}{\partial E} = \frac{3}{2} \frac{N}{E} \Rightarrow E = \frac{3}{2} N k_B T. \quad (5.144)$$

Still applies

$$\frac{p}{T} = \frac{\partial S(E, V, N)}{\partial V} = k_B N \frac{1}{V}. \quad (5.145)$$

This gives the *thermal equation of state of ideal gases*

$$pV = N k_B T. \quad (5.146)$$

For the isochoric heat capacity of the ideal gas, Eq. (5.144)

$$C^{(V)} = \frac{3}{2} k_B N. \quad (5.147)$$

Applies to the corresponding specific size

$$c^{(V)} = \frac{\frac{3}{2} k_B N}{Nm} = \frac{3 k_B}{2 m}. \quad (5.148)$$

So you can get the energy E

$$E = C^{(V)} T = N m c^{(V)} T \quad (5.149)$$

note down. For the isobaric heat capacity, Eq. (5.60)

$$C^{(p)} = T \left(\frac{\partial S}{\partial T} \right)_p = k_B T N \frac{\partial}{\partial T} \left(\ln \left(\frac{k_B T}{p} \right) + \frac{3}{2} \ln \left(\frac{3}{2} N k_B T \right) \right) = k_B T N \left(\frac{1}{T} + \frac{3}{2} \frac{1}{T} \right) = \frac{5}{2} N k_B. \quad (5.150)$$

For the enthalpy H of the ideal gas follows

$$H = E + pV = \frac{5}{2} N k_B T = C^{(p)} T. \quad (5.151)$$

For the Gibbs potential G of the ideal gas one obtains

$$G = E - ST + pV = H - ST = C^{(p)} T - ST. \quad (5.152)$$

Still applies

$$c^{(p)} - c^{(V)} = \frac{N}{m} k_B = \frac{N}{m N_A} R = R_s. \quad (5.153)$$

For the chemical potential with the equations (5.85) and (5.95)

$$\mu = \frac{E - TS + pV}{N} = \frac{C^{(p)} T}{N} - \frac{ST}{N} + k_B T = T \left(\frac{C^{(p)}}{N} - \frac{S}{N} + k_B \right), \quad (5.154)$$

where it was used that the Gibbs potential is an extensive size. An equivalent formulation of Eq. (5.146) is

$$p = \frac{N k_B T}{V} = \frac{n N_A k_B T}{V} = \frac{n R T}{V} = \frac{m R T}{V M} = \varrho R_s T \quad (5.155)$$

with the individual gas constant $R_s := \frac{R}{M}$.

The equation of state applies to a gas, not to a gas mixture. However, air consists of various gases. Now the equation of state should be extended to such a mixture. So let a gas with $N \in \mathbb{N}$ components be given. For $1 \leq i \leq N$ let p_i be the partial pressure of the i -th gas component. Since there are no WWs between the components, the following applies:

$$p = \sum_{i=1}^N p_i = \sum_{i=1}^N \varrho_i R_i T = \varrho T \sum_{i=1}^N R_i \frac{\varrho_i}{\varrho} = T R_\varrho \sum_{i=1}^N \frac{m_i}{m} \frac{1}{M_i}. \quad (5.156)$$

With the definition

$$M := \frac{1}{\sum_{i=1}^N \frac{m_i}{m} \frac{1}{M_i}} \quad (5.157)$$

becomes

$$p = \varrho \frac{R}{M} T = \varrho R_s T \quad (5.158)$$

also for a gas mixture. The average molar mass according to Eq. (5.157) can be easily calculated by weighting the molar masses of the components with their volume fractions:

$$M = \frac{\mathbf{I}}{\sum_{i=1}^N \frac{m_i}{m} \frac{n_i}{m_i}} = \frac{\sum_{i=1}^N n_i M_i}{\sum_{i=1}^N n_i} = \sum_{i=1}^N \frac{n_i}{n} M_i, \quad (5.159)$$

Here n_i is the amount of substance of the i -th component and n is the total amount of substance. You can write in mass density terms

$$M = \frac{m}{n} = \frac{m}{\sum_i \frac{m_i}{M_i}} = \frac{\varrho}{\sum_i \frac{\varrho_i}{M_i}} = \frac{\mathbf{I}}{\frac{1}{\varrho} \sum_i \frac{\varrho_i}{M_i}}. \quad (5.160)$$

For the molar mass of moist air M_h applies

$$M_h = \frac{\mathbf{I}}{\frac{\varrho_d}{M_d \varrho_h} + \frac{\varrho_v}{\varrho_h} \frac{1}{M_v}}. \quad (5.161)$$

So you have

$$\frac{\mathbf{I}}{M_h} = \frac{\mathbf{I}}{M_d} \left(\mathbf{I} - \frac{\varrho_v}{\varrho_h} \right) + \frac{\varrho_v}{\varrho_h} \frac{\mathbf{I}}{M_v}. \quad (5.162)$$

The individual gas constant of moist air is therefore

$$R_h = R_d \left(\mathbf{I} - \frac{\varrho_v}{\varrho_h} + \frac{\varrho_v}{\varrho_h} \frac{M_d}{M_v} \right). \quad (5.163)$$

One further defines the *virtual temperature* T_v as the temperature at which dry air would have the same density as moist air at the same pressure. As an equation this means

$$\begin{aligned} R_h \varrho T &= R_d \varrho T_v \Rightarrow T_v = \frac{R_h}{R_d} T = T \left(\mathbf{I} - \frac{\varrho_v}{\varrho_h} + \frac{\varrho_v}{\varrho_h} \frac{M_d}{M_v} \right) \\ &= T \left[\mathbf{I} + \frac{\varrho_v}{\varrho_h} \left(\frac{M_d}{M_v} - \mathbf{I} \right) \right]. \end{aligned} \quad (5.164)$$

The difference

$$\Delta T_v := T_v - T = T \frac{\varrho_v}{\varrho_h} \left(\frac{M_d}{M_v} - \mathbf{I} \right) \quad (5.165)$$

is called *virtual temperature surcharge*. The decisive advantage of the virtual temperature is that the location dependence of the individual gas constant R_h is absorbed into the temperature, which is particularly practical for location and time derivatives. Therefore, virtual temperature plays an important role in modeling.

Now the *moisture measurements* should be discussed. The density ϱ_v (condensation products are neglected here) is also referred to as *absolute humidity* and the vapor pressure has already been introduced. First the *relative humidity* U is given by

$$U := \frac{p_v}{p_v^{(S)}} \quad (5.166)$$

with p_v as the partial pressure of water vapor and $p_v^{(S)}$ as the saturation vapor pressure. You continue to put the *specific humidity* q through

$$q := \frac{\varrho_v}{\varrho} \quad (5.167)$$

firmly. The *mixing ratio* r is given by

$$r := \frac{\varrho_v}{\varrho_d} \quad (5.168)$$

defined. Furthermore, the *volume mixing ratio* r_V is given by

$$r_V := \frac{n_v}{n_d} \quad (5.169)$$

defined. This quantity is often used in chemical and radiation considerations where particle density rather than mass density is important. A superscript S on the symbols means that saturation is assumed. Some useful conversions are

$$\begin{aligned} q &= \frac{p_v R_h T}{R_v T p} = \frac{p_v R_h}{p R_v} = \frac{p_v}{p} \frac{R_d}{R_v} \left(\mathbf{1} - \frac{\varrho_v}{\varrho_h} + \frac{\varrho_v}{\varrho_h} \frac{M_d}{M_v} \right) \\ &= \frac{p_v}{p} \left(\frac{M_v}{M_d} (\mathbf{1} - q) + q \right) = \frac{p_v}{p} \left(q \left(\mathbf{1} - \frac{M_v}{M_d} \right) + \frac{M_v}{M_d} \right) \\ \Rightarrow q \left(\mathbf{1} + \left(\frac{M_v}{M_d} - \mathbf{1} \right) \frac{p_v}{p} \right) &= \frac{M_v}{M_d} \frac{p_v}{p} \Rightarrow q = \frac{\frac{M_v}{M_d} \frac{p_v}{p}}{\frac{p}{p_v} + \frac{M_v}{M_d} - \mathbf{1}}, \end{aligned} \quad (5.170)$$

$$\begin{aligned} r &= \frac{\varrho_v}{\varrho_d} = \frac{p_v R_d T}{R_v T p_d} = \frac{p_v}{p_d} \frac{M_v}{M_d} = \frac{p_v}{p - p_v} \frac{M_v}{M_d} = \frac{\frac{M_v}{M_d}}{\frac{p}{p_v} - \mathbf{1}}, \\ r_V &= \frac{n_v}{n_d} = \frac{p_v}{p_d} = \frac{\varrho_v R_v}{\varrho_d R_d}. \end{aligned} \quad (5.171)$$

Common approximations are

$$q \approx \frac{\frac{M_v}{M_d}}{\frac{p}{p_v} - \mathbf{1}} = r, \quad q \approx \frac{M_v}{M_d} \frac{p_v}{p}, \quad r \approx \frac{M_v}{M_d} \frac{p_v}{p}. \quad (5.172)$$

5.4 Classic systems

Classical phase space coordinates are continuous and therefore difficult to grasp statistically. Semi-classical derivations are easier, in which one starts from the QM and then carries out the classical transition $\hbar \rightarrow 0$.

Let N particles be enclosed in a cubic volume $V = L^3$. For every wave vector component of the one-particle wave function applies

$$k_n L = n\pi \Leftrightarrow k_n = \frac{n\pi}{L} \quad (5.173)$$

with $n \in \mathbb{N}$ and $n \geq \mathbf{1}$. If you integrate over the entire k -space, you can replace the sums with integrals:

$$\sum_{\mathbf{k}} \dots = \frac{V^N}{(2\pi)^{3N}} \int \dots \int \dots dk_1 \dots dk_{3N} \quad (5.174)$$

The factor $\mathbf{1}/2$ before each integral is obtained by including negative k values in the integration. In momentum space one obtains

$$\sum_{\mathbf{k}} \dots = \frac{V^N}{(2\pi\hbar)^{3N}} \int \dots d^3N p. \quad (5.175)$$

Now this should be generalized to the phase space. Consider a particle in a 1D potential well $0 \leq x \leq L$ with $L > 0$, there exist solutions of the SG of the form

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(n \frac{\pi}{L} x\right), \quad (5.176)$$

Here let $n \in \mathbb{N}$ with $n \geq 1$, the energy eigenvalues are through

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \quad (5.177)$$

given. For the phase space volume $V(E)$ of a state with energy E applies

$$V(E) = \int_0^L \int_{p^2/2m \leq E} dp dx = L \sqrt{2mE}. \quad (5.178)$$

For a given energy $E \gg 1$, the number of states $N(E)$ with self-energies $E_n \leq E$ is approximately given by

$$N(E) \approx \frac{L}{\pi \hbar} \sqrt{2mE}. \quad (5.179)$$

So you get

$$\frac{V(E)}{N(E)} = \frac{2L \sqrt{2mE} \pi \hbar}{\sqrt{2mE} L} = 2\pi \hbar. \quad (5.180)$$

This result applies generally, i.e. also for more complicated potentials. In the case of f degrees of freedom, a microstate occupies the phase space volume $(2\pi \hbar)^f$. If you sum over all microstates r and replace this again with an integral, you get

$$\sum_r \dots = \frac{1}{(2\pi \hbar)^f} \int \dots dx dp. \quad (5.181)$$

An averaging operator results

$$\sum_r P_r \dots = \frac{1}{(2\pi \hbar)^f} \int \rho'(x, p) \dots dx dp \quad (5.182)$$

with the probabilities P_r of the microstates and a modified probability density $\rho'(x, p)$.

5.4.0.1 Maxwell distribution

If you put in Eq. (5.182) is the canonical partition function

$$P_r = \frac{1}{Z} \exp\left(-\frac{E_r}{k_B T}\right) \quad (5.183)$$

one, you get

$$\frac{1}{Z} \sum_r \exp\left(-\frac{E_r}{k_B T}\right) \dots = \frac{1}{Z (2\pi \hbar)^f} \int \exp\left(-\frac{E(x, p)}{k_B T}\right) \dots dx dp \quad (5.184)$$

If the integration depends only on the momentum, it follows

$$\frac{1}{Z} \sum_r \exp\left(-\frac{E_r}{k_B T}\right) \dots = \frac{V}{Z (2\pi \hbar)^f} \int \exp\left(-\frac{E(p)}{k_B T}\right) \dots dp \quad (5.185)$$

You interpret

$$\rho(p) = \frac{V}{Z(\hbar)^3} \exp\left(-\frac{E(p)}{k_B T}\right) \quad (5.186)$$

as probability density. Now consider exactly one particle and assume Cartesian momenta, so that:

$$\rho(p) = \frac{4\pi V}{z(\hbar)^3} \exp\left(-\frac{p^2}{2mk_B T}\right) p^2 \quad (5.187)$$

For the canonical partition function z of this single particle follows

$$z(T, V) = \frac{1}{(\hbar)^3} V \int_0^\infty 4\pi \exp\left(-\frac{p^2}{2mk_B T}\right) p^2 dp = \frac{V}{2\pi^2 \hbar^3} \int_0^\infty \exp\left(-\frac{p^2}{2mk_B T}\right) p^2 dp. \quad (5.188)$$

With Eq. (A.107) follows

$$z(T, V) = \frac{V}{8\pi^2 \hbar^3} \sqrt{\pi (2mk_B T)^3} = \frac{V}{\hbar^3} \left(\frac{mk_B T}{2\pi}\right)^{3/2}. \quad (5.189)$$

This follows

$$\rho(p) = \frac{\hbar^3}{V} \left(\frac{2\pi}{mk_B T}\right)^{3/2} \frac{4\pi V}{(\hbar)^3} \exp\left(-\frac{p^2}{2mk_B T}\right) p^2 = \sqrt{\frac{2}{m^3 \pi k_B^3 T^3}} \exp\left(-\frac{p^2}{2mk_B T}\right) p^2. \quad (5.190)$$

The speed distribution is therefore:

$$\rho(v) = \sqrt{\frac{2m^3}{\pi k_B^3 T^3}} \exp\left(-\frac{mv^2}{2k_B T}\right) v^2. \quad (5.191)$$

This is the *Maxwell distribution*. The maximum $v_{\max}$ is obtained from the condition

$$0 = 2ve^{-\frac{mv^2}{2k_B T}} - \frac{mv^3}{k_B T} e^{-\frac{mv^2}{2k_B T}} \Leftrightarrow v_{\max} = \sqrt{\frac{2k_B T}{m}}. \quad (5.192)$$

If you substitute the molar mass of dry air and 20° C for m , you get $v_{\max} \approx 4 \cdot 10^2$ m/s. The expected value of this distribution is

$$\bar{v} = \sqrt{\frac{2m^3}{\pi k_B^3 T^3}} \int_0^\infty e^{-\frac{mv^2}{2k_B T}} v^3 dv. \quad (5.193)$$

With $C = \frac{m}{2k_B T}$ in Eq. (A.108) follows

$$\bar{v} = \sqrt{\frac{2m^3}{\pi k_B^3 T^3}} \frac{2k_B^2 T^2}{m^2} = \sqrt{\frac{8k_B T}{\pi m}}. \quad (5.194)$$

The corresponding vector probability density is $\rho(\mathbf{v})$

$$\rho(\mathbf{v}) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right). \quad (5.195)$$

The expected value of the relative speed of two particles of the same mass is also important. This applies to this

$$\mathbf{v}_{\text{rel}} = \mathbf{v}_2 - \mathbf{v}_1. \quad (5.196)$$

For the probability density $\rho(\mathbf{v}_1, \mathbf{v}_2)$ of two particle velocities $\mathbf{v}_1, \mathbf{v}_2$ applies

$$\rho(\mathbf{v}_1, \mathbf{v}_2) = \left(\frac{m}{2\pi k_B T} \right)^3 \exp \left(-\frac{m(v_1^2 + v_2^2)}{2k_B T} \right). \quad (5.197)$$

This gives you the abbreviations

$$a := \left(\frac{m}{2\pi k_B T} \right)^{3/2}, \quad b := \frac{m}{2k_B T} \quad (5.198)$$

the relation

$$\begin{aligned} \rho(\mathbf{v}_{\text{rel}}) &= a^2 \int \exp \left[-b(v_1^2 + v_1^2 + v_{\text{rel}}^2 + 2\mathbf{v}_{1,x}v_{\text{rel},x} + 2\mathbf{v}_{1,y}v_{\text{rel},y} + 2\mathbf{v}_{1,z}v_{\text{rel},z}) \right] dv_1^3 \\ &= a^2 e^{-bv_{\text{rel}}^2} \int \exp \left[-2b(v_1^2 + v_{1,x}v_{\text{rel},x} + v_{1,y}v_{\text{rel},y} + v_{1,z}v_{\text{rel},z}) \right] dv_1^3 \\ &= a^2 e^{-bv_{\text{rel}}^2} \int \exp \left[-2b \left(\left(v_{1,x} + \frac{v_{\text{rel},x}}{2} \right)^2 + \dots - \frac{v_{\text{rel}}^2}{4} \right) \right] dv_1^3 \\ &= a^2 e^{-\frac{b}{2}v_{\text{rel}}^2} \int e^{-2bv_1^2} dv_1^3 = a e^{-\frac{b}{2}v_{\text{rel}}^2} \int a e^{-b(\sqrt{2}v_1)^2} dv_1^3 = a e^{-\frac{b}{2}v_{\text{rel}}^2} \frac{\mathbf{I}}{2^{3/2}}. \end{aligned} \quad (5.199)$$

The last step follows from the normalization of the distribution Eq. (5.195). This means that the probability density of the magnitude of the relative speed applies

$$\rho(v_{\text{rel}}) = \frac{4\pi a}{2^{3/2}} e^{-\frac{b}{2}v_{\text{rel}}^2} v_{\text{rel}}^2. \quad (5.200)$$

For the expected value follows

$$\overline{v_{\text{rel}}} = \int_0^\infty \frac{4\pi a}{2^{3/2}} e^{-\frac{b}{2}v_{\text{rel}}^2} v_{\text{rel}}^3 dv_{\text{rel}} = \sqrt{2} \int_0^\infty 4\pi a e^{-bv_{\text{rel}}^2} v_{\text{rel}}^3 dv_{\text{rel}} = \sqrt{2}\overline{v}. \quad (5.201)$$

5.4.0.2 Kinetic gas model

In a scattering experiment, a current density j (incident particles per area and time) falls on a target. If you multiply the current density by an area, you get a particle current. One defines the *effective cross section* σ by

$$j\sigma := \frac{dN_{\text{str}}}{dt}, \quad (5.202)$$

It therefore corresponds to the area on which particles are effectively scattered. This is now applied to a gas made of particles that are hard spheres of diameter d . It applies in this case

$$\sigma = \pi d^2. \quad (5.203)$$

A particle travels the path l , colliding with N particles:

$$N = n\sigma l \quad (5.204)$$

Here n is the particle density and σl is the volume of a cylinder with radius d in which collision partners are struck. For the *average rush hour* τ therefore applies

$$\mathbf{I} = n\sigma \overline{v_{\text{rel}}} \tau$$

$$\text{Glg. (5.201)} \quad \Leftrightarrow \quad \tau = \frac{\mathbf{I}}{\sqrt{2}n\sigma\overline{v}}. \quad (5.205)$$

For the mean free path λ follows

$$\lambda = \frac{1}{\sqrt{2}n\sigma}. \quad (5.206)$$

Inhomogeneous properties of a gas are equalized through transport processes. This will be understood here using a simple model; the values determined for the transport constants should be understood as estimates. So let q be any property of the gas. q depends only on z , $q = q(z)$. The velocity distribution is isotropic, which is represented here by the fact that just $1/6$ of all particles fly in each Cartesian coordinate direction. In doing so, they transport their properties on average with a length λ . This gives the current density j_z at $z = z_0$

$$j_z = \frac{\text{Transport}}{\text{Zeit x Fläche}} = \frac{1}{6} ((n\bar{v}q)(z_0 - \lambda) - (n\bar{v}q)(z_0 + \lambda)) \approx \frac{1}{6} \frac{\partial (n\bar{v}q)}{\partial z} (-2\lambda) = -\frac{\lambda}{3} \frac{\partial (n\bar{v}q)}{\partial z}. \quad (5.207)$$

This can be noted as:

$$j_z = -C \frac{\partial q}{\partial z}, \quad (5.208)$$

if one assumes that q is not correlated with other quantities. For $q = 1$ and homogeneous v one obtains *Diffusion*,

$$C \rightarrow D \approx \frac{\bar{v}\lambda}{3}, \quad (5.209)$$

D is the *diffusion constant*. With the continuity equation

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial z} (j_z) \quad (5.210)$$

follows the *diffusion equation*

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial z^2}. \quad (5.211)$$

or in 3D

$$\frac{\partial n}{\partial t} = D \Delta n. \quad (5.212)$$

If one sets $q = mu$ with u as the flow velocity in the x-direction, one examines the momentum current density. u is obtained by averaging the particle velocities, where $u \ll \bar{v}$ should apply.

$$\begin{aligned} j_z &= \frac{\text{Impuls}}{\text{Zeit x Fläche}} = \frac{1}{6} ((n\bar{v}mu)(z_0 - \lambda) - (n\bar{v}mu)(z_0 + \lambda)) \approx \frac{1}{6} \frac{\partial (n\bar{v}mu)}{\partial z} (-2\lambda) \\ &= -\frac{\lambda, mn\bar{v}}{3} \frac{\partial u}{\partial z}, \end{aligned} \quad (5.213)$$

where $\bar{v}$ and n are assumed to be homogeneous. If the velocity field $u(z)$ is between two horizontal plates, where the lower one is stationary and the upper one is moved with a constant, positive speed in the x-direction, then there must be a force per area A

$$\frac{F}{A} = \eta \frac{\partial u}{\partial z} \quad (5.214)$$

are spent to maintain the flow field. This equation defines the *dynamic viscosity* η . The horizontal momentum flows in the z-direction, which means that stationarity is the same

$$\eta \approx \frac{n\lambda\bar{v}m}{3}. \quad (5.215)$$

Internal friction in a fluid is therefore diffusive momentum transport due to viscosity. If c is the heat capacity per particle, cT is the heat energy per particle. If you set $q = cT$, you get

$$\begin{aligned} j_z &= \frac{\text{Wärme}}{\text{Zeit x Fläche}} = \frac{1}{6} ((n\bar{v}cT)(z_o - \lambda) - (n\bar{v}cT)(z_o + \lambda)) \approx \frac{1}{6} \frac{\partial (n\bar{v}cT)}{\partial z} (-2\lambda) \\ &= -\frac{\lambda cn\bar{v}}{3} \frac{\partial T}{\partial z}, \end{aligned} \quad (5.216)$$

The size

$$\kappa \approx \frac{\lambda \bar{v}}{3} \quad (5.217)$$

is called *temperature conductivity*, which is equal to the diffusion constant in the kinetic gas model. Therefore applies

$$j_z = -cn\kappa \frac{\partial T}{\partial z} \quad (5.218)$$

This can be done in three dimensions

$$\mathbf{j}_q = -\rho c_s \kappa \nabla T \quad (5.219)$$

generalize, where the heat capacity per particle c has been replaced by the specific heat capacity c_s . A formal continuity equation also applies to heat conduction, as long as heat conduction constitutes the only heat power density:

$$\frac{\partial (ncT)}{\partial t} + \nabla \cdot \mathbf{j}_q = 0 \quad (5.220)$$

This can be done too

$$\frac{\partial \tilde{I}}{\partial t} + \nabla \cdot \mathbf{j}_q = 0 \quad (5.221)$$

generalize, here $\tilde{I}$ is the internal energy density. This is the *heat conduction equation*. If n , c and κ are time and location dependent, Eq. (5.220) to

$$\frac{\partial T}{\partial t} = \kappa \Delta T. \quad (5.222)$$

5.4.1 Clausius-Clapeyron equation

A phase is a macroscopic manifestation of matter, for example solid, liquid or gaseous. However, even within a solid there can be different phases that differ, for example, in their magnetic properties or lattice structures. First of all, a two-phase equilibrium is assumed, for example consisting of liquid water and water vapor. The liquid phase is denoted by 1, the gaseous phase by 2. The entire system is in thermodynamic equilibrium, so that (p, T) is the same in both systems. The subsystems are open, so particle exchange takes place. The equilibrium condition according to Eq. (5.54) is then

$$\mu_1(T, p) = \mu_2(T, p), \quad (5.223)$$

where μ denotes the chemical potential. We are now interested in the pressure $p_S(T)$ at which both phases coexist. This means

$$\mu_1(T, p_S(T)) = \mu_2(T, p_S(T)). \quad (5.224)$$

This is an implicit equation to the unknown function $p_S(T)$. The equation is completely differentiated according to T :

$$\frac{\partial \mu_1(T, p)}{\partial T} + \frac{\partial \mu_1(T, p)}{\partial p} \frac{dp_S(T)}{dT} = \frac{\partial \mu_2(T, p)}{\partial T} + \frac{\partial \mu_2(T, p)}{\partial p} \frac{dp_S(T)}{dT} \quad (5.225)$$

Now insert the equations (5.105) and (5.107):

$$-\frac{S_1}{N_1} + \frac{V_1}{N_1} \frac{dp_S}{dT} = -\frac{S_2}{N_2} + \frac{V_2}{N_2} \frac{dp_S}{dT} \quad (5.226)$$

It applies to a state variable Z

$$\frac{Z_i}{N_i} = \frac{Z_i}{m_i} \frac{m_i}{N_i} = z_i M_i \quad (5.227)$$

with mass m_i and specific size

$$z_i := \frac{Z_i}{m_i}. \quad (5.228)$$

This results in the definitions $\Delta s := s_2 - s_1$ and $\Delta v := v_2 - v_1$

$$\Delta s = \Delta v \frac{dp_S}{dT}. \quad (5.229)$$

You can also get the specific phase transition heat

$$c := T \Delta s \quad (5.230)$$

use:

$$\boxed{\frac{dp_S}{dT} = \frac{c}{T \Delta v}} \quad (5.231)$$

This is the *Clausius-Clapeyron equation*. This equation can be solved exactly for simple functions $c = c(T)$. For the volume per particle v applies

$$v = \frac{V}{N} = \frac{V}{n N_A} = \frac{VM}{M n N_A} = \frac{M}{N_A \rho}, \quad (5.232)$$

This can be applied to a liquid, for example, with the density $\rho = \rho_l$. For an ideal gas applies

$$v = \frac{R_s T}{p} = \frac{R_s T}{p_S}, \quad (5.233)$$

thus follows

$$T \Delta v = \frac{R_s T^2}{p_S} - \frac{MT}{N_A \rho_l} \Rightarrow \frac{1}{T \Delta v} = \frac{p_S N_A \rho_l}{N_A \rho_l R_s T^2 - p_S MT}. \quad (5.234)$$

Thus, one can note in the case of a liquid and an ideal gas

$$\frac{dp_S}{dT} = \frac{c p_S N_A \rho_l}{N_A \rho_l R_s T^2 - p_S MT}. \quad (5.235)$$

In meteorology the approximation is often used

$$T\Delta v \approx \frac{R_s T^2}{p_S} \quad (5.236)$$

made so that follows

$$\frac{1}{p_S} \frac{dp_S}{dT} = \frac{c}{R_s T^2}. \quad (5.237)$$

In the case of a temperature-independent phase transition enthalpy c , this can be solved analytically, in which case the following applies

$$p_S = p_S(T) = k \exp\left(-\frac{T_o}{T}\right), \quad (5.238)$$

because that follows

$$\frac{dp_S}{dT} = \frac{T_o}{T^2} p_S. \quad (5.239)$$

This implies

$$T_o = \frac{c}{R_s}, \quad (5.240)$$

the constant k remains undetermined at this point.

With regard to the atmosphere, the saturation vapor pressure curve of water is of particular interest. Since the heat of vaporization or sublimation of water is temperature-dependent in a way that cannot be precisely determined analytically, there is no exact expression for the saturation vapor pressure curve for water. The formulas recommended in [16] can help here. Above liquid water, $T \in [-45, 60]^\circ \text{C}$

$$e(t) = 6,112 \exp\left(\frac{17,62t}{243,12 + t}\right), \quad (5.241)$$

over ice holds for $T \in [-65, 0]^\circ \text{C}$

$$e(t) = 6,112 \exp\left(\frac{22,46t}{272,62 + t}\right), \quad (5.242)$$

where t denotes the temperature in $^\circ \text{C}$ and e denotes the respective saturation vapor pressure in hPa.

5.4.2 Osmotic pressure

We assume a solution of a substance B in a substance A , where the substances do not interact with each other. The partition function Ω of the system then holds:

$$\Omega = \Omega_A \Omega_B. \quad (5.243)$$

For the entropy S of the system follows

$$S = k_B \ln(\Omega) = k_B \ln(\Omega_A \Omega_B) = k_B \ln(\Omega_A) + k_B \ln(\Omega_B). \quad (5.244)$$

From Eq. (5.142) follows

$$\Omega_B \propto V^{N_B} \Rightarrow S = S_A + k_B N_B \ln(V) + f(E, N_B) \quad (5.245)$$

with a function $f = f(E, N_B)$, which does not depend on the volume. For the pressure p of the system follows

$$p \stackrel{\text{Glg. (5.46)}}{=} T \left(\frac{\partial S}{\partial V} \right)_E = T \left(\frac{\partial S_A}{\partial V} \right)_E + T \frac{k_B N_B}{V} = p_A + T \frac{k_B N_B}{V} =: p_A + p_{\text{osm}}. \quad (5.246)$$

The pressure difference p_{osm} compared to the pure phase A is called *osmotic pressure*, for which the following applies

$$p_{\text{osm}} = k_B T n_B \quad (5.247)$$

with the concentration $n_B := \frac{N_B}{V}$ of the solute. Eq. (5.247) is called *van't Hoff's law*.

5.4.3 Vapor pressure over a solution

At a given pressure p , the phase transition occurs at a temperature T_s between phase A , which is liquid (e.g. water), and phase C , which is gaseous or solid. This is described by a function $p_S = p_S(T_s)$, which solves the Clausius-Clapeyron equation Eq. (5.231) is. If you now dissolve a substance B in A (e.g. salt), which is limited to A , T_s shifts by ΔT_s . Designate

$$c := \frac{N_B}{N_A} = \frac{N_B/V}{N_A/V} = \frac{n_B}{n_A} \quad (5.248)$$

as the ratio of solute and solvent concentrations. For the chemical potential $\mu_A = \mu_A(T, p_A)$ applies

$$\begin{aligned} \mu_A(T, p_A) &= \mu_A(T, p - p_{\text{osm}}) \stackrel{p_{\text{osm}} \ll p}{\approx} \mu_A(T, p) - p_{\text{osm}} \left(\frac{\partial \mu}{\partial p} \right)_T \stackrel{\text{Glg. (5.247)}}{=} \mu_A(T, p) - k_B T n_B \left(\frac{\partial \mu}{\partial p} \right)_T \\ &\stackrel{\text{Glg. (5.108)}}{=} \mu_A(T, p) - k_B T n_B \frac{V}{N_A} = \mu_A(T, p) - c k_B T. \end{aligned} \quad (5.249)$$

Within the solution applies

$$\mu_{A,B}(T, p) = \mu_A(T, p_A) \stackrel{\text{Glg. (5.249)}}{\approx} \mu_A(T, p) - c k_B T. \quad (5.250)$$

Now an equilibrium condition is needed. Since we are dealing with particle exchange, the chemical potential of the solution A , B must be equated with that of the other phase C :

$$\begin{aligned} \mu_{A,B}(T, p) &= \mu_C(T, p) \\ T=T_s \pm \Delta T_s \quad \mu_{A,B}(T_s + \Delta T_s, p) &= \mu_C(T_s + \Delta T_s, p) \\ \text{Glg. (5.249)} \quad \mu_A(T_s + \Delta T_s, p) - c k_B T &= \mu_C(T_s + \Delta T_s, p) \end{aligned} \quad (5.251)$$

From Eq. (5.128) follows

$$\left(\frac{\partial \mu_A}{\partial T} \right)_p = -s_A, \quad (5.252)$$

What

$$\mu_A(T_s + \Delta T_s, p) \approx \mu_A(T_s, p) - s_A \Delta T_s \quad (5.253)$$

implied. The same applies to phase C

$$\mu_C(T_s + \Delta T_s, p) = \mu_C(T_s, p) - s_C \Delta T_s. \quad (5.254)$$

Putting the last two equations into Eq. (5.251), you get

$$\mu_A(T_s, p) - s_A \Delta T_s - ck_B T_s = \mu_C(T_s, p) - s_C \Delta T_s. \quad (5.255)$$

In the last step, a small term $ck_B \Delta T_s$ was omitted. At $c = 0$ applies

$$\mu_A(T_s, p) = \mu_C(T_s, p), \quad (5.256)$$

which corresponds to the phase boundary in the absence of the solute. Thus follows

$$\begin{aligned} -s_A \Delta T_s - ck_B T_s &= -s_C \Delta T_s \\ \Leftrightarrow \Delta T_s &= c \frac{k_B T_s}{s_C - s_A}. \end{aligned} \quad (5.257)$$

For the entropy difference applies

$$s_C - s_A = \frac{L_{A \rightarrow C}}{T_s}, \quad (5.258)$$

here $L_{A \rightarrow C}$ is the phase transition enthalpy in the transition from A to C . Thus you get

$$\Delta T_s = c \frac{k_B T_s^2}{L_{A \rightarrow C}}. \quad (5.259)$$

Two cases can be distinguished here:

- C is gaseous: This implies $L_{A \rightarrow C} > 0$, which in turn leads to $\Delta T_s > 0$, which corresponds to a boiling point increase. This is the case, for example, over the ocean surface.
- C is fixed: This implies $L_{A \rightarrow C} < 0$, which in turn leads to $\Delta T_s < 0$, which corresponds to a freezing point depression. This reduces the freezing point of ocean water to below zero degrees Celsius.

Instead of the change in boiling or freezing point, the influence of a solution on the saturation vapor pressure can also be determined. Instead of Eq. (5.251) For this you start with (5.260)

$$\mu_A(T, p_s + \Delta p_s) - ck_B T = \mu_C(T, p_s + \Delta p_s) \quad (5.260)$$

From Eq. (5.128) follows

$$\left(\frac{\partial \mu_A}{\partial p} \right)_T = v_A, \quad (5.261)$$

What

$$\mu_A(T, p_s + \Delta p_s) = \mu_A(T, p_s) + \int_{p_s}^{p_s + \Delta p_s} \left(\frac{\partial \mu_A}{\partial p} \right)_T dp = \mu_A(T, p_s) + \int_{p_s}^{p_s + \Delta p_s} v_A dp \quad (5.262)$$

implied. The same applies to phase C

$$\mu_C(T, p_s + \Delta p_s) = \mu_C(T, p_s) + \int_{p_s}^{p_s + \Delta p_s} \left(\frac{\partial \mu_C}{\partial p} \right)_T dp = \mu_C(T, p_s) + \int_{p_s}^{p_s + \Delta p_s} v_C dp. \quad (5.263)$$

Putting the last two equations into Eq. (5.260), you get

$$\mu_A(T, p_s) + \int_{p_s}^{p_s + \Delta p_s} v_A dp - ck_B T = \mu_C(T, p_s) + \int_{p_s}^{p_s + \Delta p_s} v_C dp. \quad (5.264)$$

Analogous to Eq. (5.256) applies

$$\mu_A(T, p_s) = \mu_C(T, p_s), \quad (5.265)$$

it follows from this

$$\int_{p_s}^{p_s+\Delta p_s} v_A dp - ck_B T = \int_{p_s}^{p_s+\Delta p_s} v_C dp \Rightarrow \int_{p_s}^{p_s+\Delta p_s} \frac{dp}{n_A} - ck_B T = \int_{p_s}^{p_s+\Delta p_s} \frac{dp_s}{n_C}. \quad (5.266)$$

In this case, since A is liquid and C is gas, $n_A \gg n_C$, which applies

$$-ck_B T \approx \int_{p_s}^{p_s+\Delta p_s} \frac{dp}{n_C} \quad (5.267)$$

leads. With the equation of state of ideal gases follows

$$-ck_B T = k_B T \int_{p_s}^{p_s+\Delta p_s} \frac{dp}{p_s} = k_B T \ln \left(\frac{p_s + \Delta p_s}{p_s} \right)$$

$$\Leftrightarrow \ln \left(\frac{p_s + \Delta p_s}{p_s} \right) = -c. \quad (5.268)$$

In the case of small concentrations $c \ll 1$ one obtains approximately

$$\frac{\Delta p_s}{p_s} = -c, \quad (5.269)$$

which is called *Raoult's law*.

5.4.4 Boltzmann equation

This section aims to establish a connection between statistical physics and hydrodynamics. The central factor here is function

$$f = f(\mathbf{r}, \mathbf{v}, t), \quad (5.270)$$

this is the probability density for encountering particles at time t in the phase space volume at $\mathbf{r}, \mathbf{v}$, where:

$$N = \int_{\mathbb{R}^6} f(\mathbf{r}, \mathbf{v}, t) d^3 v d^3 r \quad (5.271)$$

with N as the particle number. The total derivative of f is $\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} \right) f(\mathbf{r}, \mathbf{v}, t)$, which Equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} \right) f(\mathbf{r}, \mathbf{v}, t) = 0 \quad (5.272)$$

is called *shockless Boltzmann equation*. Here $\frac{D\mathbf{v}}{Dt} = \frac{\mathbf{F}}{m}$ with $\mathbf{F}$ as the sum of external forces (electromagnetic field, gravity, apparent forces) was used. Internal interactions caused by particle collisions (pressure gradient acceleration, viscosity) have not yet been taken into account; a term F_{int} is used for them. This term will now be developed step by step. He should describe how

1. particles are scattered into a small phase space volume at $(\mathbf{r}, \mathbf{v})$,
2. particles are scattered out of a small phase space volume at $(\mathbf{r}, \mathbf{v})$.

First, it is expected that F_{int} is an integral over all velocities:

$$F_{\text{int}} = \int_{\mathbb{R}^3} \dots d^3 v_i \quad (5.273)$$

A position integral is not useful because collisions only take place locally. Furthermore, it is expected that the loss of particles in the phase space volume $(\mathbf{r}, \mathbf{v})$ is proportional to $f(\mathbf{r}, \mathbf{v}, t)$, i.e

$$F_{\text{int}} = \int_{\mathbb{R}^3} -f(\mathbf{r}, \mathbf{v}, t) + \dots d^3 v_i \quad (5.274)$$

At the point $\mathbf{v}_i$, collisions with particles in a small phase space volume at $(\mathbf{r}, \mathbf{v}_i)$ are considered, so one continues

$$F_{\text{int}} = \int_{\mathbb{R}^3} -f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_i, t) + \dots d^3 v_i. \quad (5.275)$$

The number of collisions per time is proportional to the relative velocity $\mathbf{V} := \mathbf{v} - \mathbf{v}_i$, one obtains

$$F_{\text{int}} = \int_{\mathbb{R}^3} -f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_i, t) |\mathbf{V}| + \dots d^3 v_i. \quad (5.276)$$

The current density itself is not enough to determine the number of scattering processes per time: if all particles are ideal mass points, for example, there will be no collisions at all. This is described by the cross section σ , which is why we use it

$$F_{\text{int}} = \int_{\mathbb{R}^3} -f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_i, t) |\mathbf{V}| \sigma + \dots d^3 v_i. \quad (5.277)$$

The velocities of the particles before the collision are $\mathbf{v}$ and $\mathbf{v}_i$, those after the collision are denoted by $\mathbf{v}'$ and $\mathbf{v}'_i$. One further defines the relative velocity after the collision by $\mathbf{V}' := \mathbf{v}'_i - \mathbf{v}'$, where $|\mathbf{V}| \text{ applies} = |\mathbf{V}'|$. Denote by Ω the solid angle between $\mathbf{V}$ and $\mathbf{V}'$. Particles are scattered into the solid angle element $d\Omega$ in proportion to $\frac{d\sigma}{d\Omega} d\Omega$, this leads to

$$F_{\text{int}} = \int_{\mathbb{R}^3} \int_{\Omega} -f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_i, t) |\mathbf{V}| \frac{d\sigma}{d\Omega} d\Omega + \dots d^3 v_i. \quad (5.278)$$

Analogously, a scattering process from $\mathbf{v}'$ and $\mathbf{v}'_i$ to $\mathbf{v}$ and $\mathbf{v}_i$ takes place, this shows

$$F_{\text{int}} = \int_{\mathbb{R}^3} \int_{\Omega} [f(\mathbf{r}, \mathbf{v}', t) f(\mathbf{r}, \mathbf{v}'_i, t) - f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_i, t)] |\mathbf{V}| \frac{d\sigma}{d\Omega} d\Omega d^3 v_i. \quad (5.279)$$

The sizes $\mathbf{v}'$ and $\mathbf{v}'_i$ are determined by the scattering problem $(\mathbf{v}, \mathbf{v}_i, \Omega)$ as well as conservation of momentum and energy). If you write this on the right side of Eq. (5.272), you get

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} \right) f(\mathbf{r}, \mathbf{v}, t) \\ &= \int_{\mathbb{R}^3} \int_{\Omega} [f(\mathbf{r}, \mathbf{v}', t) f(\mathbf{r}, \mathbf{v}'_i, t) - f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_i, t)] |\mathbf{V}| \frac{d\sigma}{d\Omega} d\Omega d^3 v_i. \end{aligned} \quad (5.280)$$

This is the Boltzmann equation. This can be used as a classical analogue of the master equation Eq. (15.137) can be understood. It is important to note that no assumptions were made about the nature of the interactions that lead to the collisions. This is implicit in the cross section $\frac{d\sigma}{d\Omega}$.

The central quantities of hydrodynamics can be written in terms of f :

$$\begin{aligned}
N &= \int_{\mathbb{R}^6} f(\mathbf{r}, \mathbf{v}', t) d^3 v' d^3 r \stackrel{!}{=} \int_{\mathbb{R}^3} n(\mathbf{r}, t) d^3 v' \Rightarrow n(\mathbf{r}, t) = \int_{\mathbb{R}^3} f(\mathbf{r}, \mathbf{v}', t) d^3 v', \\
\rho(\mathbf{r}, t) &= mn(\mathbf{r}, t) = \int_{\mathbb{R}^3} mf(\mathbf{r}, \mathbf{v}', t) d^3 v', \\
\rho(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t) &= \int_{\mathbb{R}^3} mf(\mathbf{r}, \mathbf{v}', t) \mathbf{v}' d^3 v', \\
\mathbf{v}(\mathbf{r}, t) &= \frac{\rho(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)}{\rho(\mathbf{r}, t)} = \frac{\int_{\mathbb{R}^3} mf(\mathbf{r}, \mathbf{v}', t) \mathbf{v}' d^3 v'}{\int_{\mathbb{R}^3} mf(\mathbf{r}, \mathbf{v}', t) d^3 v'} = \frac{\int_{\mathbb{R}^3} f(\mathbf{r}, \mathbf{v}', t) \mathbf{v}' d^3 v'}{\int_{\mathbb{R}^3} f(\mathbf{r}, \mathbf{v}', t) d^3 v'}
\end{aligned} \tag{5.281}$$

5.5 capillarity

Imagine an interface A that coincides with the $\mathbb{R}^2$. If you expand this by a factor $d\varepsilon$ in the x-direction, you can see this as an execution of the figure

$$(x, y)^T \mapsto (x(1 + d\varepsilon), y)^T \tag{5.282}$$

interpret. The energy of the system decreases

$$dU = A\sigma d\varepsilon \tag{5.283}$$

to, here the proportionality constant σ is the *mechanical surface tension*. It applies

$$\sigma = \frac{1}{A} \frac{dU}{d\varepsilon}. \tag{5.284}$$

Now imagine a cylindrical disk with a radius r and an opening angle φ , which lies on the $\mathbb{R}^2$:

$$Z := \left\{ (x, y, z)^T \in \mathbb{R}^3 \mid |x| \leq r \sin(\varphi) \wedge 0 \leq z \leq \sqrt{r^2 - x^2} - r(1 - \cos(\varphi)) \right\} \tag{5.285}$$

The force acts on a surface element $dA = r \sin(\varphi) dy$ in the z-direction

$$F_z = -2dy\sigma \sin(\varphi). \tag{5.286}$$

In this case, the sign of r is **negative**, the *capillary pressure* p_r built up by F_z is positive. Therefore applies

$$p_r = -\frac{\sigma}{r}. \tag{5.287}$$

With Eq. (B.43) follows η in the case of a surface deflection

$$p_k \approx -\sigma \frac{\partial^2 \eta}{\partial x^2}. \tag{5.288}$$

So far only the curvature in one spatial direction has been considered. If you take both into account, it turns out

$$p_r = -\frac{2\sigma}{r}. \tag{5.289}$$

5.5.1 Kelvin equation

Until now it was assumed that the phase boundary was flat or that the surface tension was zero. In general, the equilibrium condition is Eq. (5.223) depends on the radius R of the interface:

$$\mu_1(R, T, V) = \mu_2(R, T, V) \quad (5.290)$$

Here the dependency on p was replaced by a dependency on V . In the further course of the derivation, only R is included as an argument, since T and V are considered constant. For the particle density $n = N/V$, according to Eq. (5.111)

$$n = \left(\frac{\partial p}{\partial \mu} \right)_{T, V} \stackrel{T, V \text{ const.}}{\Rightarrow} d\mu = \frac{dp}{n}. \quad (5.291)$$

Eq. (5.290) is implied

$$\begin{aligned} \mu_1(R) - \mu_1(\infty) &= \mu_2(R) - \mu_2(\infty) \\ \Leftrightarrow \int_{\infty}^R \frac{d\mu_1(r)}{dr} dr &= \int_{\infty}^R \frac{d\mu_2(r)}{dr} dr. \end{aligned} \quad (5.292)$$

This is now substituted to $p_i = p_i(r_i)$:

$$\begin{aligned} \int_{p_1(\infty)}^{p_1(R)} \frac{d\mu_1(r_1(p_1))}{dr_1} \frac{dr_1}{dp_1} dp_1 &= \int_{p_2(\infty)}^{p_2(R)} \frac{d\mu_2(r_2(p_2))}{dr_2} \frac{dr_2}{dp_2} dp_2 \\ \Leftrightarrow \int_{p_1(\infty)}^{p_1(R)} \frac{d\mu_1(p_1)}{dp_1} dp_1 &= \int_{p_2(\infty)}^{p_2(R)} \frac{d\mu_2(p_2)}{dp_2} dp_2 \end{aligned} \quad (5.293)$$

It applies

$$p_1(\infty) = p_2(\infty) = p_S. \quad (5.294)$$

1 again denotes the liquid phase and 2 the gas phase. You define

$$p_R := p_2(R). \quad (5.295)$$

With Eq. (5.289) follows

$$p_1(R) = p_R + \frac{2\gamma}{R}. \quad (5.296)$$

Thus you get

$$\int_{p_S}^{p_R + \frac{2\gamma}{R}} \frac{d\mu_1(p_1)}{dp_1} dp_1 = \int_{p_S}^{p_R} \frac{d\mu_2(p_2)}{dp_2} dp_2. \quad (5.297)$$

If you put Eq. (5.291), follows

$$\int_{p_S}^{p_R + \frac{2\gamma}{R}} \frac{1}{n_1(p_1)} dp_1 = \int_{p_S}^{p_R} \frac{1}{n_2(p_2)} dp_2. \quad (5.298)$$

If the liquid phase is assumed to be incompressible, $n_l = n_l > 0$ is constantly independent of p . With the equation of state of ideal gases $p_2 = n_2 k_B T$ follows

$$\begin{aligned} \frac{p_R + \frac{2\gamma}{R} - p_S}{n_l} &= k_B T \int_{p_S}^{p_R} \frac{1}{p_2} dp_2 = k_B T \ln \left(\frac{p_R}{p_S} \right) \\ \Leftrightarrow \frac{N_A}{M} k_B T \ln \left(\frac{p_R}{p_S} \right) &= \frac{N_A}{M} \frac{p_R + \frac{2\gamma}{R} - p_S}{n_l} \\ \Leftrightarrow R_s T \ln \left(\frac{p_R}{p_S} \right) &= \frac{N_A}{M} \frac{p_R + \frac{2\gamma}{R} - p_S}{n_l}, \end{aligned} \quad (5.299)$$

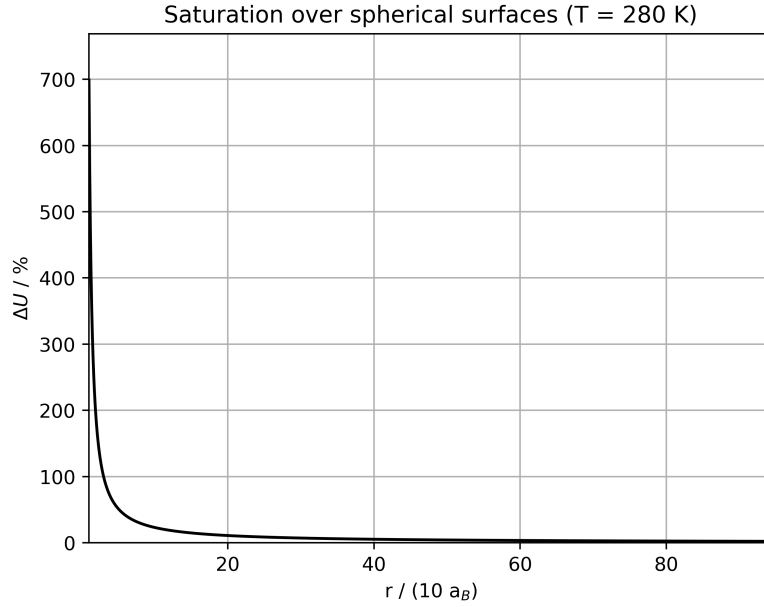


Figure 5.1: Difference between the saturation moisture over a curved surface and over a flat surface using water as an example.

where M is the molar mass of the substance under consideration. Assuming

$$\frac{2\gamma}{R} \gg p_R - p_S \quad (5.300)$$

This results in the *Kelvin equation*

$$\ln \left(\frac{p_R}{p_S} \right) = \frac{2\gamma}{R_s T R \rho_l}. \quad (5.301)$$

The size

$$\Delta U := \frac{p_R}{p_S} - 1 = \exp \left(\frac{2\gamma}{R_s T R \rho_l} \right) - 1 \geq 0 \quad (5.302)$$

is the saturation moisture over a curved surface relative to the saturation moisture over a flat surface. Fig. 5.1 illustrates this using H_2O as an example.

5.6 Photon gas

Imagine a cavity of temperature T in equilibrium with electromagnetic radiation. We are looking for the spectral energy density $u(\omega)$ in the cavity. The properties of electromagnetic waves were discussed in Sect. 3.3. These are transverse waves. If the wave vector points in the z direction, $\mathbf{k} = k\mathbf{e}_z$, this follows for the electric field in the case of standing waves

$$\mathbf{E}(z, t) = (E_{o,x}\mathbf{e}_x + E_{o,y}\mathbf{e}_y) \sin(kz) \sin(\omega t). \quad (5.303)$$

Any phases were neglected. The B field can be determined from this. The cavity is cubic with volume $V = L^3$, and the walls are metallic. In this case, the parallel component of the electric field disappears at the surface, otherwise currents would be excited and energy would be dissipated. From this follow the discrete k -values

$$k_i L = i\pi \Leftrightarrow k_i = \frac{\pi}{L} i \quad (5.304)$$

with $i \in \mathbb{N}$ and $i \geq 1$, negative values of i must be neglected because this does not result in new solutions. Sums over k_i values can again be replaced by integrals:

$$\sum_{k_i} \dots = \frac{L}{\pi} \int_0^\infty \dots dk = \frac{L}{2\pi} \int_{-\infty}^\infty \dots dk. \quad (5.305)$$

For a sum over all modes in the cavity applies

$$\sum_{m=1}^2 \sum_{\mathbf{k}} \dots = 2 \sum_{\mathbf{k}} \dots = 2 \left(\frac{L}{2\pi} \right)^3 \int \dots d^3 k = \frac{2V}{(2\pi)^3} \int \dots d^3 k. \quad (5.306)$$

m runs over the two possible polarization directions. For the energies $E = E(\mathbf{k}, m)$, according to Eq. (4.6)

$$E(\mathbf{k}, m) = \hbar\omega(k) = \hbar ck. \quad (5.307)$$

A microstate r of the system is given by the population numbers

$$r = (n_{\mathbf{k},m}) \quad (5.308)$$

given, i.e. the number of excitations for each vibration mode, one excitation is one photon. The energy of the microstate is $E_r(V)$

$$E_r(V) = \sum_{m,\mathbf{k}} \hbar\omega(k) n_{\mathbf{k},m} = \hbar c \sum_{m,\mathbf{k}} k n_{\mathbf{k},m}. \quad (5.309)$$

Now the average occupation numbers $\bar{n}_{\mathbf{k},m}$ have to be determined. For this we start from the grand canonical partition function of a system without a polarization degree of freedom, i.e. $m = 1$:

$$\begin{aligned} Y &= \sum_r \exp[-\beta(E_r - \mu N_r)] = \sum_{n_{\mathbf{p}_1}=0}^{\infty} \exp[-\beta(E_{\mathbf{p}_1} - \mu) n_{\mathbf{p}_1}] \cdot \sum_{n_{\mathbf{p}_2}=0}^{\infty} \exp[-\beta(E_{\mathbf{p}_2} - \mu) n_{\mathbf{p}_2}] \cdot \dots \\ &\stackrel{\text{Glg. (A.8)}}{=} \prod_{\mathbf{p}} \frac{1}{1 - \exp(-\beta(E_{\mathbf{p}} - \mu))}. \end{aligned} \quad (5.310)$$

It follows

$$\begin{aligned} \bar{n}_{\mathbf{p}_i} &= \frac{1}{Y} \sum_r n_{\mathbf{p}_i} \exp[-\beta(E_r - \mu N_r)] = \frac{1}{Y} \sum_{n_{\mathbf{p}_1}=0}^{\infty} \dots \sum_{n_{\mathbf{p}_i}=0}^{\infty} \dots n_{\mathbf{p}_i} \exp[-\beta(E_{\mathbf{p}_i} - \mu) n_{\mathbf{p}_i}] \dots \\ &= \frac{1}{Y} \sum_{n_{\mathbf{p}_1}=0}^{\infty} \dots \left(\frac{1}{\beta} \frac{\partial}{\partial \mu} \sum_{n_{\mathbf{p}_i}=0}^{\infty} \exp[-\beta(E_{\mathbf{p}_i} - \mu) n_{\mathbf{p}_i}] \right) \dots = \frac{1}{Y} \sum_{n_{\mathbf{p}_1}=0}^{\infty} \dots \left(\frac{1}{\beta} \frac{\partial}{\partial \mu} \frac{1}{1 - \exp[-\beta(E_{\mathbf{p}_i} - \mu)]} \right) \dots \\ &= \frac{1}{Y} \sum_{n_{\mathbf{p}_1}=0}^{\infty} \dots \left(\frac{\exp[-\beta(E_{\mathbf{p}_i} - \mu)]}{(1 - \exp[-\beta(E_{\mathbf{p}_i} - \mu)])^2} \right) \dots = \frac{\exp[-\beta(E_{\mathbf{p}_i} - \mu)]}{1 - \exp[-\beta(E_{\mathbf{p}_i} - \mu)]}. \end{aligned} \quad (5.311)$$

This is the *Bose distribution*, it applies to particles with integer spin:

$$\boxed{\bar{n}_{\mathbf{p}} = \frac{1}{e^{\beta(E_{\mathbf{p}} - \mu)} - 1}} \quad (5.312)$$

The energy eigenvalues $E_r(V)$ do not depend on the number of phonons N , so the following applies

$$\mu = \frac{\overline{\partial E_r(V)}}{\partial N} = 0, \quad (5.313)$$

the chemical potential disappears. Therefore applies

$$\bar{n}_{\mathbf{k},m} = \frac{1}{\exp(\beta E_k) - 1}. \quad (5.314)$$

It follows

$$\begin{aligned} E(T, V) = \overline{E_r(T, V)} &= \sum_{m,\mathbf{k}} E_k \bar{n}_k = \frac{2V}{(2\pi)^3} \int \frac{\hbar c k}{\exp(\beta \hbar c k) - 1} d^3 k = \frac{2V}{(2\pi)^3} 4\pi \int_0^\infty \frac{\hbar c k^3}{\exp(\beta \hbar c k) - 1} dk \\ &= V \int_0^\infty \underbrace{\frac{\hbar}{c^3 \pi^2} \frac{\omega^3}{\exp(\beta \hbar \omega) - 1}}_{=u(\omega)} d\omega. \end{aligned} \quad (5.315)$$

$$u(\omega) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1}. \quad (5.316)$$

This is the *Planck's radiation law*. The ideas in this section are very specific, but Planck's distribution always applies when matter of temperature T is in equilibrium with electromagnetic radiation. This equilibrium can always be assumed due to the high speed of the waves (speed of light). However, there may be deviations in the spectrum, such as absorption lines. Within a cavity in thermal equilibrium, the radiation is isotropic, so the spectral radiance applies

$$J(\omega) = \frac{u(\omega)}{4\pi} c = \frac{\hbar}{4\pi^3 c^2} \frac{\omega^3}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1}. \quad (5.317)$$

The spectral intensity $I(\omega)$ of a radiating surface is calculated from this:

$$I(\omega) = \int_{\vartheta=0}^{\pi/2} \int_{\varphi=0}^{2\pi} J(\omega) \cos(\vartheta) \sin(\vartheta) d\vartheta d\varphi = 2\pi \frac{1}{2} J(\omega) = \frac{\hbar}{4\pi^2 c^2} \frac{\omega^3}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1}. \quad (5.318)$$

If you integrate this over the entire spectrum, the radiated power density follows

$$\frac{P}{A} = \int_0^\infty I(\omega) d\omega = \frac{\hbar}{4\pi^2 c^2} \int_0^\infty \frac{\omega^3}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1} d\omega = \frac{k_B^4 T^4}{4\pi^2 c^2 \hbar^3} \int_0^\infty \frac{x^3}{e^x - 1} dx \quad (5.319)$$

With Eq. (A.99) follows

$$P = P(T) = \frac{k_B^4 \pi^2}{60 c^2 \hbar^3} T^4. \quad (5.320)$$

This is the *Stefan-Boltzmann law*, is defined

$$\sigma := \frac{k_B^4 \pi^2}{60 c^2 \hbar^3} \quad (5.321)$$

as the *Stefan-Boltzmann constant*. Real bodies emit at a temperature T in the direction specified by ϑ and φ at an angular frequency ω a factor of $J(\omega, T)$

$$\varepsilon = \varepsilon(\omega, T, \vartheta, \varphi) \quad (5.322)$$

different spectral radiance:

$$J_{\text{real}}(\omega, T, \vartheta, \varphi) = \varepsilon(\omega, T, \vartheta, \varphi) J(\omega, T). \quad (5.323)$$

The factor ε is called *emissivity*. Imagine a small area dA on the inner surface of the cavity. This area absorbs a power density

$$\frac{dP_{\text{abs}}}{dA} = \int_{\omega=0}^{\infty} \int_{\vartheta=0}^{\pi/2} \int_{\varphi=0}^{2\pi} a(\omega, T, \vartheta, \varphi) J(\omega, T) \cos(\vartheta) \sin(\vartheta) d\varphi d\vartheta d\omega, \quad (5.324)$$

Here the absorption coefficient $a(\omega, T, \vartheta, \varphi)$ was introduced. Since a thermodynamic equilibrium is assumed, the emitted power density applies

$$\frac{dP_{\text{emt}}}{dA} = \int_{\omega=0}^{\infty} \int_{\vartheta=0}^{\pi/2} \int_{\varphi=0}^{2\pi} \varepsilon(\omega, T, \vartheta, \varphi) J(\omega, T) \cos(\vartheta) \sin(\vartheta) d\varphi d\vartheta d\omega = \frac{dP_{\text{abs}}}{dA}. \quad (5.325)$$

It follows

$$\int_{\omega=0}^{\infty} \int_{\vartheta=0}^{\pi/2} \int_{\varphi=0}^{2\pi} (\varepsilon(\omega, T, \vartheta, \varphi) - a(\omega, T, \vartheta, \varphi)) J(\omega, T) \cos(\vartheta) \sin(\vartheta) d\varphi d\vartheta d\omega = 0. \quad (5.326)$$

Since the spectral energy density of the cavity is constant, even

$$\int_{\vartheta=0}^{\pi/2} \int_{\varphi=0}^{2\pi} [\varepsilon(\omega, T, \vartheta, \varphi) - a(\omega, T, \vartheta, \varphi)] \sin(\vartheta) \cos(\vartheta) d\varphi d\vartheta = 0. \quad (5.327)$$

You define it

$$\varepsilon(\omega, T) := \int_{\vartheta=0}^{\pi/2} \int_{\varphi=0}^{2\pi} \varepsilon(\omega, T, \vartheta, \varphi) \sin(\vartheta) \cos(\vartheta) d\varphi d\vartheta. \quad (5.328)$$

and analogously for the absorption coefficient, follows

$$\varepsilon(\omega, T) = a(\omega, T). \quad (5.329)$$

Now we look specifically at the direction given by ϑ and φ . Here dA is the spectral radiance

$$\begin{aligned} J_{\text{out}}(\omega, T) &= J(\omega, T) \\ &= J(\omega, T) \left(\varepsilon(\omega, T, \vartheta, \varphi) + \int_{\varphi'=0}^{2\pi} \int_{\vartheta'=0}^{\pi/2} s(\vartheta', \varphi', \vartheta, \varphi, \omega, T) \cos(\vartheta') \sin(\vartheta') d\vartheta' d\varphi' \right) \end{aligned} \quad (5.330)$$

out of. The expression in brackets results in one. The *scattering cross section* $s(\vartheta', \varphi', \vartheta, \varphi, \omega, T)$ was defined. It describes the extent to which radiation incident from the direction (ϑ', φ') is redirected in the direction (ϑ, φ) without being absorbed and re-emitted in between. The following applies to the incident spectral radiance

$$\begin{aligned} J_{\text{in}}(\omega, T) &= J(\omega, T) \\ &= J(\omega, T) \left(a(\omega, T, \vartheta, \varphi) + \int_{\varphi'=0}^{2\pi} \int_{\vartheta'=0}^{\pi/2} s(\vartheta, \varphi, \vartheta', \varphi', \omega, T) \cos(\vartheta') \sin(\vartheta') d\vartheta' d\varphi' \right) \end{aligned} \quad (5.331)$$

The expression in brackets must return to one. Since the Maxwell equations, like the Schrödinger equation, are invariant against time reversal, the following applies

$$s(\mathcal{J}, \varphi, \mathcal{J}', \varphi', \omega, T) = s(\mathcal{J}', \varphi', \mathcal{J}, \varphi, \omega, T). \quad (5.332)$$

It follows

$$\varepsilon(\omega, T, \mathcal{J}, \varphi) = a(\omega, T, \mathcal{J}, \varphi) \quad (5.333)$$

This is called *Kirchhoff's radiation law*. Since a body can never absorb more than the radiation that hits it, $a \leq \mathbf{1}$ applies, so it follows

$$\varepsilon \leq \mathbf{1}. \quad (5.334)$$

Bodies with $\varepsilon(\mathcal{J}, \varphi, \omega) = \mathbf{1}$ are called *black bodies*, so the Stefan-Boltzmann law only applies to black bodies.

Part II

Governing equations

The governing equations form the system of equations that determine the temporal development of the atmosphere. First, however, their condition must be described.

A particle is a small volume of air ΔV , which is so large that on a long-term average it contains such a large number of gas molecules that a continuous picture of matter can be assumed. The atmosphere $A \subseteq \mathbb{R}^3$ is the gas envelope of the Earth. The openness makes sense so that a directional derivation in every direction is possible at every point. The definition of the upper bound depends on the problem being addressed. At the lower limit, the atmosphere is limited by the earth's surface, including the movements that take place there, so the amount A is time-dependent, $A = A(t)$. All meteorological fields are assumed to be differentiable as often as required for the calculations. *Air* consists of *dry air* and *Tracers*. These include:

- water vapor
- liquid or solid water
- Aerosols that do not consist of water
- gaseous components present in variable concentrations

6.1 gas phase

Moist air is a mixture of dry air and water vapor. The number of *tracer classes* taken into account, in particular the *condensate classes*, is considered sufficient when incorrect predictions are no longer due to coarseness in the equation system used for the prediction, but to errors in the initial and/or boundary conditions. The following state variables are defined:

- The density of dry air $\rho_d : A \rightarrow \mathbb{R}$ is defined by

$$\rho_d := \frac{1}{\Delta V} \sum_{i=1}^{N_d} m_i^{(d)}. \quad (6.1)$$

Here, N_d is the number of gas atoms other than H_2O and other separately considered trace gases present in the volume ΔV , and the $m_i^{(d)}$ are their masses.

- The *wind vector* $\mathbf{v} : A \rightarrow \mathbb{R}^3$ is defined by

$$\mathbf{v} := \frac{1}{\sum_{j=1}^{N_g} m_j^{(g)}} \sum_{i=1}^{N_g} m_i^{(g)} \mathbf{v}_i^{(g)}, \quad (6.2)$$

where $\mathbf{v}_i^{(g)}$ is the velocity of the i -th molecule of the gaseous portion of the air in ΔV .

- The temperature $T : A \rightarrow \mathbb{R}$ of the moist air. Let
- $p : A \rightarrow \mathbb{R}$ be the pressure.

6.2 Second continuum transition

The derivation of the Navier-Stokes equations is based on a continuous conception of matter, which was motivated by a continuum transition. The continuum transition is a heuristic idea based on the assumption that matter will eventually become continuous if you just zoom out enough to blur the grittiness of matter in the form of atoms and molecules. Mathematically, this means using continuously differentiable fields to describe the system instead of a number of trajectories.

You are faced with a similar problem if you include phase transitions and condensates in the description. You could now describe the condensates using trajectory curves, while still treating the gas phase as a fluid. However, this has two disadvantages: First of all, for such a formulation you have to answer the technical question of what size something is considered to be condensate; In addition, the computational effort required for this is enormous. Instead, you do the so-called *Second phase transition*, which also considers the mass densities and other properties of the condensates as continuously differentiable functions. Of course, this is not exact in the sense that the Maxwell equations are exact, but the fundamental problem is already inherent in the Navier-Stokes equations themselves.

The following state variables are also introduced for the condensates, which from now on are also referred to as *Tracer*:

- The densities of the tracer classes $\rho_i : A \rightarrow \mathbb{R}$ are defined analogously to ρ_d .
- Let the $Q_i : A \rightarrow \mathbb{R}$ be the charge densities of the tracers.
- The mass flux density $\mathbf{j}_i : A \rightarrow \mathbb{R}^3$ of the i -th tracer class is defined by

$$\mathbf{j}_i := \rho_i \sum_{k=1}^{N_i} \mathbf{v}_k^{(i)}, \quad (6.3)$$

where $\mathbf{v}_k^{(i)}$ is the velocity of the k th particle of the corresponding tracer class in ΔV .

- Let the temperature $T_i : A \rightarrow \mathbb{R}$ be that of the i -th tracer class; all particles of a class should have the same temperature. The gaseous tracers have the temperature of moist air.
- Furthermore, consider the field of spectral radiance $L_\lambda : A \times [0, \infty) \times [0, \pi] \times [0, 2\pi) \rightarrow \mathbb{R}$.
- The *electric field* $\mathbf{E}$ as well as the *magnetic flux density* $\mathbf{B}$ must also be taken into account (e.g. for thunderstorms and the *ionosphere*).

The totality of all these quantities is an *atmospheric state* Z . The aim of this chapter is to formulate prognostic equations in such a way that the state trajectory is determined by initial conditions and boundary conditions. Each state is considered a quasi-stationary state. Through thermodynamic equations of state or other diagnostic equations that arise from approximate or approximate relations between the elements of Z , a state can already be determined by a real subset of Z or by a bijection on this subset.

The i -th condensate class has the *microscopic density* ρ'_i , which means, for example, the density of water $\sim 10^3 \text{ kgm}^{-3}$ in contrast to the density averaged over a particle. The ρ'_i are assumed to be constants that do not depend on external conditions for them

$$\rho'_i = \frac{m_i}{V_i}, \quad (6.4)$$

where m_i is the mass of component i and V_i is the volume occupied by it. The density of air is generally given by:

$$\rho = \frac{m_g + \sum_{i \in \{\text{Kondensatklassen}\}} m_i}{V_g + \sum_{i \in \{\text{Kondensatklassen}\}} V_i}. \quad (6.5)$$

The general rule applies to the density of the component ρ_i

$$\rho_i = \frac{m_i}{v_h} = \frac{m_i}{V_g + \sum_{i \in \{\text{Kondensatklassen}\}} V_i}. \quad (6.6)$$

The following applies to the density ρ_g of the gaseous air

$$\rho_g = \frac{m_g}{v_h} = \frac{m_g}{V_g + \sum_{i \in \{\text{Kondensatklassen}\}} V_i}. \quad (6.7)$$

For the microscopic densities of gaseous air one obtains

$$\begin{aligned} \rho'_g &= \frac{m_g}{V_g} = \frac{m_g}{V - \sum_{i \in \{\text{Kondensatklassen}\}} V_i} = \frac{1}{\frac{V}{m_g} - \sum_{i \in \{\text{Kondensatklassen}\}} \frac{V_i}{m_g}} \\ &= \frac{1}{\frac{1}{\rho_g} - \sum_{i \in \{\text{Kondensatklassen}\}} \frac{V_i}{m_i} \frac{m_i}{m_g}} = \frac{1}{1 - \sum_{i \in \{\text{Kondensatklassen}\}} \frac{\rho_i}{\rho'_i}}. \end{aligned} \quad (6.8)$$

The microscopic density of water vapor ρ'_v is also referred to as *microscopic humidity*. The same applies to them

$$\rho'_v = \frac{m_v}{V_g} = \frac{\rho_v}{1 - \sum_{i \in \{\text{Kondensatklassen}\}} \frac{\rho_i}{\rho'_i}}. \quad (6.9)$$

This therefore applies to the equation of state of air

$$p = T_g R_g \rho'_g. \quad (6.10)$$

6.2.1 Descriptive information loss

In statistical physics, the description moves from the microstate to the macrostate and sees this description as statistically complete. Similarly, one may question whether the description developed in the previous two sections is complete. This would only be the case (assuming the second continuum transition) if an infinite number of tracer classes were introduced and a continuous temperature distribution was assumed in each particle class. Except for the restrictive assumption that all particles of a tracer class have the same temperature, the above description has the potential to be a complete description under certain assumptions.

6.2.2 Forcings and time derivations

Phase transition rates matter to the first law of thermodynamics because they are associated with latent heat flows, as well as to the continuity equations that they are mass flows. However, the first law is formulated materially for a specific particle and not in local time like the continuity equation. The question arises as to whether there is a distinction between total and local time derivatives in the phase transition rates, since these quantities are also time derivatives. To answer this question, imagine a measuring device that measures the mass $m(t)$, which has changed phase up to a time $t > 0$ in a stationary control volume V . Measure for the phase transition rate q

$$q = \frac{m(t)}{tV}. \quad (6.11)$$

Imagine a second measuring device that measures the mass $m'(t)$, which has changed phase up to a time $t > 0$ in a particle $V'(t)$ that moves with the wind field. Let $V'(0) = V(0)$. Then this meter measures the phase transition rate

$$q' = \frac{m'(t)}{tV'(t)}. \quad (6.12)$$

In the case $t \rightarrow 0$ goes $V' \rightarrow V$. Therefore applies

$$\begin{aligned} \lim_{t \rightarrow 0} (q - q') &= \lim_{t \rightarrow 0} \left[\frac{m(t)}{Vt} - \frac{m'(t)}{V'(t)t} \right] = \lim_{t \rightarrow 0} \frac{m(t)}{Vt} - \lim_{t \rightarrow 0} \frac{m'(t)}{V'(t)t} \\ &= \frac{1}{V} \lim_{t \rightarrow 0} \frac{m(t)}{t} - \lim_{t \rightarrow 0} \frac{1}{V'(t)} \lim_{t \rightarrow 0} \frac{m'(t)}{t} \\ &= \frac{1}{V} \lim_{t \rightarrow 0} \frac{m(t)}{t} - \frac{1}{V} \lim_{t \rightarrow 0} \frac{m'(t)}{t} = \frac{1}{V} \lim_{t \rightarrow 0} \frac{m(t) - m'(t)}{t} \end{aligned} \quad (6.13)$$

according to the calculation rules for functional limit values. With the true space- and time-dependent condensation rate $q_r(\mathbf{r}, t)$ one can

$$m(t) = \int_0^t \int_V q_r(\mathbf{r}, t') d^3r dt' \quad (6.14)$$

as well as

$$m'(t) = \int_0^t \int_{V'(t')} q_r(\mathbf{r}, t') d^3r dt' \quad (6.15)$$

note down. This gives you

$$\begin{aligned}
 m(t) - m'(t) &= \int_{\circ}^t \int_V q_r(\mathbf{r}, t) d^3r dt' - \int_{\circ}^t \int_{V'(t)} q_r(\mathbf{r}, t) d^3r dt' \\
 &= \int_{\circ}^t \left[\int_V q_r(\mathbf{r}, t) d^3r - \int_{V'(t)} q_r(\mathbf{r}, t) d^3r \right] dt'.
 \end{aligned} \tag{6.16}$$

According to the main theorem of differential and integral calculus follows

$$\lim_{t \rightarrow \circ} \frac{m(t) - m'(t)}{t} = \frac{1}{V} \lim_{t \rightarrow \circ} \left[\int_V q_r(\mathbf{r}, t) d^3r - \int_{V'(t)} q_r(\mathbf{r}, t) d^3r \right] = \circ. \tag{6.17}$$

So $q - q' = \circ$ for the limit $t \rightarrow \circ$. The phase transition rates in the particle system are measured in the same way as in the system at rest, so that the distinction between total and local time derivatives does not occur here. This applies analogously to all other source strengths and forcings.

7 CONTINUITY EQUATIONS

7.1 Basics

The continuity equation is the balance equation of the mass. Let $\Omega \subseteq \mathbb{R}^3$ be an open subset, ρ a density and $\mathbf{j}$ the corresponding flux density. Then using Gauss's theorem and a source density Q

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega} \rho d^3r &= - \int_{\partial\Omega} \mathbf{j} \cdot d\mathbf{n} + \int_{\Omega} Q d^3r = - \int_{\Omega} \nabla \cdot \mathbf{j} - Q d^3r \\ \Rightarrow \int_{\Omega} \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} - Q d^3r &= 0. \end{aligned} \quad (7.1)$$

Since the integrand is continuous, it is already homogeneous and constantly equal to zero. If $\left| \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} - Q \right| > \varepsilon > 0$ holds at a point $\mathbf{r}_0 \in \Omega$, then there exists an open environment $\omega \subseteq \Omega$ with $\mathbf{r}_0 \in \omega$ and $\int_{\omega} \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} - Q d^3r \neq 0$ in contradiction to Eq. (7.1). It therefore applies

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = Q. \quad (7.2)$$

In specific volume terms a this can be written as

$$-\frac{1}{a^2} \frac{\partial a}{\partial t} - \frac{1}{a^2} \mathbf{v} \cdot \nabla a + \frac{1}{a} \nabla \cdot \mathbf{v} = 0 \quad \Leftrightarrow \quad \frac{\partial a}{\partial t} = a \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla a. \quad (7.3)$$

note down. This is now noted separately for all components of the air:

$\frac{\partial \rho_d}{\partial t} + \nabla \cdot \mathbf{j}_d = Q_d \quad (7.4)$
$\frac{\partial \rho_v}{\partial t} + \nabla \cdot \mathbf{j}_v = Q_v \quad (7.5)$
$\frac{\partial \rho_i}{\partial t} + \nabla \cdot \mathbf{j}_i = Q_i \quad (7.6)$

This applies

$$\mathbf{j}_d = \rho_d \mathbf{v} - D_d \nabla \rho_d, \quad \mathbf{j}_v = \rho_v \mathbf{v} - D_v \nabla \rho_v. \quad (7.7)$$

The D_d, D_v are the diffusion coefficients for dry and moist air, respectively. You can at first

$$Q_d = 0 \quad (7.8)$$

hold onto.

7.2 Specification of source terms

Now the Q_x should be specified in more detail in the equations (7.4) - (7.6). There are five processes that contribute to them:

- Diffusion
- Phase transitions
- collisions
- decays
- for gases, ions and electrons also chemical reactions and radiation interactions

The last point will be ignored in the rest of the section; this will only be about the condensates. Diffusion only occurs with the gaseous components, so in Q_d there is a term $D_d \Delta \varphi_d$ and in Q_v there is a term $D_v \Delta \varphi_v$, here D_d and D_v are the diffusion coefficients of dry air and water vapor in air, respectively. Dry air is not affected by the other processes, so

$$Q_d = D_d \Delta \varphi_d \quad (7.9)$$

applies.

7.2.1 Collisions

If two particles of the condensate classes j and k meet, one can specify a probability $0 \leq P_{j,k} \leq 1$ that they will then form a particle. This has a well-defined class $R_{j,k}$. Furthermore, let $\sigma_{j,k}$ be the cross section of the collisions of particles of classes j and k . For example, if j are spheres with radius r_j and k are spheres with radius r_k , then $\sigma_{j,k} = \pi (r_j + r_k)^2$. Let the average relative velocity between the particles of classes j and k be $\overline{v_{\text{rel}}}(j, k)$. Then a particle of class j flies through a volume $\sigma_{j,k} \overline{v_{\text{rel}}}(j, k) t$ in time t relative to the particles of class k . The average collision time $\tau_{j,k}$ is defined by requiring that exactly one particle of class k is in this volume, i.e

$$n_k \sigma_{j,k} \overline{v_{\text{rel}}}(j, k) \tau_{j,k} \stackrel{!}{=} 1. \quad (7.10)$$

All particles of group j participate in collision processes, therefore the total collision rate of particles j with particles k is given by

$$\frac{n_j}{\tau_{j,k}} = n_j n_k \sigma_{j,k} \overline{v_{\text{rel}}}(j, k). \quad (7.11)$$

If $\tilde{m}_i$ is the mass of the particles of the group $i = R_{j,k}$, this results in a corresponding source strength

$$\tilde{m}_i \sigma_{j,k} n_j n_k \overline{v_{\text{rel}}}(j, k) P_{j,k}. \quad (7.12)$$

Furthermore, a negative proportion of the swelling strength must also be taken into account, which occurs because particles of their original condensate class are lost when they combine with other particles. This leads to

$$Q_i^{(\text{Kollisionen})} = \tilde{m}_i \sum_j \sum_{k \leq j} \sigma_{j,k} n_j n_k \overline{v_{\text{rel}}}(j, k) P_{j,k} (\delta_{i, R_{j,k}} - \delta_{j,i} - \delta_{k,i}). \quad (7.13)$$

Because of mass conservation, this requires that the particle masses $\tilde{m}_i$ are integer multiples of a minimum mass so that no mass artificially disappears or arises during collisions.

7.2.2 decays

Decay processes are now being investigated. The following applies to the change in particle density n_j due to decay

$$dn_j = -n_j \mathcal{J}_j dt \Leftrightarrow \frac{dn_j}{dt} = -\mathcal{J}_j n_j, \quad (7.14)$$

here $\mathcal{J}_j$ is the decay constant. The product of the decay is a particle of class k and one of class l with probability $Z_{j,k,l}$; the normalization applies here

$$1 = \sum_k \sum_{l \leq k} Z_{j,k,l}, \quad (7.15)$$

where $Z_{j,j,l} = Z_{j,k,j} = 0$, that is, the product of a decay must not be equal to the reactant. Positive and negative terms must be taken into account for each condensate class i , so that:

$$Q_i^{(\text{Zerfälle})} = \tilde{m}_i \sum_j \sum_k \sum_{l \leq k} \mathcal{J}_j n_j Z_{j,k,l} (\delta_{i,k} + \delta_{i,l} - \delta_{j,i}). \quad (7.16)$$

7.3 Phase transitions

Finally, phase transitions are discussed. These can take place in two ways.

7.3.1 Condensation and resublimation

First, condensation and resublimation can lead directly to the creation of new particles of class i , and evaporation and sublimation can lead to their destruction, respectively. The corresponding mass flux densities are denoted by $\tilde{q}'_{v,i}$ in the first case and $\tilde{q}'_{i,v}$ in the second case. Through this process you get terms

$$Q_v^{(\pm \text{Entstehung})} = \sum_j \tilde{q}'_{j,v} - \tilde{q}'_{v,j}, \quad (7.17)$$

$$Q_i^{(\pm \text{Entstehung})} = \tilde{q}'_{v,i} - \tilde{q}'_{i,v}. \quad (7.18)$$

7.3.2 growth

Large condensation products such as hailstones do not form instantaneously, but rather grow, among other things, through condensation or resublimation of water vapor on smaller particles. They can also disappear again in the opposite way. During a time interval Δt , condense or resublime a mass m_i of particles of class i within a volume ΔV . This causes them to grow and become heavier, but it was discussed in Chap. 6 specifies that all particles of class i should have the same mass $\tilde{m}_i$. If this is the only process that takes place, it is due to conservation of mass

$$\rho_{g(i)}(t) \Delta V + m_i = \rho_{g(i)}(t + \Delta t) \Delta V. \quad (7.19)$$

Here $g(i)$ is the condensate class that arises from i through growth. This follows

$$\frac{\partial \rho_{g(i)}}{\partial t} = \frac{1}{\Delta V} \frac{dm_i}{dt} =: \tilde{q}''_{v,i}. \quad (7.20)$$

This is initially confusing because condensation on particles i changes the density $\rho_{g(i)}$; This results from the fact that no new particles of class i are formed during this type of phase transition. In the case of evaporation or sublimation one obtains

$$\frac{\partial \rho_{d(i)}}{\partial t} =: \tilde{q}''_{i,v}, \quad (7.21)$$

where $d(i)$ is the condensate class formed from i by shrinkage.

7.3.3 Freezing and melting

Thirdly, condensates can transform into one another by freezing or melting; the corresponding swelling strengths are denoted by $\tilde{q}'''_{j,k}$. You receive

$$Q_i^{(\text{Umwandlung})} = \sum_j \tilde{q}'''_{j,i} - \tilde{q}'''_{i,j}. \quad (7.22)$$

7.4 Summary

The source strengths are summarized as follows:

$$Q_d = D_d \Delta \rho_d \quad (7.23)$$

$$Q_v = \sum_i \left(\tilde{q}'_{i,v} - \tilde{q}'_{v,i} + \tilde{q}''_{i,v} - \tilde{q}''_{v,i} \right) + D_v \Delta \rho_v \quad (7.24)$$

$$\begin{aligned} Q_i = & \tilde{m}_i \sum_j \sum_{k \leq j} \sigma_{j,k} n_j n_k \overline{v_{\text{rel}}}(j, k) P_{j,k} (\delta_{i,R_{j,k}} - \delta_{j,i} - \delta_{k,i}) + \tilde{q}'_{v,i} - \tilde{q}'_{i,v} \\ & + \tilde{m}_i \sum_j \sum_k \sum_{l \leq k} \lambda_j n_j Z_{j,k,l} (\delta_{i,k} + \delta_{i,l} - \delta_{j,i}) + \left(\tilde{q}''_{g(i),v} + \tilde{q}''_{v,d(i)} \right) + \sum_j \tilde{q}'''_{j,i} - \tilde{q}'''_{i,j} \end{aligned} \quad (7.25)$$

The exact calculation of the $P_{j,k}$, λ_j and $Z_{j,k,l}$ as well as the phase transition rates is the task of smaller-scale numerical methods and would exceed the aim of this book; this is analogous to the spectra.

Now the mass flux densities $\mathbf{j}_i$ have to be specified. Let v_i be the equilibrium sink speed of the particles i , then one can from

$$\mathbf{j}_i = \rho_i \mathbf{v} - \mathbf{k}_{\rho_i} v_i \quad (7.26)$$

go out. For the precipitation P_i of the condensate class i applies

$$P_i = -\mathbf{j}_i(z_{\text{SFC}}), \quad (7.27)$$

where SFC refers to the earth's surface. These equations are also applicable to aerosols.

7.4.1 Conversion to specific sizes

The specific humidity $q = \rho_i / \rho$ is also often used (def. see equation (5.167)), since it is a conserved quantity in the case of a component i advected by the wind field:

$$\frac{Dq}{Dt} = -\frac{q}{\rho} \frac{D\rho}{Dt} + \frac{1}{\rho} \frac{D\rho_i}{Dt} = q \nabla \cdot \mathbf{v} - q \nabla \cdot \mathbf{v} = 0 \quad (7.28)$$

The source terms of q are those of ρ_i divided by the density of the medium ρ .

8 MOMENTUM EQUATION

The momentum $\mathbf{p}$ of a particle ΔV with N_h gas molecules and N_c condensate nuclei is through

$$\mathbf{p} = \sum_{i=1}^{N_h+N_c} m_i \mathbf{v}_i \stackrel{\text{Glg. (6.2)}}{=} \mathbf{v} \sum_{j=1}^{N_h} m_j + \sum_{j=N_h+1}^{N_h+N_c} m_j (\mathbf{v} + \Delta \mathbf{v}_j), \quad (8.1)$$

Here $\Delta \mathbf{v}_j$ is the sinking speed of the corresponding condensate class, which is assumed to be independent of density. One can note Newton's second axiom in inertial systems:

$$\frac{D\mathbf{p}}{Dt} = \rho \Delta V \frac{D}{Dt} \mathbf{v} = \mathbf{F}_{\text{int}} + \mathbf{F}_{\text{ext}} \quad (8.2)$$

The force is the sum of internal forces and external forces. Assuming that the internal forces consist of pairwise interactions of the particles that satisfy Newton's Third Axiom,

$$\mathbf{F}_{\text{int}} = \sum_{i,j=1}^N \mathbf{F}_{i,j} = \sum_{i=1}^N \sum_{j=i+1}^N \mathbf{F}_{i,j} + \mathbf{F}_{j,i} \stackrel{\text{Newton III}}{=} \mathbf{0}. \quad (8.3)$$

Here $\mathbf{F}_{i,j}$ is the force on the i -th particle due to the j -th particle. Two types of forces come into question for $\mathbf{F}_{\text{ext}}$:

- Force fields and charge and mass distributions
- Interactions with neighboring particles

The first point usually only includes the gravity field. For the weight $\mathbf{F}_g$ applies

$$\mathbf{F}_g = \sum_{i=1}^N m_i \mathbf{g} = \rho \Delta V \mathbf{g}. \quad (8.4)$$

The force acting due to the pressure on the open ball $\Omega := B_r(\mathbf{r}_o)$ with radius r with $\Delta V = \frac{4}{3}\pi r^3$ and center $\mathbf{r}_o$ applies

$$\mathbf{F}_p = - \int_{\partial \Delta V} p d\mathbf{A}. \quad (8.5)$$

Here we assume a spherical particle, then it follows

$$\mathbf{F}_p = - \int_{\partial \Delta V} p r^2 d\omega \approx - \int_{\partial \Delta V} (p(\mathbf{r}_o) + \mathbf{r} \cdot \nabla p) r^2 d\omega \quad (8.6)$$

with $d\omega$ as the solid angle element. To carry out the integration, you set up ∇p or similar. A. on the z-axis so that:

$$\nabla p = |\nabla p| \mathbf{e}_z. \quad (8.7)$$

This results in $p_o := p(\mathbf{r}_o)$

$$\begin{aligned} \mathbf{F}_p &= - \int_{\partial \Delta V} (p_o + \mathbf{r} \cdot \nabla p) r d\omega = -r \int_{\partial \Delta V} (\mathbf{r} \cdot \nabla p) r d\omega = -r^2 |\nabla p| \int_{\partial \Delta V} \cos \{ \nabla p, \mathbf{r} \} r d\omega \\ &= -r^3 |\nabla p| \int_{\vartheta=0}^{\pi} \int_{\varphi=0}^{2\pi} \cos(\vartheta) \sin(\vartheta) \begin{pmatrix} \sin(\vartheta) \cos(\varphi) \\ \sin(\vartheta) \sin(\varphi) \\ \cos(\vartheta) \end{pmatrix} d\varphi d\vartheta \\ &= -r^3 \nabla p 2\pi \int_0^{\pi} \cos^2(\vartheta) \sin(\vartheta) d\vartheta = r^3 \nabla p 2\pi \left[\frac{1}{3} \cos^3(\vartheta) \right]_0^{\pi} = -\frac{4}{3} \pi r^3 \nabla p = -\Delta V \nabla p. \end{aligned} \quad (8.8)$$

This force is called *pressure gradient force*. You receive

$$\rho \Delta V \frac{D}{Dt} \mathbf{v} = \rho \Delta V \mathbf{g} - \Delta V \nabla p, \quad (8.9)$$

If you convert this to the acceleration of the particle $\frac{D\mathbf{v}}{Dt}$, you get

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p + \mathbf{g}. \quad (8.10)$$

This equation is called *Euler equation*.

In an alternative derivation, one considers a macroscopic open set $\Omega \subseteq \mathbb{R}^3$, the momentum $\mathbf{p}$ in this set is given by

$$\mathbf{p} = \int_{\Omega} \rho \mathbf{v} d^3 r. \quad (8.11)$$

At this point you carry out the *momentum flux density tensor* Π

$$\Pi_{i,j} := \rho U_i U_j \quad (8.12)$$

for $i, j \leq 3$ a. For $i \leq 3$

$$\Pi \cdot \mathbf{e}_i = \sum_{j=1}^3 \rho v_j v_i \mathbf{e}_j = v_i \rho \mathbf{v} \quad (8.13)$$

the flow of the momentum density in the $\mathbf{e}_i$ -direction. For a general unit vector $\mathbf{e}$, $\Pi \cdot \mathbf{e}$ is the flux of momentum density in the $\mathbf{e}$ -direction. Thus, with the findings of section 6.2.2

$$\begin{aligned} \frac{\partial \mathbf{p}}{\partial t} &= \int_{\Omega} \frac{\partial (\rho \mathbf{v})}{\partial t} d^3 r = \int_{\Omega} -\nabla p + \rho \mathbf{g} d^3 r - \int_{\partial \Omega} \Pi \cdot d\mathbf{n} \\ &\Rightarrow \int_{\Omega} \frac{\partial (\rho \mathbf{v})}{\partial t} d^3 r = \int_{\Omega} -\nabla p + \rho \mathbf{g} - \nabla \cdot \Pi d^3 r \\ &\Rightarrow \int_{\Omega} \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla p + \nabla \cdot \Pi - \rho \mathbf{g} d^3 r = \mathbf{0}. \end{aligned} \quad (8.14)$$

So it already applies

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla p + \nabla \cdot \Pi - \rho \mathbf{g} = \mathbf{0}. \quad (8.15)$$

For the divergence of Π follows

$$\begin{aligned} (\nabla \cdot \Pi)_i &= \sum_{j=1}^3 \frac{\partial}{\partial x_j} (\rho v_i v_j) = \sum_{j=1}^3 v_i v_j \frac{\partial \rho}{\partial x_j} + \rho v_j \frac{\partial v_i}{\partial x_j} + \rho v_i \frac{\partial v_j}{\partial x_j} \\ &= v_i \mathbf{v} \cdot \nabla \rho + \rho (\mathbf{v} \cdot \nabla) v_i + \rho v_i \nabla \cdot \mathbf{v}, \end{aligned} \quad (8.16)$$

so applies

$$\nabla \cdot \Pi = \mathbf{v} (\mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v}) + (\rho \mathbf{v} \cdot \nabla) \mathbf{v}. \quad (8.17)$$

Thus follows

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \frac{\partial \rho}{\partial t} + \nabla p + \mathbf{v} (\mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v}) + (\rho \mathbf{v} \cdot \nabla) \mathbf{v} - \rho \mathbf{g} = \mathbf{0}. \quad (8.18)$$

With the continuity equation you finally get

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \mathbf{g}. \quad (8.19)$$

8.1 Apparent forces

Newton's axioms only apply in inertial systems. In relation to the Earth, one considers the center of the Earth to be unaccelerated, even if it orbits the Sun, and only considers the rotation of the Earth. Let $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ denote the basis of the resting coordinates (see section D.1). If you measure accelerations in this KS, you can link them to the acting forces using Newton's second axiom. However, if you choose a base rotating at the angular velocity of the Earth, further acceleration terms arise that do not arise from physical forces. The base of the global coordinates is in resting coordinates

$$\mathbf{e}_x(t) = \begin{pmatrix} \cos(\omega t) \\ \sin(\omega t) \\ 0 \end{pmatrix}, \quad \mathbf{e}_y(t) = \begin{pmatrix} -\sin(\omega t) \\ \cos(\omega t) \\ 0 \end{pmatrix}, \quad \mathbf{e}_z(t) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (8.20)$$

with the angular velocity of the Earth's rotation $\boldsymbol{\omega} = (0, 0, \omega)^T$. Let a particle with the position vector $\mathbf{r} = \mathbf{r}(t) = x(t)\mathbf{e}_x(t) + y(t)\mathbf{e}_y(t) + z(t)\mathbf{e}_z(t)$ be given. Then applies to the speed

$$\mathbf{v} = \dot{\mathbf{r}} = \dot{x}\mathbf{e}_x + y\dot{\mathbf{e}}_x + \dot{y}\mathbf{e}_y + z\dot{\mathbf{e}}_y + x\dot{\mathbf{e}}_x + y\dot{\mathbf{e}}_y + z\dot{\mathbf{e}}_z. \quad (8.21)$$

The following applies to the time derivatives of the basis vectors

$$\dot{\mathbf{e}}_x = \omega \begin{pmatrix} -\sin(\omega t) \\ \cos(\omega t) \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \omega \end{pmatrix} \times \begin{pmatrix} \cos(\omega t) \\ \sin(\omega t) \\ 0 \end{pmatrix} = \boldsymbol{\omega} \times \mathbf{e}_x, \quad (8.22)$$

$$\dot{\mathbf{e}}_y = \omega \begin{pmatrix} -\cos(\omega t) \\ -\sin(\omega t) \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \omega \end{pmatrix} \times \begin{pmatrix} -\sin(\omega t) \\ \cos(\omega t) \\ 0 \end{pmatrix} = \boldsymbol{\omega} \times \mathbf{e}_y, \quad (8.23)$$

$$\dot{\mathbf{e}}_z = 0 = \boldsymbol{\omega} \times \mathbf{e}_z. \quad (8.24)$$

The velocity vector is therefore written as

$$\mathbf{v} = \mathbf{v}' + x\boldsymbol{\omega} \times \mathbf{e}_x + y\boldsymbol{\omega} \times \mathbf{e}_y + z\boldsymbol{\omega} \times \mathbf{e}_z = \mathbf{v}' + \boldsymbol{\omega} \times \mathbf{r}, \quad (8.25)$$

For the speed measured in the canceled system, $\mathbf{v}' = \dot{x}\mathbf{e}_x + \dot{y}\mathbf{e}_y + \dot{z}\mathbf{e}_z$ was written and the linearity of the vector product Eq.en (A.147) - (A.148) exploited. Newton's Second Axiom is a statement about the acceleration $\frac{D\mathbf{v}}{Dt}$, so we derive the above equation again in time:

$$\frac{D\mathbf{v}}{Dt} = \left(\frac{D\mathbf{v}'}{Dt} \right)' + \boldsymbol{\omega} \times \mathbf{v}' + \boldsymbol{\omega} \times (\mathbf{v}' + \boldsymbol{\omega} \times \mathbf{r}) = \left(\frac{D\mathbf{v}'}{Dt} \right)' + 2\boldsymbol{\omega} \times \mathbf{v}' + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}), \quad (8.26)$$

where $\left(\frac{D\mathbf{v}'}{Dt} \right)'$ is the acceleration measured in the rotating system. One is interested in the acceleration in global coordinates, i.e. in the vector $\left(\frac{D\mathbf{v}'}{Dt} \right)'$.

$$\left(\frac{D\mathbf{v}'}{Dt} \right)' = \frac{D\mathbf{v}}{Dt} - 2\boldsymbol{\omega} \times \mathbf{v}' - \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}) \quad (8.27)$$

The location-dependent term $-\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})$ is the centrifugal acceleration, the speed-dependent term $-2\boldsymbol{\omega} \times \mathbf{v}'$ is the Coriolis acceleration. For the IS acceleration $\frac{D\mathbf{v}}{Dt}$, the accelerations that result from the forces according to Newton's second axiom must be used. In particular, note that the Coriolis force does no work because it is perpendicular to the velocity vector.

8.2 Stress tensor

stress refers to all the forces that a fluid exerts on itself. O.B.d. A. imagine a cube whose sides are parallel to the coordinate surfaces of a Cartesian coordinate system. The stress is determined by the *stress tensor*

$$T = \begin{pmatrix} T_{x,x} & T_{x,y} & T_{x,z} \\ T_{y,x} & T_{y,y} & T_{y,z} \\ T_{z,x} & T_{z,y} & T_{z,z} \end{pmatrix} \quad (8.28)$$

described. The elements of this tensor have the dimension of a pressure (force per area). The i -th line of T describes forces acting on the faces of the cube (anti)parallel to the i -axis. The entry in the j th column denotes the force acting on this surface in the j direction if the normal of the surface under consideration is parallel to the i axis, otherwise the signs are swapped. This causes compressive forces to always be negative.

First, the case of a fluid at rest is considered. In this case the stress must be isotropic. It corresponds to the pressure p , so in this case the stress tensor applies

$$T_{i,j} = -p\delta_{i,j}. \quad (8.29)$$

The sign comes from the convention that compressive forces are always negative. Now note the decomposition

$$T = -p + \tau. \quad (8.30)$$

Imagine a fluid particle $[-\frac{\Delta}{2}, \frac{\Delta}{2}]^3$ with $\Delta > 0$. The z -component D_z of the torque acting on this particle D is proportional to

$$\begin{aligned} D_z &\propto T_{1,2} + \frac{\Delta}{2} \frac{\partial T_{1,2}}{\partial x} + T_{1,2} - \frac{\Delta}{2} \frac{\partial T_{1,2}}{\partial x} - \left(T_{2,1} + \frac{\Delta}{2} \frac{\partial T_{2,1}}{\partial y} + T_{2,1} - \frac{\Delta}{2} \frac{\partial T_{2,1}}{\partial y} \right) \\ &= 2T_{1,2} - 2T_{2,1}, \end{aligned} \quad (8.31)$$

where the values of T are evaluated at the center of the coordinate system. Assuming vanishing torque:

$$T_{1,2} = T_{2,1}. \quad (8.32)$$

This assumption is comparable to the concept of quasi-static change of state in statistical physics. By changing the orientation of the coordinate system, this also applies to all other off-diagonal indices, so T is symmetrical. Therefore the tensor τ must also be symmetric.

The size $\frac{\partial v_i}{\partial x_j}$ is called *velocity gradient tensor*. You can take notes for this one

$$\frac{\partial v_i}{\partial x_j} = S_{i,j} + \frac{1}{2}R_{i,j} \quad (8.33)$$

with

$$S_{i,j} := \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad R_{i,j} := \frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i}. \quad (8.34)$$

$S_{i,j}$ is called *stress tensor*, which is symmetrical, and $R_{i,j}$ is called *rotation tensor*, which is antisymmetric. The elements of the rotation tensor correspond to the rotation of fluid particles, but not to deformation or acceleration. Only the elements of the stress tensor are relevant for the stress. Therefore you can make notes

$$\tau_{i,j} = \sum_{n,m} K_{i,j,m,n} S_{m,n} \quad (8.35)$$

with a complex fourth-order tensor K , whose elements describe how the fluid reacts to deformations. The totals run from one to three. This formulation allows all elements of τ to be linearly linked in pairs with all elements of S .

If one assumes a medium whose material properties are independent of direction, which is the case for ideal gases, K must be independent of the orientation of the coordinate system. This implies that K is isotropic. An isotropic tensor of the fourth order has the form

$$K_{i,j,m,n} = \lambda \delta_{i,j} \delta_{m,n} + \mu \delta_{i,m} \delta_{j,n} + \gamma \delta_{i,n} \delta_{j,m}, \quad (8.36)$$

where $\lambda, \mu, \gamma \in \mathbb{C}$ are scalars. Since both τ and S are symmetric, they do not change when i and j are swapped. The same must also apply to K . This implies

$$\gamma = \mu. \quad (8.37)$$

This leads to

$$K_{i,j,m,n} = \lambda \delta_{i,j} \delta_{m,n} + 2\mu \delta_{i,m} \delta_{j,n}. \quad (8.38)$$

μ is called *dynamic viscosity* and λ is called *Lamé constant*. Putting this into Eq. (8.35), you get

$$\tau_{i,j} = \sum_{n,m} (\lambda \delta_{i,j} \delta_{m,n} + 2\mu \delta_{i,m} \delta_{j,n}) S_{m,n} = \lambda \delta_{i,j} \sum_m S_{m,m} + 2\mu S_{i,j}. \quad (8.39)$$

From Eq. (8.34) follows

$$\sum_m S_{m,m} = \nabla \cdot \mathbf{v}. \quad (8.40)$$

Therefore applies

$$T_{i,j} = -p \delta_{i,j} + \lambda \delta_{i,j} \nabla \cdot \mathbf{v} + 2\mu S_{i,j} \quad (8.41)$$

For $i = j$ we get from this

$$T_{i,i} = -p + \lambda \nabla \cdot \mathbf{v} + 2\mu S_{i,i}. \quad (8.42)$$

If you sum this over $i = 1, 2, 3$, it follows

$$\begin{aligned} \sum_i T_{i,i} &= -3p + (2\mu + 3\lambda) \nabla \cdot \mathbf{v} \\ \Rightarrow p &= -\frac{1}{3} T_{i,i} + \sum_i T_{i,i} + \left(\frac{2}{3} \mu + \lambda \right) \nabla \cdot \mathbf{v}. \end{aligned} \quad (8.43)$$

From this, in contrast to the thermodynamic pressure, one can derive a *average pressure*

$$\bar{p} := -\frac{1}{3} T_{i,i} \quad (8.44)$$

derive. This applies to this one

$$p - \bar{p} = \sum_i T_{i,i} + \left(\frac{2}{3} \mu + \lambda \right) \nabla \cdot \mathbf{v}. \quad (8.45)$$

Now define the *bulk viscosity* μ_v by

$$\mu_v := \frac{2}{3} \mu + \lambda \Rightarrow p - \bar{p} = \sum_i T_{i,i} + \mu_v \nabla \cdot \mathbf{v}. \quad (8.46)$$

The *Stokes Assumption*

$$\mu_v = 0 \quad (8.47)$$

is often justified, but is not done further. For the Lamé constant λ is obtained in bulk viscosity terms

$$\lambda = \mu_v - \frac{2}{3}\mu. \quad (8.48)$$

Putting this into Eq. (8.41), you get

$$T_{i,j} = -p\delta_{i,j} + \left(\mu_v - \frac{2}{3}\mu\right)\delta_{i,j}\nabla \cdot \mathbf{v} + 2\mu S_{i,j}. \quad (8.49)$$

Another spelling is:

$$T_{i,j} = -p\delta_{i,j} + \tau_{i,j} = -p\delta_{i,j} + 2\mu \left(S_{i,j} - \frac{1}{3}\nabla \cdot \mathbf{v}\delta_{i,j} \right) + \mu_v \nabla \cdot \mathbf{v}\delta_{i,j}. \quad (8.50)$$

The assumption that T depends linearly on S is an approximation that is correct for most fluids. Such fluids are called *Newtonian fluids*. In meteorology it is not necessary to go beyond this.

In Cartesian coordinates with $\mathbf{v} = (u, v, w)^T$, Eq. (8.50)

$$T = \begin{pmatrix} -p + 2\mu \frac{\partial u}{\partial x} + \left(\mu_v - \frac{2}{3}\mu\right)\nabla \cdot \mathbf{v} & \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) & -p + 2\mu \frac{\partial v}{\partial y} + \left(\mu_v - \frac{2}{3}\mu\right)\nabla \cdot \mathbf{v} & \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) & \mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) & -p + 2\mu \frac{\partial w}{\partial z} + \left(\mu_v - \frac{2}{3}\mu\right)\nabla \cdot \mathbf{v} \end{pmatrix}. \quad (8.51)$$

From this we can calculate the frictional acceleration $\mathbf{f}_R$:

$$\begin{aligned} \mathbf{f}_R &= \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau} = \frac{1}{\rho} \begin{pmatrix} 2\mu \frac{\partial^2 u}{\partial x^2} + \left(\mu_v - \frac{2}{3}\mu\right) \frac{\partial \nabla \cdot \mathbf{v}}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial y \partial x} \right) + \mu \left(\frac{\partial^2 u}{\partial z^2} + \frac{\partial^2 w}{\partial z \partial x} \right) \\ \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 u}{\partial x \partial y} \right) + 2\mu \frac{\partial^2 v}{\partial y^2} + \left(\mu_v - \frac{2}{3}\mu\right) \frac{\partial \nabla \cdot \mathbf{v}}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial z^2} + \frac{\partial^2 w}{\partial z \partial y} \right) \\ \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 u}{\partial x \partial z} \right) + \mu \left(\frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 v}{\partial y \partial z} \right) + 2\mu \frac{\partial^2 w}{\partial z^2} + \left(\mu_v - \frac{2}{3}\mu\right) \frac{\partial \nabla \cdot \mathbf{v}}{\partial z} \end{pmatrix} \\ &= \frac{\mu}{\rho} \Delta \mathbf{v} + \frac{1}{\rho} \begin{pmatrix} \mu \frac{\partial^2 u}{\partial x^2} + \left(\mu_v - \frac{2}{3}\mu\right) \frac{\partial \nabla \cdot \mathbf{v}}{\partial x} + \mu \frac{\partial^2 v}{\partial y \partial x} + \mu \frac{\partial^2 w}{\partial z \partial x} \\ \mu \frac{\partial^2 u}{\partial x \partial y} + \mu \frac{\partial^2 v}{\partial y^2} + \left(\mu_v - \frac{2}{3}\mu\right) \frac{\partial \nabla \cdot \mathbf{v}}{\partial y} + \mu \frac{\partial^2 w}{\partial z \partial y} \\ \mu \frac{\partial^2 u}{\partial x \partial z} + \mu \frac{\partial^2 v}{\partial y \partial z} + \mu \frac{\partial^2 w}{\partial z^2} + \left(\mu_v - \frac{2}{3}\mu\right) \frac{\partial \nabla \cdot \mathbf{v}}{\partial z} \end{pmatrix} \\ &= r \Delta \mathbf{v} + \frac{\mu_v}{\rho} \nabla (\nabla \cdot \mathbf{v}) + \frac{\mu}{\rho} \begin{pmatrix} \frac{\partial^2 u}{\partial x^2} - \frac{2}{3} \frac{\partial \nabla \cdot \mathbf{v}}{\partial x} + \frac{\partial^2 v}{\partial y \partial x} + \frac{\partial^2 w}{\partial z \partial x} \\ \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial y^2} - \frac{2}{3} \frac{\partial \nabla \cdot \mathbf{v}}{\partial y} + \frac{\partial^2 w}{\partial z \partial y} \\ \frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 v}{\partial y \partial z} + \frac{\partial^2 w}{\partial z^2} - \frac{2}{3} \frac{\partial \nabla \cdot \mathbf{v}}{\partial z} \end{pmatrix} \\ &= r \Delta \mathbf{v} + \frac{\mu_v}{\rho} \nabla (\nabla \cdot \mathbf{v}) + \frac{r}{3} \begin{pmatrix} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 v}{\partial y \partial x} + \frac{\partial^2 w}{\partial z \partial x} \\ \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 w}{\partial z \partial y} \\ \frac{\partial^2 u}{\partial x \partial z} + \frac{\partial^2 v}{\partial y \partial z} + \frac{\partial^2 w}{\partial z^2} \end{pmatrix} = r \Delta \mathbf{v} + \left(\frac{\mu_v}{\rho} + \frac{r}{3} \right) \nabla (\nabla \cdot \mathbf{v}) \end{aligned}$$

$$\Leftrightarrow \mathbf{f}_R = r \Delta \mathbf{v} + \left(\frac{\mu_v}{\rho} + \frac{r}{3} \right) \nabla (\nabla \cdot \mathbf{v}) \quad (8.52)$$

It was assumed that the viscosities were homogeneous. For the friction, other values than those given in Eq. (8.52) obtained expression is used. Therefore, from now on, the derivations will mostly use a general expression

$$\mathbf{f}_R = \begin{pmatrix} f_{R,x} \\ f_{R,y} \\ f_{R,z} \end{pmatrix} \equiv \begin{pmatrix} f_R^{(H)} \\ f_{R,z} \end{pmatrix} \quad (8.53)$$

carried for frictional acceleration. This makes sense despite the relative smallness of friction in the atmosphere due to its importance for the energy cascade (see section 8.2.4).

A scale analysis of the frictional acceleration for the synoptic scale gives $10^{-5} 10^{-11} = 10^{-16} \text{ m/s}^2$, the typical acceleration is 10^{-4} m/s^2 , so the friction on the synoptic scale is twelve orders of magnitude smaller than the acceleration and is therefore completely negligible. It nevertheless has an important thermodynamic significance as it is responsible for the dissipation of kinetic energy. The dissipated kinetic energy is converted into thermal energy. Fluids without friction are called *ideal fluids*.

8.2.1 Incompressible limit case

In the case of incompressibility the equation holds because $S_{m,m} = \nabla \cdot \mathbf{v} = 0$

$$T_{i,j} = -p\delta_{i,j} + 2\mu S_{i,j}. \quad (8.54)$$

From this it follows

$$\frac{1}{\rho} \nabla \cdot T \stackrel{\text{Glg. (8.52)}}{=} r \Delta \mathbf{v}. \quad (8.55)$$

8.2.2 Dissipation

The friction term $\mathbf{f}_R$ dissipates specific kinetic energy $k = \frac{1}{2} \mathbf{v}^2$ into internal energy $i = c^{(V)} T$. The momentum equation in an IS is

$$\frac{D\mathbf{v}}{Dt} = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \mathbf{g} + \mathbf{f}_R \quad (8.56)$$

ring. In this case, the material change in the specific kinetic energy k applies

$$\frac{Dk}{Dt} = \frac{D}{Dt} \left(\frac{1}{2} \mathbf{v}^2 \right) = \mathbf{v} \cdot \frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p \cdot \mathbf{v} + \mathbf{v} \cdot \mathbf{g} + \mathbf{v} \cdot \mathbf{f}_R = -\frac{1}{\rho} \sum_{i=1}^3 v_i \frac{\partial p}{\partial x_i} + \sum_{i=1}^3 v_i g_i + \frac{1}{\rho} \sum_{i,j=1}^3 v_j \frac{\partial \tau_{i,j}}{\partial x_i}. \quad (8.57)$$

Multiplying this by ρ gives

$$\rho \frac{Dk}{Dt} = - \sum_{i=1}^3 v_i \frac{\partial p}{\partial x_i} + \sum_{i=1}^3 \rho v_i g_i + \sum_{i,j=1}^3 v_j \frac{\partial \tau_{i,j}}{\partial x_i}. \quad (8.58)$$

Let $\Omega = \Omega(t) \subseteq \mathbb{R}^3$ be a connected control volume. Then the total energy in this area in the absence of heat flows (except dissipation) applies:

$$\frac{d}{dt} \int_{\Omega(t)} \rho (k + i) d^3 r = \int_{\Omega(t)} \rho \mathbf{v} \cdot \mathbf{g} d^3 r + \int_{\partial\Omega(t)} \mathbf{f} \cdot \mathbf{v} dA. \quad (8.59)$$

Here $\mathbf{v}$ is the force acting on the surface of the control volume. For these, the definitions at the beginning of Section 8.2 apply

$$\int_{\partial\Omega(t)} \mathbf{f} \cdot \mathbf{v} dA = \int_{\partial\Omega(t)} \sum_{i,j=1}^3 n_i T_{i,j} v_j dA = \int_{\Omega(t)} \sum_{i,j=1}^3 \frac{\partial (T_{i,j} v_j)}{\partial x_i} d^3 r. \quad (8.60)$$

For the integrand one obtains

$$\sum_{i,j=1}^3 \frac{\partial (T_{i,j} v_j)}{\partial x_i} = \sum_{i,j=1}^3 v_j \frac{\partial T_{i,j}}{\partial x_i} + T_{i,j} \frac{\partial v_j}{\partial x_i} = \sum_{i,j=1}^3 v_j \frac{\partial \tau_{i,j}}{\partial x_i} + \sum_{i,j=1}^3 \tau_{i,j} \frac{\partial v_j}{\partial x_i} - \sum_{i=1}^3 v_i \frac{\partial p}{\partial x_i} - \sum_{i=1}^3 p \frac{\partial v_i}{\partial x_i}. \quad (8.61)$$

Putting this into Eq. (8.59), you get

$$\frac{d}{dt} \int_{\Omega(t)} \rho (k+i) d^3r = \int_{\Omega(t)} \rho \sum_{i=1}^3 g_i v_i + \sum_{i,j=1}^3 v_j \frac{\partial \tau_{ij}}{\partial x_i} + \sum_{i,j=1}^3 \tau_{ij} \frac{\partial v_j}{\partial x_i} - \sum_{i=1}^3 v_i \frac{\partial p}{\partial x_i} - \sum_{i=1}^3 p \frac{\partial v_i}{\partial x_i} d^3r. \quad (8.62)$$

If you let Ω shrink to the size of a fluid particle, you get

$$\frac{D [\rho (k+i)]}{Dt} = \sum_{i=1}^3 \rho v_i g_i + \sum_{i,j=1}^3 v_j \frac{\partial \tau_{ij}}{\partial x_i} + \sum_{i,j=1}^3 \tau_{ij} \frac{\partial v_j}{\partial x_i} - \sum_{i=1}^3 v_i \frac{\partial p}{\partial x_i} - \sum_{i=1}^3 p \frac{\partial v_i}{\partial x_i}. \quad (8.63)$$

If you subtract Eq. (8.58), one gets

$$\frac{D (\rho i)}{Dt} = \sum_{i,j=1}^3 \tau_{ij} \frac{\partial v_j}{\partial x_i} - \sum_{i=1}^3 p \frac{\partial v_i}{\partial x_i} = -p \nabla \cdot \mathbf{v} + \sum_{i,j=1}^3 \tau_{ij} \frac{\partial v_j}{\partial x_i} \equiv -p \nabla \cdot \mathbf{v} + \rho \varepsilon. \quad (8.64)$$

The specific dissipation rate, or short *Dissipation* ε , is defined by

$$\varepsilon := \frac{1}{\rho} \sum_{i,j=1}^3 \tau_{ij} \frac{\partial v_j}{\partial x_i} \stackrel{\text{Glg.en (8.34) - (8.34)}}{=} \frac{1}{\rho} \sum_{i,j=1}^3 \tau_{ij} \left(S_{ij} - \frac{1}{2} R_{ij} \right) \stackrel{R_{ij} \text{ antisymmetrisch}}{=} \frac{1}{\rho} \sum_{i,j=1}^3 \tau_{ij} S_{ij}. \quad (8.65)$$

It will be as a result of this section

$$\varepsilon = \frac{1}{\rho} \sum_{i,j=1}^3 \tau_{ij} S_{ij} = \frac{1}{\rho} \sum_{i,j=1}^3 \tau_{ij} \frac{\partial v_j}{\partial x_i} \quad (8.66)$$

noted.

8.2.3 Thermodynamic meaning of friction

Friction is usually thought of as a braking force. This is not always the case in fluids. To see this, we use the one-dimensional flow field

$$u = \mathbf{z} + \sin(x) > \mathbf{o} \quad (8.67)$$

out, ignoring units for the moment. Such a field is realistic, it is a background wind with a superimposed wave. If the medium is incompressible, the frictional acceleration is a_R up to a constant

$$a_R = \frac{\partial^2 u}{\partial x^2} = -\sin(x). \quad (8.68)$$

Thus, the work done by friction can

$$ua_R = -u \sin(x) = -(\mathbf{z} + \sin(x)) \sin(x) = -\mathbf{z} \sin(x) - \sin^2(x) \quad (8.69)$$

have both signs. It is therefore possible in fluids for friction to produce kinetic energy. Nevertheless, the mean value of Eq. (8.75) negative, on average the friction dissipates kinetic energy in this case too. However, this is not yet a generally valid derivation of the dissipative effect of friction.

However, if the equations are integrated globally, the negative effect of friction on the integral of kinetic energy can also be seen formally. For this purpose, a one-dimensional incompressible medium is initially assumed, which is limited to the area $[\mathbf{o}, L]$, the boundary conditions are $u(x = \mathbf{o}, L) = \mathbf{o}$. Thus one obtains by means of partial integration

$$\int_{\mathbf{o}}^L ua_R dx = \int_{\mathbf{o}}^L u \frac{\partial^2 u}{\partial x^2} dx = \left[u \frac{\partial u}{\partial x} \right]_{\mathbf{o}}^L - \int_{\mathbf{o}}^L \left(\frac{\partial u}{\partial x} \right)^2 dx = - \int_{\mathbf{o}}^L \left(\frac{\partial u}{\partial x} \right)^2 dx \leq \mathbf{o}. \quad (8.70)$$

Accordingly applies

$$\int_0^L q dx = - \int_0^L u a_R dx \geq 0, \quad (8.71)$$

The friction destroys globally integrated kinetic energy by means of a heat power density q in favor of the internal energy. Locally, however, friction can produce kinetic energy, which is associated with $q < 0$. The boundary conditions are therefore crucial for the thermodynamic role of friction.

Both trains of thought can also be generalized in three dimensions. To do this, first start with a three-dimensional wind field of the shape

$$\mathbf{v}(\mathbf{r}) = \mathbf{u} (2 + \sin(\mathbf{k} \cdot \mathbf{r})) \quad (8.72)$$

out of. From this it follows

$$\mathbf{v} \cdot \Delta \mathbf{v} = -k^2 u^2 \sin(\mathbf{k} \cdot \mathbf{r}) (2 + \sin(\mathbf{k} \cdot \mathbf{r})). \quad (8.73)$$

This expression takes both signs, so even in the three-dimensional case the frictional acceleration can locally produce kinetic energy. The work that the frictional acceleration does can be calculated locally

$$\mathbf{v} \cdot \Delta \mathbf{v} = \sum_{i,j=1}^3 v_i \frac{\partial^2 v_i}{\partial x_j^2} \quad (8.74)$$

note down. Since this expression is isotropic, further consideration can be limited to the terms with x-derivative:

$$\sum_{i=1}^3 v_i \frac{\partial^2 v_i}{\partial x^2} \quad (8.75)$$

Now look at the quantity

$$\Omega := [0, L_x] \times [0, L_y] \times [0, L_z] \quad (8.76)$$

with the boundary conditions

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \nabla \mathbf{v} \cdot \mathbf{n} = 0 \quad (8.77)$$

on $\partial\Omega$, here $\mathbf{n}$ is a normal vector on $\partial\Omega$. If one now integrates Eq. (8.75) on Ω , one obtains

$$\int_{\Omega} \sum_{i=1}^3 v_i \frac{\partial^2 v_i}{\partial x^2} d^3 r = \int_{z=0}^{L_z} \int_{y=0}^{L_y} \int_{x=0}^{L_x} \sum_{i=1}^3 v_i \frac{\partial^2 v_i}{\partial x^2} dx dy dz. \quad (8.78)$$

If you just do the integration over x, you get

$$\int_0^{L_x} \sum_{i=1}^3 v_i \frac{\partial^2 v_i}{\partial x^2} dx = \int_0^{L_x} v_x \frac{\partial^2 v_x}{\partial x^2} + v_y \frac{\partial^2 v_y}{\partial x^2} + v_z \frac{\partial^2 v_z}{\partial x^2} dx. \quad (8.79)$$

If you integrate again partially, it follows

$$\begin{aligned} \int_0^{L_x} v_x \frac{\partial^2 v_x}{\partial x^2} + v_y \frac{\partial^2 v_y}{\partial x^2} + v_z \frac{\partial^2 v_z}{\partial x^2} dx &= \left[v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_y}{\partial x} + v_z \frac{\partial v_z}{\partial x} \right]_0^L - \int_0^{L_x} \left(\frac{\partial v_x}{\partial x} \right)^2 + \left(\frac{\partial v_y}{\partial x} \right)^2 + \left(\frac{\partial v_z}{\partial x} \right)^2 dx \\ &= - \int_0^{L_x} \left(\frac{\partial v_x}{\partial x} \right)^2 + \left(\frac{\partial v_y}{\partial x} \right)^2 + \left(\frac{\partial v_z}{\partial x} \right)^2 dx \leq 0. \end{aligned} \quad (8.80)$$

This implies

$$\int_{\Omega} \mathbf{v} \cdot \Delta \mathbf{v} d^3 r \leq 0. \quad (8.81)$$

Accordingly, in this case too, friction destroys kinetic energy.

Both observations can also be generalized to the three-dimensional compressible case. To do this, one starts again with a wind field of the form Eq. (8.72), but this time with the additional condition $\mathbf{u} \cdot \mathbf{k} = 0$. This implies

$$\nabla \cdot \mathbf{v} = \mathbf{k} \cdot \mathbf{u} \cos(\mathbf{k} \cdot \mathbf{r}) = 0. \quad (8.82)$$

Thus, the term with $\nabla \cdot \mathbf{v}$ falls into Eq. (8.52) with this special wind field, which, in analogy to the three-dimensional incompressible case, means that the work done by the friction force $\mathbf{v} \cdot \mathbf{f}_R$ can take on both signs.

If you multiply Eq. (8.52) with $\rho \mathbf{v}$, one obtains

$$\rho \mathbf{v} \cdot \mathbf{f}_R = \mu \mathbf{v} \cdot \Delta \mathbf{v} + \left(\mu_v + \frac{\mu}{3} \right) \mathbf{v} \cdot \nabla (\nabla \cdot \mathbf{v}). \quad (8.83)$$

Assuming that the viscosities are homogeneous, the following applies analogously to the incompressible case

$$\int_{\Omega} \mu \mathbf{v} \cdot \Delta \mathbf{v} d^3 r \leq 0. \quad (8.84)$$

Calculate for the second term

$$\int_0^{L_x} u \frac{\partial \nabla \cdot \mathbf{v}}{\partial x} dx = [u \nabla \cdot \mathbf{v}]_0^{L_x} - \int_0^{L_x} \frac{\partial u}{\partial x} \nabla \cdot \mathbf{v} dx. \quad (8.85)$$

With the kinematic boundary condition $u(x=0, L_x) = 0$ the first term is omitted. Therefore applies

$$\int_{\Omega} \mathbf{v} \cdot \nabla (\nabla \cdot \mathbf{v}) d^3 r = - \int_{\Omega} (\nabla \cdot \mathbf{v})^2 d^3 r \leq 0. \quad (8.86)$$

This also applies in the compressible case

$$\int_{\Omega} \rho \mathbf{v} \cdot \mathbf{f}_R d^3 r \leq 0. \quad (8.87)$$

8.2.4 Thermodynamic significance of dissipation

According to Eq. (8.66)

$$\begin{aligned} \varepsilon &= \frac{1}{\rho} \sum_{i,j=1}^3 \tau_{i,j} S_{i,j} \stackrel{\text{Glg. (8.50)}}{=} \frac{1}{\rho} \sum_{i,j=1}^3 \left[2\mu \left(S_{i,j} - \frac{1}{3} \nabla \cdot \mathbf{v} \delta_{i,j} \right) + \mu_v \nabla \cdot \mathbf{v} \delta_{i,j} \right] S_{i,j} \\ &= \frac{2\mu}{\rho} \sum_{i,j=1}^3 S_{i,j}^2 - \frac{2}{3} \frac{\mu}{\rho} \sum_{i,j=1}^3 \nabla \cdot \mathbf{v} \delta_{i,j} S_{i,j} + \frac{\mu_v}{\rho} \sum_{i,j=1}^3 \nabla \cdot \mathbf{v} \delta_{i,j} S_{i,j} \\ &\stackrel{\text{Glg. (8.34)}}{=} \frac{2\mu}{\rho} \sum_{i,j=1}^3 S_{i,j}^2 - \frac{2}{3} \frac{\mu}{\rho} \sum_{i,j=1}^3 \nabla \cdot \mathbf{v} \delta_{i,j} \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \frac{\mu_v}{\rho} \sum_{i,j=1}^3 \nabla \cdot \mathbf{v} \delta_{i,j} \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \end{aligned}$$

$$\begin{aligned}
&= \frac{2\mu}{\rho} \sum_{i,j=1}^3 S_{i,j}^2 - \frac{2}{3} \frac{\mu}{\rho} \nabla \cdot \mathbf{v} \sum_{i,j=1}^3 \delta_{i,j} \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \frac{\mu_v}{\rho} \nabla \cdot \mathbf{v} \sum_{i,j=1}^3 \delta_{i,j} \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \\
&= \frac{2\mu}{\rho} \sum_{i,j=1}^3 S_{i,j}^2 - \frac{2}{3} \frac{\mu}{\rho} (\nabla \cdot \mathbf{v})^2 + \frac{\mu_v}{\rho} (\nabla \cdot \mathbf{v})^2 = \frac{2\mu}{\rho} \sum_{i,j=1}^3 S_{i,j}^2 + \left(\frac{\mu_v}{\rho} - \frac{2}{3} \frac{\mu}{\rho} \right) (\nabla \cdot \mathbf{v})^2.
\end{aligned} \tag{8.88}$$

According to Eq. (8.48) applies

$$\mu_v - \frac{2}{3}\mu = \mathcal{L}, \tag{8.89}$$

here $\mathcal{L} \geq 0$ is the Lamé constant. Therefore applies

$$\boxed{\varepsilon \geq 0.} \tag{8.90}$$

According to Eq., the friction destroys (8.87) kinetic energy on a global average, but can also produce kinetic energy locally, as shown in Sect. 8.2.4. The dissipation, on the other hand, is always positive. So local applies

$$\rho \mathbf{v} \cdot \mathbf{f}_R + \rho \varepsilon \stackrel{\text{i. A.}}{\neq} 0. \tag{8.91}$$

However, it is expected that on a global average the dissipation produces exactly as much internal energy as the friction destroys kinetic energy. To show this, one calculates

$$\begin{aligned}
\int_{\Omega} \rho \varepsilon + \rho \mathbf{v} \cdot \mathbf{f}_R d^3r &\stackrel{\text{Glg. (8.66)}}{=} \int_{\Omega} \sum_{i,j=1}^3 \tau_{i,j} \frac{\partial v_j}{\partial x_i} + \rho \mathbf{v} \cdot \mathbf{f}_R d^3r = \int_{\Omega} \sum_{i,j=1}^3 \tau_{i,j} \frac{\partial v_j}{\partial x_i} + \rho \sum_{i,j=1}^3 \frac{1}{\rho} v_j \frac{\partial \tau_{i,j}}{\partial x_i} d^3r \\
&= \int_{\Omega} \sum_{i,j=1}^3 \tau_{i,j} \frac{\partial v_j}{\partial x_i} + \sum_{i,j=1}^3 v_j \frac{\partial \tau_{i,j}}{\partial x_i} d^3r = \int_{\Omega} \sum_{i,j=1}^3 \tau_{i,j} \frac{\partial v_j}{\partial x_i} + v_j \frac{\partial \tau_{i,j}}{\partial x_i} d^3r \\
&= \int_{\Omega} \sum_{i,j=1}^3 \frac{\partial (\tau_{i,j} v_j)}{\partial x_i} d^3r.
\end{aligned} \tag{8.92}$$

As an example, you first consider only the terms with partial derivatives with respect to x and assume $\Omega = [0, L_x] \times [0, L_z] \times [0, L_y]$:

$$\begin{aligned}
\int_0^{L_x} \sum_{j=1}^3 \frac{\partial (\tau_{x,j} v_j)}{\partial x} dx &= \left[\sum_{j=1}^3 \tau_{x,j} v_j \right]_0^{L_x} = [\tau_{x,x} u + \tau_{x,y} v + \tau_{x,z} w]_0^{L_x} \stackrel{u(x=0, L_x)=0}{=} [\tau_{x,y} v + \tau_{x,z} w]_0^{L_x} \\
&= \left[v \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + w \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right]_0^{L_x} \\
&\stackrel{u(x=0, L_x)=0}{=} \left[v \mu \frac{\partial v}{\partial x} + w \mu \frac{\partial w}{\partial x} \right]_0^{L_x} = \mu \left[v \frac{\partial v}{\partial x} + w \frac{\partial w}{\partial x} \right]_0^{L_x}
\end{aligned} \tag{8.93}$$

With the boundary condition

$$\nabla \mathbf{v} \cdot \mathbf{n} = 0 \tag{8.94}$$

are partial derivatives of tangential wind components orthogonal to the surface equal to zero. Thus follows

$$\int_0^{L_x} \sum_{j=1}^3 \frac{\partial (\tau_{x,j} v_j)}{\partial x} dx = 0. \tag{8.95}$$

This also applies to the other spatial directions through cyclic swapping. So it is indeed

$$\int_{\Omega} \rho \varepsilon + \rho \mathbf{v} \cdot \mathbf{f}_R d^3r = 0. \quad (8.96)$$

8.3 Addition of forces

If you put Eq. (B.131) and Eq. (8.52) in Eq. (8.10), this results

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p + \mathbf{v} \times \mathbf{f} + \mathbf{g} + \mathbf{f}_R. \quad (8.97)$$

$\mathbf{f} := \boldsymbol{\omega} \times \mathbf{r}$ is the *Coriolis vector*. With a renaming, the acceleration $\left(\frac{D\mathbf{v}'}{Dt}\right)'$ was also denoted by $\frac{D\mathbf{v}}{Dt}$, see Eq. (B.131). $\mathbf{v}$ is the speed measured in the rotating system. The centrifugal acceleration term was absorbed in $\mathbf{g}$.

The acceleration $\frac{D\mathbf{v}}{Dt}$ can be divided into a local time derivative $\frac{\partial \mathbf{v}}{\partial t}$ and an advective part:

$$\frac{D\mathbf{v}}{Dt} = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \quad (8.98)$$

For the advective part, Eq. (B.57)

$$(\mathbf{v} \cdot \nabla) \mathbf{v} = \frac{1}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times (\nabla \times \mathbf{v}). \quad (8.99)$$

Define the *specific kinetic energy* k by

$$k := \frac{1}{2} \mathbf{v}^2, \quad (8.100)$$

follows

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{1}{\rho} \nabla p + \mathbf{v} \times (\mathbf{f} + \nabla \times \mathbf{v}) - \nabla k + \mathbf{g} + \mathbf{f}_R. \quad (8.101)$$

Now equation (8.97) is written down component by component with respect to the location-dependent orthonormal basis of the spherical coordinates. For the vector $\mathbf{f}$ applies

$$\mathbf{f} = |\mathbf{f}| \begin{pmatrix} 0 \\ \cos(\varphi) \\ \sin(\varphi) \end{pmatrix} =: \begin{pmatrix} 0 \\ f^r \\ f^\varphi \end{pmatrix}. \quad (8.102)$$

$f := \boldsymbol{\kappa} \cdot \mathbf{r}$ bezeichnet man als den *Coriolis-Parameter*. Damit folgt

$$\mathbf{v} \times \mathbf{f} = \begin{pmatrix} f^r v^\varphi - f^\varphi v^r \\ -f^\varphi v^\theta \\ f^\varphi v^\theta \end{pmatrix}. \quad (8.103)$$

If you insert this into the equation of motion, it follows

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} - \frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + g_x - f'w + fv + f_{R,x}, \quad (8.104)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} + \frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + g_y - fu + f_{R,y}, \quad (8.105)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} - \frac{u^2 + v^2}{a+z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + g_z + f'u + f_{R,z}. \quad (8.106)$$

8.4 Boundary conditions

If you want to apply a system of differential equations to a set Ω , you need boundary conditions. Let Ω be limited by condensed matter. Let $\mathbf{n}$ be a normal vector on $\partial\Omega$, then the boundary condition for the wind field is $\mathbf{v}$

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad (8.107)$$

since particles cannot overcome the fixed boundary $\partial\Omega$. This is called *kinematic boundary condition*. This boundary condition is often also required at the upper edge of the atmosphere, which is not a physical reality but a necessary constraint. Another commonly used boundary condition is

$$\mathbf{v}(\partial\Omega) = 0, \quad (8.108)$$

what is called *adhesion condition*. This can be understood as a parameterization of the kinematic boundary condition for small-scale effects on rough surfaces. The term *soil friction* describes the influence of the validity of the kinematic boundary condition on the earth's surface on the dynamics of a geofluid. If a phase interface is in motion, such as the sea surface, one requires that the normal component of the velocity in each medium converges to a common limit as it is approached. For the parallel components this must be the case. A. However, this does not apply.

If the pressure field is continuous, then A applies at a phase boundary

$$\lim_{r \uparrow A} p = \lim_{r \downarrow A} p, \quad (8.109)$$

where the two limit values represent the different sides of the phase interface. This applies except for any surface tension that may be present, which is precisely a discontinuity in the pressure field at an interface. Eq. (8.109) is called *dynamic boundary condition*.

9.1 Ideal monatomic gas

This section is about the thermodynamics of an atmosphere that consists of an ideal, monatomic gas with the individual gas constant R_s .

9.1.1 First law as a temperature equation

The starting point is Eq. (5.82). Differentiation according to time results in:

$$\frac{dE}{dt} + p \frac{dV}{dt} = \frac{dQ_T}{dt} + \mu \frac{dN}{dt}. \quad (9.1)$$

With the equations (5.149) and (5.154) follows

$$\begin{aligned} c^{(V)} m \frac{dT}{dt} + c^{(V)} T \frac{dm}{dt} + p \frac{dV}{dt} &= \frac{dQ_T}{dt} + T \left(\frac{C^{(v)}}{N} - \frac{S}{N} + k_B \right) \frac{dN}{dt} \\ &= \frac{dQ_T}{dt} + T \left(\frac{C^{(v)}}{N} - \frac{S}{N} + \frac{pV}{NT} \right) \frac{dN}{dt}. \end{aligned} \quad (9.2)$$

Division by the mass m of the particle under consideration yields

$$\frac{1}{m} p \frac{dV}{dt} = p \frac{d}{dt} \left(\frac{V}{m} \right) + \frac{pV}{m^2} \frac{dm}{dt} = -\frac{p}{\rho^2} \frac{d\rho}{dt} + \frac{p}{m\rho} \frac{dm}{dt} \quad (9.3)$$

the equation

$$\begin{aligned} c^{(V)} \frac{dT}{dt} - \frac{p}{\rho^2} \frac{d\rho}{dt} &= \frac{dq_T}{dt} - \frac{p}{m\rho} \frac{dm}{dt} + T \left(c^{(V)} - c^{(V)} - s + \frac{p}{\rho T} \right) \frac{1}{N} \frac{dN}{dt} \\ &= \frac{dq_T}{dt} - \frac{p}{m\rho} \frac{dm}{dt} + T(R_s - s) \frac{1}{N} \frac{dN}{dt} \\ &= \frac{dq_T}{dt} - \frac{p}{m\rho} \frac{dm}{dt} + R_s T \frac{1}{N} \frac{dN}{dt} - T s \frac{1}{N} \frac{dN}{dt}, \end{aligned} \quad (9.4)$$

where $s := \frac{S}{m}$ represents the specific entropy and $q_T := \frac{Q_T}{m}$ represents the specific heat. By expanding with the particle mass one obtains

$$c^{(V)} \frac{dT}{dt} - \frac{p}{\rho^2} \frac{d\rho}{dt} = \frac{dq_T}{dt} - \frac{p}{m\rho} \frac{dm}{dt} + R_s T \frac{1}{m} \frac{dm}{dt} - s T \frac{1}{m} \frac{dm}{dt}, \quad (9.5)$$

Based on the equation of state of ideal gases,

$$-\frac{p}{\rho} \frac{1}{m} \frac{dm}{dt} + R_s T \frac{1}{m} \frac{dm}{dt} = 0. \quad (9.6)$$

You define

$$\frac{dq_\rho}{dt} := \frac{1}{m} \frac{dm}{dt}. \quad (9.7)$$

However, the heat and mass flows are usually related to the volume, it is

$$q_\rho^{(V)} := \rho \frac{dq_\rho}{dt}, \quad q_T^{(V)} := \rho \frac{dq_T}{dt} \quad (9.8)$$

defined. This follows

$$c^{(V)} \frac{dT}{dt} - \frac{p}{\rho^2} \frac{d\rho}{dt} = \frac{q_T^{(V)}}{\rho} - \frac{sT}{\rho} q_\rho^{(V)} \quad (9.9)$$

It should be noted that the time derivations are material derivations

$$c^{(V)} \frac{DT}{Dt} - \frac{p}{\rho^2} \frac{D\rho}{Dt} = \frac{q_T^{(V)}}{\rho} - \frac{sT}{\rho} q_\rho^{(V)}. \quad (9.10)$$

Another form of this equation is

$$p \frac{Da}{Dt} = -c^{(V)} \frac{DT}{Dt} + \frac{q_T^{(V)}}{\rho} - \frac{sT}{\rho} q_\rho^{(V)}. \quad (9.11)$$

Using the continuity equation in the form

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v} \quad (9.12)$$

you can do this

$$c^{(V)} \frac{\partial T}{\partial t} + c^{(V)} \mathbf{v} \cdot \nabla T + \frac{p}{\rho} \nabla \cdot \mathbf{v} = \frac{q_T^{(V)}}{\rho} - \frac{sT}{\rho} q_\rho^{(V)} \quad (9.13)$$

reshape. With $p = \rho R_s T$ follows

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T + \frac{R_s T}{c^{(V)}} \nabla \cdot \mathbf{v} = \frac{\partial T}{\partial t} + \nabla \cdot (T \mathbf{v}) + \left(\frac{R_s}{c^{(V)}} - 1 \right) T \nabla \cdot \mathbf{v} = \frac{q_T^{(V)}}{c^{(V)} \rho} - \frac{sT}{c^{(V)} \rho} q_\rho^{(V)}. \quad (9.14)$$

rewrite.

9.1.2 Adiabatic

A process is adiabatic if no heat is transferred, $dQ = 0$. The first law then reads with the state variables of the ideal gas

$$c^{(V)} m \frac{dT}{Dt} = -p \frac{Dv}{Dt}. \quad (9.15)$$

A process coordinate is a quantity as a function of which all other state variables can be written. Time is always a possible process coordinate, but volume is used here. Using the chain rule we get:

$$c^{(V)} m \frac{dT}{dp} \frac{dp}{dV} = -p. \quad (9.16)$$

From the equation of state $pV = nRT$ it follows $T = \frac{pV}{nR}$, so the total derivative of the temperature with respect to the pressure for this process is

$$\frac{dT}{dp} = \frac{\partial T}{\partial p} + \frac{\partial T}{\partial V} \frac{dV}{dp} = \frac{V}{nR} + \frac{p}{nR} \frac{dV}{dp}. \quad (9.17)$$

Putting this into Eq. (9.16), you get

$$\begin{aligned} c^{(V)} m \frac{dp}{dV} \left(\frac{V}{nR} + \frac{p}{nR} \frac{dV}{dp} \right) &= -p \Leftrightarrow \frac{c^{(V)}}{R_s} V \frac{dp}{dV} + \frac{c^{(V)}}{R_s} p = -p \\ &\Leftrightarrow V \frac{dp}{dV} = -p \left(1 + \frac{R_s}{c^{(V)}} \right). \end{aligned} \quad (9.18)$$

If you do the approach with a $z > 0$

$$p(V) = p_0 \left(\frac{V_0}{V} \right)^z, \quad (9.19)$$

follows

$$\frac{dp}{dV} = -z p_0 V_0^z V^{-z-1} = -z p_0 \left(\frac{V_0}{V} \right)^z \frac{1}{V} = -z \frac{p}{V} \quad (9.20)$$

and by comparing coefficients one obtains

$$-z p = -p \left(1 + \frac{R_s}{c^{(V)}} \right) \Leftrightarrow z = 1 + \frac{R_s}{c^{(V)}} = \frac{c^{(p)}}{c^{(V)}}. \quad (9.21)$$

From this it follows

$$z = \frac{c^{(p)}}{c^{(V)}}. \quad (9.22)$$

$z > 1$ bezeichnet man als den *Adiabaten- oder Isentropenexponenten*. Glg. (9.19) bezeichnet man als *Adiabate*.

9.1.3 Entropy as a prognostic variable

If you put the equations of state (5.144) and (7.2) into Eq. (5.142), follows ignoring the approximately sign

$$\begin{aligned} S(E, V, N) &= k_B \frac{3N}{2} \ln(c) + k_B N \ln \left(\frac{V}{N} \right) + k_B \frac{3N}{2} \ln \left(\frac{E}{N} \right) \\ &= k_B \frac{3N}{2} \ln(c) + k_B N \ln \left(\frac{k_B T}{p} \right) + k_B \frac{3N}{2} \ln \left(\frac{3}{2} k_B T \right) \\ &= k_B N \ln(k_B T) + k_B \frac{3N}{2} \ln \left(\frac{3}{2} k_B T \right) - N k_B \ln(p) + k_B \frac{3N}{2} \ln(c) \\ &= k_B \frac{5N}{2} \ln(k_B T) + k_B \frac{3N}{2} \ln \left(\frac{3}{2} \right) - N k_B \ln(p) + k_B \frac{3N}{2} \ln(c) \\ &= k_B \frac{5N}{2} \ln(T) - N k_B \ln(p) + k_B \frac{5N}{2} \ln(k_B) + k_B \frac{3N}{2} \ln \left(\frac{3}{2} \right) + k_B \frac{3N}{2} \ln(c) \\ &= k_B \frac{5N}{2} \ln(T) - N k_B \ln(p) + N k_B \ln \left(k_B^{\frac{5}{2}} \right) + N k_B \ln \left[\left(\frac{3}{2} \right)^{\frac{3}{2}} \right] + N k_B \ln \left(c^{\frac{3}{2}} \right) \\ &= k_B \frac{5N}{2} \ln(T) - N k_B \ln(p) + N k_B \ln \left[k_B^{\frac{5}{2}} \left(\frac{3}{2} \right)^{\frac{3}{2}} c^{\frac{3}{2}} \right] \\ &= k_B \frac{5N}{2} \ln(T) - N k_B \ln(p) + N k_B \ln \left[\left(\frac{3 k_B}{2} c \right)^{\frac{3}{2}} k_B \right]. \end{aligned} \quad (9.23)$$

From Eq. (5.143) is known

$$c = \frac{Me^{5/3}}{3\pi\hbar^2}, \quad (9.24)$$

where M denotes the mass of the particles. From this it follows

$$\begin{aligned} S(E, V, N) &= k_B \frac{5N}{2} \ln(T) - Nk_B \ln(p) + Nk_B \ln \left[\left(\frac{3k_B}{2} \frac{Me^{5/3}}{3\pi\hbar^2} \right)^{\frac{3}{2}} k_B \right] \\ &= k_B \frac{5N}{2} \ln(T) - Nk_B \ln(p) + Nk_B \ln \left[\left(\frac{Me^{5/3}k_B}{2\pi\hbar^2} \right)^{\frac{3}{2}} k_B \right]. \end{aligned} \quad (9.25)$$

With

$$c' := k_B \ln \left[\left(\frac{Me^{5/3}k_B}{2\pi\hbar^2} \right)^{\frac{3}{2}} k_B \right] \quad (9.26)$$

can be abbreviated

$$S(E, V, N) = k_B \frac{5N}{2} \ln(T) - Nk_B \ln(p) + Nc' \quad (9.27)$$

note down. Thus you get

$$\begin{aligned} S(E, V, N) &= C^{(p)} \ln(T) - Nk_B \ln(p) + Nc' \\ &= C^{(p)} \ln \left[\theta \left(\frac{p}{p_o} \right)^{\frac{R_s}{c^{(p)}}} \right] - Nk_B \ln(p) + Nc' \\ &= C^{(p)} \ln(\theta) + R_s m \ln \left(\frac{p}{p_o} \right) - Nk_B \ln(p) + Nc' \\ &= C^{(p)} \ln(\theta) + k_B N \ln(p) - Nk_B \ln(p) - Nk_B \ln(p_o) + Nc' \\ &= C^{(p)} \ln(\theta) - Nk_B \ln(p_o) + Nk_B \ln \left[\left(\frac{k_B Me^{5/3}}{2\pi\hbar^2} \right)^{\frac{3}{2}} k_B \right] \\ &= C^{(p)} \ln(\theta) + Nk_B \ln \left[\frac{k_B}{p_o} \left(\frac{k_B Me^{5/3}}{2\pi\hbar^2} \right)^{\frac{3}{2}} \right] = C^{(p)} \ln(\theta) + \frac{2C^{(p)}}{5} \ln \left[\frac{k_B}{p_o} \left(\frac{k_B Me^{5/3}}{2\pi\hbar^2} \right)^{\frac{3}{2}} \right] \\ &= C^{(p)} \ln(\theta) + mc''. \end{aligned} \quad (9.28)$$

With

$$c'' := \frac{2C^{(p)}}{5} \ln \left[\frac{k_B}{p_o} \left(\frac{k_B Me^{5/3}}{2\pi\hbar^2} \right)^{\frac{3}{2}} \right]. \quad (9.29)$$

This therefore applies to the specific entropy s

$$s = c^{(p)} \ln(\theta) + c'' \quad (9.30)$$

with molar mass M .

You can also use s as a state variable. It is valid

$$\varrho \frac{Ds}{Dt} = c^{(p)} \frac{\varrho}{\theta} \frac{D\theta}{Dt} = \frac{1}{T} \left(q_T^{(V)} - s T q_\varphi^{(V)} \right). \quad (9.31)$$

Add the product of the entropy s with the continuity equation

$$s \frac{\partial \rho}{\partial t} + s \mathbf{v} \cdot \nabla_{\rho} + s \rho \nabla \cdot \mathbf{v} = s q_{\rho}^{(V)} \quad (9.32)$$

added, follows with the definition

$$\tilde{s} := \rho s. \quad (9.33)$$

the equation

$$\frac{\partial \tilde{s}}{\partial t} + \nabla \cdot (\tilde{s} \mathbf{v}) = \frac{q_T^{(V)}}{T}. \quad (9.34)$$

It should be clear at this point that the constant c'' is not irrelevant. Namely replace

$$s \rightarrow s - \tilde{c} \quad (9.35)$$

with an arbitrary constant $\tilde{c}$, then Eq. (9.34)

$$\frac{\partial \tilde{s}}{\partial t} + \nabla \cdot (\tilde{s} \mathbf{v}) = \frac{q_T^{(V)}}{T} + \tilde{c} q_{\rho}^{(V)}. \quad (9.36)$$

If you want to get rid of c'' and use $c^{(p)} \ln(\theta)$ directly as an expression for the entropy, this can only be done by neglecting mass source terms. These do not contribute to the evolution of the entropy density.

With the name change

$$c \rightarrow \frac{c''}{M} \quad (9.37)$$

results as a diagnostic for the potential temperature

$$\theta = \exp\left(\frac{s - c}{c^{(p)}}\right) = \exp\left(\frac{\frac{\tilde{s}}{\rho} - c}{c^{(p)}}\right) = \exp\left(-\frac{c}{c^{(p)}}\right) \exp\left(\frac{\tilde{s}}{c^{(p)} \rho}\right). \quad (9.38)$$

With

$$\theta = T \left(\frac{p_{\circ}}{p}\right)^{R_s/c^{(p)}} = T \left(\frac{p_{\circ}}{\rho R_s T}\right)^{R_s/c^{(p)}} = \left(\frac{p_{\circ}}{R_s}\right)^{R_s/c^{(p)}} T^{c^{(V)}/c^{(p)}} \rho^{-R_s/c^{(p)}} \quad (9.39)$$

you continue to receive

$$T = \left(\frac{R_s}{p_{\circ}}\right)^{R_s/c^{(V)}} \exp\left(-\frac{c}{c^{(V)}}\right) \rho^{R_s/c^{(V)}} \exp\left(\frac{\tilde{s}}{c^{(V)} \rho}\right). \quad (9.40)$$

With

$$\beta := \left(\frac{R_s}{p_{\circ}}\right)^{R_s/c^{(V)}} \exp\left(-\frac{c}{c^{(V)}}\right) \quad (9.41)$$

you can do this shorter than

$$T = \beta \rho^{R_s/c^{(V)}} \exp\left(\frac{\tilde{s}}{c^{(V)}\rho}\right) \quad (9.42)$$

note down. This is the equation of state of ideal gases in entropy formulation.

The forms of the first law of thermodynamics derived in this section are evolutionary equations for entropy and therefore look more like a formulation of the second law. However, they were derived purely from the first law and the thermal equation of state of ideal gases. However, the equation of state itself was derived from the state function, which contains the same information as the entropy. Accordingly, it is expected that the equations derived in this section are closely related to the Second Law. However, this should not obscure the fact that the First and Second Laws are independent statements and one cannot be proven from the other. In Section 10.1 it will be shown that a thermodynamic quantity, which is conserved in adiabatic processes in the ideal gas, is a bijection of the specific entropy.

9.1.3.1 Potential temperature as a prognostic variable

The *potential temperature* θ is the temperature that a gas parcel would have if it were brought adiabatically to an arbitrary reference pressure p_o . If you replace using the equation of state in the adiabatic equation. (9.19) the volume by the temperature is obtained

$$p_o = p \left(\frac{V}{V_o}\right)^z = p \left(\frac{T p_o}{p \theta}\right)^z \Leftrightarrow T_o^z = T^z \left(\frac{p_o}{p}\right)^{z-1} \Leftrightarrow \theta = T \left(\frac{p_o}{p}\right)^{\frac{R_s}{c^{(p)}}} \quad (9.43)$$

One obtains the expression for the potential density ρ_θ

$$\rho_\theta = \rho \left(\frac{p_o}{p}\right)^{\frac{1}{z}}. \quad (9.44)$$

In meteorology, $p_o := 1000$ hPa. The *dry adiabatic temperature gradient* refers to the decrease in temperature with height during adiabatic ascent of a dry air particle. You can easily derive the value using the potential temperature. Yes, it applies

$$\frac{dT}{dz} = \theta \frac{dp}{dz} \frac{R_s}{c^{(p)}} \frac{1}{p_o} \left(\frac{p}{p_o}\right)^{\frac{R_s}{c^{(p)}}-1}, \quad (9.45)$$

since one assumes an adiabatic process and the potential temperature does not change. p_o is the reference pressure, which is also intended to denote the level at which the derivation is carried out. If one uses the hydrostatic approximation and the equation of state of ideal gases, it follows

$$\frac{dT}{dz} = -\theta g \rho_o \frac{R_s}{c^{(p)}} \frac{1}{p_o} = -\frac{g}{c^{(p)}} \approx -0.98 \frac{\text{K}}{100 \text{ m}}, \quad (9.46)$$

one defines the dry adiabatic gradient Γ_d as the magnitude of the decrease

$$\Gamma_d := \frac{g}{c^{(p)}} \approx 0.98 \frac{\text{K}}{100 \text{ m}}. \quad (9.47)$$

The dry adiabatic temperature gradient is not a temperature gradient in the true sense, it is the derivative of the function $T = T(z)$, which describes the adiabatic uplift of a particle. This function is also called dry adiabates. It is not the vertical component of the atmospheric temperature gradient ∇T . This does not have to correspond at all, not even approximately, to the dry adiabatic. It is valid

$$\begin{aligned} \frac{\partial T}{\partial z} &= \theta \frac{\partial p}{\partial z} \frac{R_s}{c^{(p)}} \frac{1}{p_o} \left(\frac{p}{p_o}\right)^{\frac{R_s}{c^{(p)}}-1} + \frac{\partial \theta}{\partial z} \left(\frac{p}{p_o}\right)^{\frac{R_s}{c^{(p)}}} = -\frac{g}{c^{(p)}} - g \frac{p}{R_s T} \frac{\partial \theta}{\partial p} \left(\frac{p}{p_o}\right)^{\frac{R_s}{c^{(p)}}} \\ &\Rightarrow g \frac{p}{R_s \theta} \frac{\partial \theta}{\partial p} = -(\Gamma_d - \Gamma) \end{aligned} \quad (9.48)$$

with

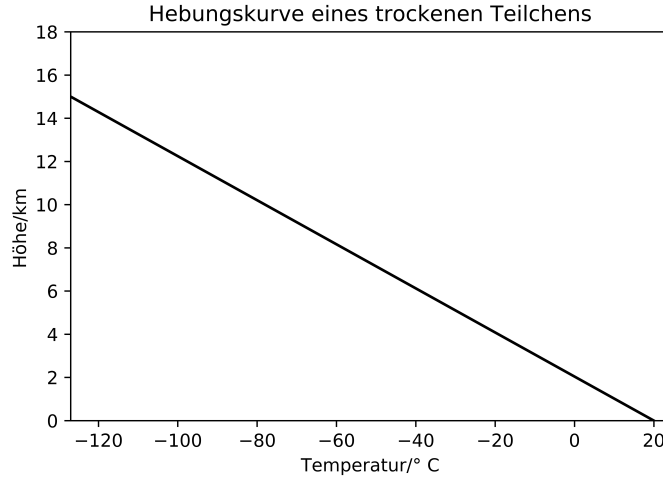


Figure 9.1: The adiabatic uplift of a dry air particle, this curve is also known as the uplift curve.

$$\Gamma := -\frac{\partial T}{\partial z}. \quad (9.49)$$

The material derivation of Eq. (9.43) is

$$\frac{DT}{Dt} = \frac{D\theta}{Dt} \left(\frac{p}{p_o} \right)^{R_s/c^{(p)}} + \theta \frac{dp}{dt} \frac{1}{p_o} \frac{R_s}{c^{(p)}} \left(\frac{p}{p_o} \right)^{R_s/c^{(p)}-1} = \frac{T}{\theta} \frac{D\theta}{Dt} + \frac{T}{p} \omega \frac{R_s}{c^{(p)}} = \frac{T}{\theta} \frac{D\theta}{Dt} + \frac{\omega}{\rho c^{(p)}}. \quad (9.50)$$

From this it follows

$$\begin{aligned} c^{(V)} \frac{T}{\theta} \frac{D\theta}{Dt} + \frac{T}{p} \omega \frac{R_s}{c^{(p)}} c^{(V)} + p \frac{D}{Dt} \frac{R_s T}{p} &= \frac{q_T^{(V)}}{\rho} - \frac{sT}{\rho} q_\rho^{(V)} \\ \Leftrightarrow \frac{D\theta}{Dt} \frac{T}{\theta} + \frac{\omega T}{p} \frac{R_s}{c^{(p)}} - \frac{R_s T}{p c^{(V)}} \omega + \frac{R_s}{c^{(V)}} \frac{DT}{Dt} &= \frac{q_T^{(V)}}{c^{(V)} \rho} - \frac{sT}{c^{(V)} \rho} q_\rho^{(V)} \\ \Leftrightarrow \frac{T}{\theta} \frac{D\theta}{Dt} + \frac{\omega R_s T}{p} \left(\frac{1}{c^{(p)}} - \frac{1}{c^{(V)}} \right) &+ \frac{R_s}{c^{(V)}} \left(\frac{T}{\theta} \frac{D\theta}{Dt} + \frac{T}{p} \omega \frac{R_s}{c^{(p)}} \right) = \frac{q_T^{(V)}}{c^{(V)} \rho} - \frac{sT}{c^{(V)} \rho} q_\rho^{(V)} \\ \Leftrightarrow \frac{T}{\theta} \frac{D\theta}{Dt} \frac{c^{(p)}}{c^{(V)}} + \frac{\omega R_s T}{p} \frac{c^{(V)} - c^{(p)} + R_s}{c^{(V)} c^{(p)}} &= \frac{q_T^{(V)}}{c^{(V)} \rho} - \frac{sT}{c^{(V)} \rho} q_\rho^{(V)}. \end{aligned} \quad (9.51)$$

This means that the first law of thermodynamics for a gas reads in terms of potential temperature

$$\frac{D\theta}{Dt} = \frac{\theta}{T c^{(p)}} \left(q_T^{(V)} - sT q_\rho^{(V)} \right). \quad (9.52)$$

Multiplying this equation by ρ gives

$$\rho \frac{\partial \theta}{\partial t} + \rho \mathbf{v} \cdot \nabla \theta = \frac{\theta}{T c^{(p)}} \left(q_T^{(V)} - sT q_\rho^{(V)} \right). \quad (9.53)$$

Add the product of the potential temperature with the continuity equation

$$\theta \frac{\partial \rho}{\partial t} + \theta \mathbf{v} \cdot \nabla \rho + \theta \rho \nabla \cdot \mathbf{v} = \theta q_\ell^{(V)} = \frac{\theta}{T c^{(p)}} T c^{(p)} q_\ell^{(V)} \quad (9.54)$$

added, follows

$$\frac{\partial (\rho \theta)}{\partial t} + \nabla \cdot (\rho \theta \mathbf{v}) = \frac{\theta}{T c^{(p)}} \left(q_T^{(V)} + T (c^{(p)} - s) q_\ell^{(V)} \right). \quad (9.55)$$

This form is also referred to as *flow form*, whereas Eq. (9.52) *advection form*. The flow form can be understood as a formal continuity equation.

9.2 The isentropic dry atmosphere

In an isentropic atmosphere (atmosphere of homogeneous specific entropy), according to Eq. (9.30) the potential temperature is also homogeneous. This leads to a different dependence of pressure on altitude than in the case of the isothermal atmosphere. If $\Gamma_d > 0$ is the dry adiabatic temperature gradient, the temperature is $T(z) = T_o - \Gamma_d z$ with $T_o := T(z = 0)$. This follows

$$\frac{\partial p}{\partial z} = -g \rho = -g \frac{p}{R_d T} = -\frac{g}{R_d} \frac{p}{T_o - \Gamma_d z} = \frac{gp}{R_d (\Gamma_d z - T_o)} \quad (9.56)$$

as a differential equation to be solved for $p = p(z)$. You do the approach

$$p(z) = C \exp[f(z)] \quad (9.57)$$

with a continuously differentiable function $f = f(z)$ and a constant $C > 0$, it follows

$$\frac{\partial p}{\partial z} = \frac{\partial f}{\partial z} p, \quad (9.58)$$

so you get for f

$$\frac{\partial f}{\partial z} = \frac{g}{R_d (\Gamma_d z - T_o)}, \quad (9.59)$$

this is solved for

$$f = \frac{g}{R_d \Gamma_d} \ln(T_o - \Gamma_d z). \quad (9.60)$$

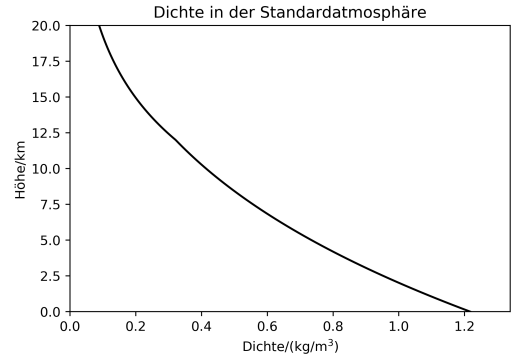
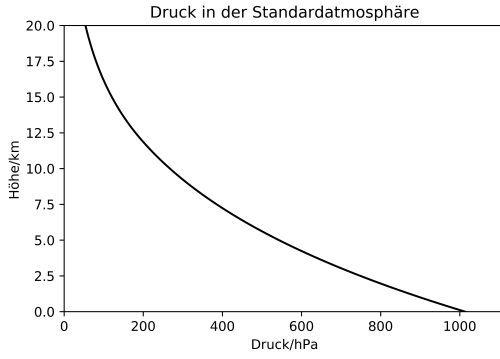
This follows for printing

$$p(z) = C \exp\left(\frac{g}{R_d \Gamma_d} \ln(T_o - \Gamma_d z)\right) = C (T_o - \Gamma_d z)^{\frac{g}{R_d \Gamma_d}}, \quad (9.61)$$

with $p(0) = p_o$ it follows $C = \frac{p_o}{T_o^{\frac{g}{R_d \Gamma_d}}}$. So it applies

$$p(z) = p_o \left(1 - \frac{\Gamma_d z}{T_o}\right)^{\frac{g}{R_d \Gamma_d}}. \quad (9.62)$$

In the troposphere, a linear decrease in temperature with altitude is more realistic than isothermia. However, the dry adiabatic gradient is climatologically too extreme. The *standard atmosphere* is assumed to be an atmosphere



with a temperature of $T_o = 290 \text{ K} = 16.85^\circ \text{ C}$ reduced to the geopotential surface zero and a linear temperature decrease $k = 0.65 \text{ K/100m}$ up to an altitude $H = 12 \text{ km}$. This is assumed to be isothermal. If you replace the dry adiabatic gradient Γ_d by k in the formula for the isentropic atmosphere (9.62) and use the barometric altitude formula above it, it follows

$$p(z) = \begin{cases} p_o \left(1 - \frac{kz}{T_o}\right)^{\frac{g}{R_d k}}, & z < H \\ p(H) \exp\left(-g \frac{z-H}{R_d T_T}\right), & z \geq H \end{cases} \quad (9.63)$$

with $T_T := T_o - kH$ as the temperature of the tropopause.

In a stable atmosphere, θ is a possible vertical coordinate, one speaks of *isentropic coordinates*, since the surfaces with the same vertical coordinate are surfaces with the same entropy.

9.3 Further forms of the first law in the atmosphere

9.3.1 Pressure as a prognostic variable

Now the definition of the potential temperature should be inserted into the equation of state:

$$p = \rho R_s \theta \left(\frac{p}{p_o}\right)^{R_s/c^{(p)}} \Rightarrow p^{1-R_s/c^{(p)}} = \rho R_s \theta \frac{1}{p_o^{R_s/c^{(p)}}} \quad (9.64)$$

$$\Rightarrow p^{1/z} = \rho R_s \theta \frac{1}{p_o^{R_s/c^{(p)}}} \Rightarrow p = (\rho R_s \theta)^z \left(\frac{1}{p_o}\right)^{z-1} \quad (9.65)$$

A prognostic equation can also be derived for p :

$$p = \rho R_s T \Rightarrow \frac{Dp}{Dt} = R_s \left(T \frac{D\rho}{Dt} + \rho \frac{DT}{Dt} \right) \quad (9.66)$$

With

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v} + q_\rho^{(V)}, \quad \frac{DT}{Dt} = \frac{T}{\theta} \frac{D\theta}{Dt} + \frac{TR_s}{c^{(p)} p} \frac{Dp}{Dt} \quad (9.67)$$

follows

$$\begin{aligned}
\frac{Dp}{Dt} &= R_s T (-\rho \nabla \cdot \mathbf{v} + q_\rho) + R_s \rho \left(\frac{T}{\theta} \frac{D\theta}{Dt} + \frac{TR_s}{c^{(p)} p} \frac{Dp}{Dt} \right) \\
&= -p \nabla \cdot \mathbf{v} + R_s T q_\rho^{(V)} + \frac{p}{\theta} \frac{D\theta}{Dt} + \frac{R_s}{c^{(p)}} \frac{Dp}{Dt} \\
\Leftrightarrow \frac{c^{(V)}}{c^{(p)}} \frac{Dp}{Dt} &= -p \nabla \cdot \mathbf{v} + R_s T q_\rho^{(V)} + \frac{p}{\theta} \frac{D\theta}{Dt} \\
\Leftrightarrow \frac{\partial p}{\partial t} &= -\mathbf{v} \cdot \nabla p - \frac{c^{(p)}}{c^{(V)}} p \nabla \cdot \mathbf{v} + \frac{c^{(p)}}{c^{(V)}} R_s T q_\rho^{(V)} + \frac{p}{T \rho c^{(V)}} (q_T^{(V)} - s T q_\rho^{(V)})
\end{aligned} \tag{9.68}$$

$$\Leftrightarrow \frac{\partial p}{\partial t} = -\mathbf{v} \cdot \nabla p - \frac{c^{(p)}}{c^{(V)}} p \nabla \cdot \mathbf{v} + \frac{c^{(p)}}{c^{(V)}} R_s T q_\rho^{(V)} + \frac{R_s}{c^{(V)}} (q_T^{(V)} - s T q_\rho^{(V)}). \tag{9.69}$$

9.3.2 Exner pressure as a prognostic variable

Define the *Exner pressure* Π by

$$\Pi := \frac{T}{\theta} = \left(\frac{p}{p_\circ} \right)^{R_s/c^{(p)}} \Leftrightarrow p = \Pi^{c^{(p)}/R_s} p_\circ, \tag{9.70}$$

the connection applies

$$\begin{aligned}
p &= \rho R_s \theta \Pi \Leftrightarrow \Pi^{c^{(p)}/R_s} = \frac{\rho R_s \theta}{p_\circ} \Pi \Leftrightarrow \Pi^{c^{(V)}/R_s} = \frac{\rho R_s \theta}{p_\circ} \\
\Leftrightarrow \Pi &= \left(\frac{\rho R_s \theta}{p_\circ} \right)^{R_s/c^{(V)}}.
\end{aligned} \tag{9.71}$$

From this it follows

$$\nabla p = R_s \theta \rho \nabla \Pi + R_s \Pi \nabla (\rho \theta) = c^{(p)} \theta \rho \nabla \Pi - c^{(V)} \theta \rho \nabla \Pi + R_s \Pi \nabla (\rho \theta). \tag{9.72}$$

One finds:

$$\begin{aligned}
-c^{(V)} \theta \rho \nabla \Pi + R_s \Pi \nabla (\rho \theta) &= - \left(\frac{R_s}{p_\circ} \right)^{R_s/c^{(V)}} c^{(V)} \theta \rho \nabla (\rho \theta)^{R_s/c^{(V)}} + R_s \Pi \nabla (\rho \theta) \\
&\stackrel{\text{Glg. (9.71)}}{=} R_s \left(\Pi - \left(\frac{R_s}{p_\circ} \right)^{R_s/c^{(V)}} (\rho \theta)^{R_s/c^{(V)}} \right) \nabla (\rho \theta) = \mathbf{o}
\end{aligned} \tag{9.73}$$

So you can write for the pressure gradient acceleration

$$-\frac{\mathbf{I}}{\rho} \nabla p = -c^{(p)} \theta \nabla \Pi. \tag{9.74}$$

With Eq. (B.49) follows

$$\begin{aligned}
\nabla \cdot (\rho c^{(p)} \Pi \theta \mathbf{v}) &= \rho c^{(p)} \theta \mathbf{v} \cdot \nabla \Pi + \Pi \nabla \cdot (\rho c^{(p)} \theta \mathbf{v}) \\
\Leftrightarrow -\rho \mathbf{v} \cdot c^{(p)} \theta \nabla \Pi &= -\nabla \cdot (\rho c^{(p)} T \mathbf{v}) + c^{(p)} \Pi \nabla \cdot (\rho \theta \mathbf{v}) \\
\Leftrightarrow -\rho \mathbf{v} \cdot c^{(p)} \theta \nabla \Pi &= -\nabla \cdot (\rho h \mathbf{v}) + c^{(p)} \Pi \nabla \cdot (\rho \theta \mathbf{v})
\end{aligned} \tag{9.75}$$

with the specific enthalpy h . From this you can deduce:

- If the pressure gradient has an accelerating effect, the flow of potential temperature diverges more than the flow of enthalpy.
- If the pressure gradient has a braking effect, the flow of enthalpy diverges more than the flow of potential temperature.

Now two more prognostic equations for Π are derived. The local time derivation of Eq. (9.71) is in the adiabatic case

$$\begin{aligned}\frac{\partial \Pi}{\partial t} &= \frac{R_s}{c^{(V)}} \left(\frac{\rho R_s \theta}{p_o} \right)^{\frac{R_s}{c^{(V)}} - 1} \frac{\rho R_s \theta}{p_o} \left(\frac{1}{\theta} \frac{\partial \theta}{\partial t} + \frac{1}{\rho} \frac{\partial \rho}{\partial t} \right) = \frac{R_s}{c^{(V)} \theta \rho} \left(\frac{\rho R_s \theta}{p_o} \right)^{\frac{R_s}{c^{(V)}}} \left(\frac{\partial \theta}{\partial t} + \theta \frac{\partial \rho}{\partial t} \right) \\ &= \frac{R_s \Pi}{c^{(V)} \theta \rho} \left(\frac{\partial \theta}{\partial t} + \theta \frac{\partial \rho}{\partial t} \right) = \frac{R_s \Pi}{c^{(V)} \theta \rho} (-\rho \mathbf{v} \cdot \nabla \theta - \theta \nabla \cdot (\rho \mathbf{v})) = -\frac{R_s \Pi}{c^{(V)} \theta \rho} \nabla \cdot (\rho \theta \mathbf{v}).\end{aligned}\quad (9.76)$$

If you add the diabatic terms, it follows

$$\frac{\partial \Pi}{\partial t} = -\frac{R_s \Pi}{c^{(V)} \theta \rho} \left[\nabla \cdot (\rho \theta \mathbf{v}) - \frac{\theta}{T c^{(p)}} \left(q_T^{(V)} + T (c^{(p)} - s) q_\rho^{(V)} \right) \right]. \quad (9.77)$$

For the material derivation of Eq. (9.71) is obtained

$$\frac{D \Pi}{D t} = \frac{R_s}{c^{(V)}} \left(\frac{\rho R_s \theta}{p_o} \right)^{R_s/c^{(V)} - 1} \frac{R_s}{p_o} \frac{D(\rho \theta)}{D t} = \frac{R_s}{c^{(V)} \rho \theta} \left(\frac{\rho R_s \theta}{p_o} \right)^{R_s/c^{(V)}} \frac{D(\rho \theta)}{D t} = \frac{R_s \Pi}{c^{(V)} \rho \theta} \frac{D(\rho \theta)}{D t}. \quad (9.78)$$

With Eq. (9.55) follows

$$\frac{D \Pi}{D t} = \frac{R_s \Pi}{c^{(V)}} \left[-\nabla \cdot \mathbf{v} + \frac{1}{\rho T c^{(p)}} \left(q_T^{(V)} + T (c^{(p)} - s) q_\rho^{(V)} \right) \right]. \quad (9.79)$$

9.4 Ideal gas mixture with a homogeneous composition

N-atomic ideal gases have additional rotational and vibrational degrees of freedom compared to monatomic gases. These additional degrees of freedom increase the heat capacities and an analytical expression for the entropy is then no longer available. A monatomic ideal gas with the same average molar mass as the original gas is used as a model for this complex system, with measured values or products of a more fundamental theory used for the heat capacities. This means that the results listed in the previous section can also be transferred to dry air.

9.5 Ideal gas mixture with variable composition

Here we assume a gas mixture of $N \geq 1$ ideal monatomic gases. Eq. (9.34) can be applied and overlaid on any of these components. This applies

$$\tilde{s}_i = s_i \rho_i \quad (9.80)$$

for $1 \leq i \leq N$ and

$$s = \sum_{i=1}^N \tilde{s}_i. \quad (9.81)$$

In principle, each type of gas gets its own temperature source term $q_{T,i}$. However, to simplify matters, it is assumed that the subsequent exchange of energy between the types of gas is so fast that it can be assumed to be instantaneous. In this case you can

$$q_{T,i}^{(V)} = \frac{\varrho_i c_i^{(V)}}{\sum_{j=1}^N \varrho_j c_j^{(V)}} q_T^{(V)} \quad (9.82)$$

Therefore, Eq. (9.34)

$$\Rightarrow \frac{\partial \tilde{s}}{\partial t} + \nabla \cdot (\tilde{s} \mathbf{v}) = \frac{q_T^{(V)}}{T} \quad (9.83)$$

also with these definitions.

9.5.1 Example: moist air

One defines the so-called *virtual potential temperature* θ_v durch

$$\theta_v := T_v \left(\frac{p_o}{p} \right)^{R_d/c_d^{(p)}}, \quad (9.84)$$

here is

$$T_v = T \left[1 + \frac{\varrho_v}{\varrho_h} \left(\frac{M_d}{M_v} - 1 \right) \right] \quad (9.85)$$

those in Eq. (5.164) defined virtual temperature. The virtual potential temperature is not the potential temperature of moist air θ_h , because for this would

$$\theta_h := T \left(\frac{p_o}{p} \right)^{R_h/c_h^{(p)}} \quad (9.86)$$

apply. The virtual potential temperature is the potential temperature that dry air would have to have in order to have the same density after adiabatic compression to the reference pressure p_o like the moist air under consideration.

For the specific isochoric heat capacity of moist air $c_h^{(v)}$ applies

$$c_h^{(v)} = \frac{\varrho_d c_d^{(v)} + \varrho_v c_v^{(v)}}{\varrho_d + \varrho_v} = c_d^{(v)} \frac{\varrho_d + \varrho_v \frac{c_v^{(v)}}{c_d^{(v)}}}{\varrho_d + \varrho_v} = c_d^{(v)} \frac{\varrho_h - \varrho_v + \varrho_v \frac{c_v^{(v)}}{c_d^{(v)}}}{\varrho_h} = c_d^{(v)} \left[1 + \frac{\varrho_v}{\varrho_h} \left(\frac{c_v^{(v)}}{c_d^{(v)}} - 1 \right) \right] \quad (9.87)$$

According to Eq. (5.148) applies in ideal gas

$$\frac{c_v^{(v)}}{c_d^{(v)}} = \frac{M_d}{M_v}. \quad (9.88)$$

However, if you insert the actual values, you get

$$\frac{c_v^{(v)}}{c_d^{(v)}} = 1,945 \neq 1,608 = \frac{M_d}{M_v}. \quad (9.89)$$

This shows that although real gases can be described very well under atmospheric conditions by the thermal equation of state of ideal gases, their material properties cannot. However, if you ignore this deviation, it follows

$$c_h^{(v)} = c_d^{(v)} \left[1 + \frac{\varrho_v}{\varrho_h} \left(\frac{M_d}{M_v} - 1 \right) \right] \quad (9.90)$$

The adiabatic form of the first law of thermodynamics Eq. (9.14) can now be formulated in virtual temperature terms:

$$\begin{aligned}
 & c_h^{(v)} \frac{DT}{Dt} + R_h T \nabla \cdot \mathbf{v} = 0 \\
 \Leftrightarrow & c_d^{(v)} \left[\mathbf{1} + \frac{\rho_v}{\rho_h} \left(\frac{M_d}{M_v} - \mathbf{1} \right) \right] \frac{DT}{Dt} + R_d T_v \nabla \cdot \mathbf{v} = 0 \\
 \Leftrightarrow & c_d^{(v)} \frac{D \left\{ T \left[\mathbf{1} + \frac{\rho_v}{\rho_h} \left(\frac{M_d}{M_v} - \mathbf{1} \right) \right] \right\}}{Dt} + R_d T_v \nabla \cdot \mathbf{v} = 0 \\
 \Leftrightarrow & c_d^{(v)} \frac{DT_v}{Dt} + R_d T_v \nabla \cdot \mathbf{v} = 0
 \end{aligned} \tag{9.91}$$

The prefactor $\mathbf{1} + \frac{\rho_v}{\rho_h} \left(\frac{M_d}{M_v} - \mathbf{1} \right)$, which turns the temperature into the virtual temperature, can be included in the derivation, since the term $\propto \frac{Dq}{Dt}$ resulting from the product rule according to Eq. (7.28) is equal to zero for adiabatic processes. In humid air you can use adiabatic processes to replace the equations for dry air

$$T \rightarrow T_v \tag{9.92}$$

use if the inaccuracy according to Inq. (9.89) accepted.

9.6 Thermodynamic significance of heat conduction

Eq. (9.83)

$$\frac{\partial \tilde{s}}{\partial t} + \nabla \cdot (\tilde{s} \mathbf{v}) = \frac{q_T^{(V)}}{T} \tag{9.93}$$

is a combination of the first and second laws of thermodynamics. For $q_T^{(V)}$ applies in the absence of radiation and condensates

$$q_T^{(V)} = -\nabla \cdot \mathbf{j}_q + \varepsilon, \tag{9.94}$$

here $\mathbf{j}_q$ is the heat flux density through heat conduction. According to Eq. (5.219) applies

$$\mathbf{j}_q = -\rho c_d^{(v)} \kappa \nabla T. \tag{9.95}$$

You can now do the math

$$\frac{\nabla \cdot (\rho \kappa \nabla T)}{T} = \nabla \cdot \frac{\rho c_d^{(v)} \kappa \nabla T}{T} + \frac{\rho c_d^{(v)} \kappa}{T^2} (\nabla T)^2 = -\nabla \cdot \frac{\mathbf{j}_q}{T} + \frac{\rho c_d^{(v)} \kappa}{T^2} (\nabla T)^2. \tag{9.96}$$

Putting this into Eq. (9.93) and integrate globally, you get

$$\int_A \frac{\partial \tilde{s}}{\partial t} d^3 r = \frac{d}{dt} \int_A \tilde{s} d^3 r = \int_A -\nabla \cdot \frac{\mathbf{j}_q}{T} + \frac{\rho c_d^{(v)} \kappa}{T^2} (\nabla T)^2 d^3 r = - \int_{\partial A} \frac{\mathbf{j}_q}{T} \cdot d\mathbf{n} + \int_A \frac{\rho c_d^{(v)} \kappa}{T^2} (\nabla T)^2 d^3 r. \tag{9.97}$$

The evolution equation of the total entropy of the atmosphere

$$S = \int_A \tilde{s} d^3 r \tag{9.98}$$

in this case is:

$$\frac{dS}{dt} = \underbrace{- \int_{\partial A} \frac{j_q}{T} \cdot d\mathbf{n}}_{\text{Wechselwirkung mit der Umgebung}} + \underbrace{\int_A \frac{\rho c_d^{(v)} \kappa}{T^2} (\nabla T)^2 d^3r}_{\text{Entropieproduktion durch Wärmeleitung (nichtnegativ)}} + \underbrace{\int_A \frac{\varepsilon}{T} d^3r}_{\text{Entropieproduktion durch Dissipation (nichtnegativ)}} \quad (9.99)$$

Internal processes in an ideal gas with viscosity can therefore only produce entropy, as required by the second law of thermodynamics.

9.7 Condensates

The first law must also be formulated for the condensate classes i . To do this, one starts from Eq. (5.34) from:

$$\Delta U_i = \Delta Q_i - \Delta W_i \quad (9.100)$$

The condensates are assumed to be incompressible, i.e. $\Delta W_i = 0$. In addition to radiation, heat transfer and dissipation, phase transitions also play a role as heat sources. These work in two ways:

- They lead to latent heat flows and thus change the temperature.
- They change the composition of the components of the air and change the temperature through mixing.

The first point is discussed in Chap. 11 described in more detail. All heat flows that act on phase i per volume are combined into a source strength q_i . This is about the second point, i.e. the effect of mass flows on the temperature T_i is to be examined. Eq. (7.25) includes five types of mass fluxes, viz

- Phase transitions in which new condensate particles are formed,
- Phase transitions that take place on the surface of a particle,
- Phase transformations of condensate particles so that they change their class,
- collisions and
- Decay processes

Only processes in which matter transitions into phase i contribute to a change in temperature T_i . The class i has the specific heat capacity c_i , the m_j and m_h are the masses passing into the phase i . Then applies to the heat content before or after a mass flow

$$\begin{aligned} c_i m_i T_i(t) + c_h m_h T + \sum_{j \neq i} c_j m_j T_j &= c_i T_i(t + \Delta t) \left(m_h + m_i + \sum_{j \neq i} m_j \right) \\ \Leftrightarrow c_i m_i [T_i(t + \Delta t) - T_i(t)] &= c_h m_h T + \sum_{j \neq i} c_j m_j T_j - c_i T_i(t + \Delta t) \left(m_h + \sum_{j \neq i} m_j \right) \\ \Leftrightarrow \Delta T_i &= \frac{c_h}{c_i m_i} m_h \left(T - \frac{c_i}{c_h} T_i(t + \Delta t) \right) + \frac{1}{c_i m_i} \sum_{j \neq i} [c_j m_j T_j - c_i m_j T_i(t + \Delta t)] \\ \Leftrightarrow \frac{1}{\Delta V} \frac{dT_i}{dt} &= \frac{1}{m_i} \tilde{q}_{hi} \left(\frac{c_h}{c_i} T - T_i \right) + \frac{1}{m_i} \sum_{j \neq i} \tilde{q}_{j,i} \left(\frac{c_j}{c_i} T_j - T_i \right) \\ \Leftrightarrow \rho_i c_i \frac{dT_i}{dt} &= \tilde{q}_{hi} (c_h T - c_i T_i) + \sum_j \tilde{q}_{j,i} (c_j T_j - c_i T_i). \end{aligned} \quad (9.101)$$

It was assumed that all particles of class i have the same temperature T_i , meaning that instantaneous mixing occurs. According to Eq. (7.25) and the considerations in section 11.2 apply

$$\tilde{q}_{hi} = \tilde{q}'_{v,i} + \tilde{q}''_{v,i}. \quad (9.102)$$

Phase transformations, collisions and decay processes contribute to the $\tilde{q}_{j,i}$. According to the considerations in the derivation of Eq. (7.25) applies

$$\tilde{q}_{j,i} = \tilde{m}_j \sum_k \sigma_{j,k} n_j n_k \overline{v_{\text{rel}}}(j, k) P_{j,k} \delta_{i,R_{j,k}} + \tilde{m}_i \lambda_j n_j \sum_l (Z_{jil}) + \tilde{q}_{j,i}'''. \quad (9.103)$$

So you have

$$\begin{aligned} \rho_i c_i \frac{dT_i}{dt} = & q_i + \left(\tilde{q}'_{v,i} + \tilde{q}''_{v,i} \right) (c_h T - c_i T_i) \\ & + \sum_j \left[\tilde{m}_j \sum_k \sigma_{j,k} n_j n_k \overline{v_{\text{rel}}}(j, k) P_{j,k} \delta_{i,R_{j,k}} + \tilde{m}_i \lambda_j n_j \sum_l (Z_{jil}) + \tilde{q}_{j,i}''' \right] (c_j T_j - c_i T_i) \end{aligned} \quad (9.104)$$

The notation explicitly takes into account that what is meant is the isochoric specific heat capacity. An analogous term must also be taken into account for moist air:

$$\rho_h c_h^{(v)} \frac{DT}{Dt} = q_h + \sum_i \left(\tilde{q}'_{v,i} + \tilde{q}''_{v,i} \right) \left(c_h^{(v)} T - c_i T_i \right) \quad (9.105)$$

It makes sense to set the mass density ρ as the first prognostic variable and the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (10.1)$$

as the first prognostic equation. This is because mass density is a very fundamental quantity (it simply describes how much mass is in a given location) and the continuity equation is included in the derivation of many other prognostic equations. Due to the thermal equation of state of ideal gases, one must choose exactly one additional thermodynamic variable $q_1 \neq \rho$ in order to clearly determine the thermodynamic state of the ideal gas. You then record the Hamilton function of the atmosphere

$$H = H(\rho, q_1, \mathbf{v}) = \int_A \frac{1}{2} \rho \mathbf{v}^2 + \rho \varphi + \tilde{I}(\rho, q_1) d^3 r. \quad (10.2)$$

$\tilde{I}(\rho, q_1)$ is the internal energy density as a function of the mass density and the prognostic variable q_1 . The thermal equation of state of ideal gases is implicit in this functional context.

The scalar product of two functions of scalar functions f, g is defined

$$\langle f | g \rangle := \int_A f^*(\mathbf{r}, t) g(\mathbf{r}, t) d^3 r. \quad (10.3)$$

This corresponds to the unitary product Eq. defined in quantum mechanics. (4.1). Real- and complex-valued functions are allowed for f and g . In the case of real functions, the complex conjugation of f does not matter. For vector-valued functions one defines analogously

$$\langle f | g \rangle := \int_A \mathbf{f}^*(\mathbf{r}, t) \cdot \mathbf{g}(\mathbf{r}, t) d^3 r. \quad (10.4)$$

10.1 Reversible dry atmosphere

Let F be any functional of the atmospheric state variables. The time evolution of F can be calculated according to Eq. (2.74) using the Poisson bracket as

$$\frac{dF}{dt} = \{F, H\} + \frac{\partial F}{\partial t}. \quad (10.5)$$

note down. If F does not depend explicitly on time, which is usually the case, it follows

$$\frac{dF}{dt} = \{F, H\}. \quad (10.6)$$

To derive an explicit expression for $\{F, H\}$, one begins by entering Eq. (2.73) $K = H$ inserts:

$$\{F, H\} := \sum_{i=1}^f \left(\frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \quad (10.7)$$

The atmospheric state variables $\mathbf{u} = (\rho, q_1, \mathbf{v})^T$ are now used for the generalized coordinates. However, since F and H are functionals and are generalized coordinate functions, the Poisson bracket must first be generalized for this case. Let $f = f(\mathbf{u})$ be a scalar or vector valued function of the atmospheric state functions. One can now find a functional belonging to f

$$F[\mathbf{u}] := \int_A f(\mathbf{u}) d^3 r \quad (10.8)$$

define. If you derive this in terms of time, you get

$$\frac{dF[\mathbf{u}]}{dt} = \int_A \frac{\partial f(\mathbf{u})}{\partial t} d^3r = \int_A \frac{df(\mathbf{u})}{d\mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial t} d^3r, \quad (10.9)$$

whereby the multidimensional chain rule was used in the last step. This can be further transformed into:

$$\frac{dF[\mathbf{u}]}{dt} = \{F, H\} = \int_A \frac{df(\mathbf{u})}{d\varrho} \cdot \frac{\partial \varrho}{\partial t} d^3r + \int_A \frac{df(\mathbf{u})}{dq_1} \cdot \frac{\partial q_1}{\partial t} d^3r + \int_A \frac{df(\mathbf{u})}{d\mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} d^3r. \quad (10.10)$$

The derivatives of f are the so-called *functional derivatives* of F , one defines

$$\frac{\delta F}{\delta x} := \frac{df}{dx} \quad (10.11)$$

for $x \in \{\varrho, q_1, \mathbf{v}\}$. Therefore applies

$$\frac{dF[\mathbf{u}]}{dt} = \{F, H\} = \int_A \frac{\delta F}{\delta \varrho} \frac{\partial \varrho}{\partial t} d^3r + \int_A \frac{\delta F}{\delta q_1} \frac{\partial q_1}{\partial t} d^3r + \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} d^3r. \quad (10.12)$$

When choosing q_1 , you now limit yourself to the sizes for which

$$\frac{\partial q_1}{\partial t} = -\nabla \cdot (q_1 \mathbf{v}) \quad (10.13)$$

applies. Define $q'_1 := \frac{q_1}{\varrho}$, then Eq. (10.13)

$$\begin{aligned} \frac{\partial (\varrho q'_1)}{\partial t} &= -\nabla \cdot (\varrho q'_1 \mathbf{v}) \\ \Leftrightarrow q'_1 \frac{\partial \varrho}{\partial t} + \varrho \frac{\partial q'_1}{\partial t} &= -q'_1 \nabla \cdot (\varrho \mathbf{v}) - \varrho \mathbf{v} \cdot \nabla q'_1 \\ \text{Kontinuitätsglg.} \quad \Leftrightarrow \varrho \frac{\partial q'_1}{\partial t} &= -\varrho \mathbf{v} \cdot \nabla q'_1 \Leftrightarrow \frac{Dq'_1}{Dt} = 0. \end{aligned} \quad (10.14)$$

q'_1 is therefore a thermodynamic state variable that does not change during adiabatic processes. This implies

$$q'_1 = \frac{q_1}{\varrho} = f(s), \quad (10.15)$$

where s is the specific entropy.

Define p_x for $x \in \{\varrho, q_1, \mathbf{v}\}$ as the canonical momentum belonging to the state variable x . Due to Eq. (2.71) applies

$$\frac{\delta H}{\delta p_\varrho} = \frac{\partial \varrho}{\partial t} = -\nabla \cdot (\varrho \mathbf{v}), \quad (10.16)$$

$$\frac{\delta H}{\delta p_{q_1}} = \frac{\partial q_1}{\partial t} = -\nabla \cdot (q_1 \mathbf{v}) = -\nabla \cdot \left(\frac{q_1}{\varrho} \varrho \mathbf{v} \right), \quad (10.17)$$

$$\frac{\delta H}{\delta p_{\mathbf{v}}} = \frac{\partial \mathbf{v}}{\partial t} = -\frac{1}{\varrho} \nabla p - \frac{\eta}{\varrho} \times \varrho \mathbf{v} - \nabla \varphi - \nabla k, \quad (10.18)$$

here φ is the geopotential and k is the specific kinetic energy. For the globally integrated kinetic energy K of the atmosphere applies

$$K := \int_A \frac{1}{2} \varrho \mathbf{v}^2 d^3r. \quad (10.19)$$

The sum of globally integrated internal and potential energy I' is

$$I' := \int_A \tilde{I} + \rho \varphi d^3r = \int_A \rho \varphi + c_d^{(v)} \rho T d^3r \quad (10.20)$$

This means that $H = K + I'$, since H is the total energy of the atmosphere (H is not explicitly time dependent). It applies regardless of the choice of q_1

$$\frac{\delta I'}{\delta \mathbf{v}} = \mathbf{0} \Rightarrow \frac{\delta H}{\delta \mathbf{v}} = \frac{\delta K}{\delta \mathbf{v}} = \rho \mathbf{v}. \quad (10.21)$$

For K still applies

$$\frac{\delta K}{\delta q_1} = \mathbf{0}, \quad (10.22)$$

$$\frac{\delta K}{\delta \rho} = \frac{1}{2} \mathbf{v}^2 = k. \quad (10.23)$$

If you insert this into the equations (10.16) - (10.18), you get

$$\frac{\delta H}{\delta p_\rho} = \frac{\partial \rho}{\partial t} = -\nabla \cdot \frac{\delta H}{\delta \mathbf{v}}, \quad (10.24)$$

$$\frac{\delta H}{\delta p_{q_1}} = \frac{\partial q_1}{\partial t} = -\nabla \cdot (q_1 \mathbf{v}) = -\nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right), \quad (10.25)$$

$$\frac{\delta H}{\delta p_v} = \frac{\partial \mathbf{v}}{\partial t} = -\frac{1}{\rho} \nabla p - \frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}} - \nabla \varphi - \nabla \frac{\delta K}{\delta \rho}, \quad (10.26)$$

Now the pressure gradient must be expressed in terms of H . According to Eq. (5.91) applies

$$p = - \left(\frac{\partial E}{\partial V} \right)_{S,N}, \quad (10.27)$$

where E is the total energy of the system. The system used is an air particle, in which both the mass m and the particle number N are constant. The total energy here corresponds to the internal energy I . Therefore applies

$$p = - \left(\frac{\partial I/m}{\partial V/m} \right)_s = - \left(\frac{\partial i}{\partial V/m} \right)_s, \quad (10.28)$$

where $i = I/m$ is the specific internal energy. $\frac{V}{m} = a = \frac{1}{\rho}$ is the specific volume. Therefore applies

$$p = - \left(\frac{\partial i}{\partial a} \right)_s = - \frac{\partial \rho}{\partial a} \left(\frac{\partial i}{\partial \rho} \right)_s = \frac{1}{a^2} \left(\frac{\partial i}{\partial \rho} \right)_s = \rho^2 \left(\frac{\partial i}{\partial \rho} \right)_s. \quad (10.29)$$

It now applies

$$\left(\frac{\partial i}{\partial \rho} \right)_s = \left(\frac{\partial i}{\partial \rho} \right)_{\tilde{s}} + \left(\frac{\partial i}{\partial \tilde{s}} \right)_\rho \frac{\partial \tilde{s}}{\partial \rho}. \quad (10.30)$$

For the internal energy density $\tilde{I}$ applies

$$\tilde{I} = \rho i \Rightarrow i = \frac{\tilde{I}}{\rho}, \quad (10.31)$$

it follows from this

$$p = \rho^2 \left(\frac{\partial \tilde{I}/\rho}{\partial \rho} \right)_{\tilde{s}} + \rho^2 \left(\frac{\partial \tilde{I}/\rho}{\partial \tilde{s}} \right)_{\rho} \frac{\partial \tilde{s}}{\partial \rho} = \rho \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} - \tilde{I} + \tilde{s} \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho}. \quad (10.32)$$

This gives the pressure gradient

$$\begin{aligned} \nabla p &= \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} \nabla_{\rho} + \rho \nabla \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} - \nabla \tilde{I} + \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho} \nabla_{\tilde{s}} + \tilde{s} \nabla \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho} \\ &= \left(\left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} \nabla_{\rho} + \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho} \nabla_{\tilde{s}} - \nabla \tilde{I} \right) + \rho \nabla \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} + \tilde{s} \nabla \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho} \\ &= \rho \nabla \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} + \tilde{s} \nabla \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho}. \end{aligned} \quad (10.33)$$

This therefore applies to the pressure gradient acceleration

$$-\frac{\mathbf{I}}{\rho} \nabla p = -\nabla \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{\tilde{s}} - \tilde{s} \nabla \left(\frac{\partial \tilde{I}}{\partial \tilde{s}} \right)_{\rho}. \quad (10.34)$$

Due to Eq. (10.15) is $\frac{q_1}{\rho} = f(s)$, which

$$\left(\frac{\partial i}{\partial x} \right)_s = \left(\frac{\partial i}{\partial x} \right)_{q_1/\rho} \quad (10.35)$$

implied. Thus, Eq. (10.34) to

$$-\frac{\mathbf{I}}{\rho} \nabla p = -\nabla \left(\frac{\partial \tilde{I}}{\partial \rho} \right)_{q_1} - \frac{q_1}{\rho} \nabla \left(\frac{\partial \tilde{I}}{\partial q_1} \right)_{\rho}. \quad (10.36)$$

be generalized. This can be expressed by functional derivatives of the globally integrated internal energy I :

$$-\frac{\mathbf{I}}{\rho} \nabla p = -\nabla \left(\frac{\partial I}{\partial \rho} \right)_{q_1} - \frac{q_1}{\rho} \nabla \left(\frac{\partial I}{\partial q_1} \right)_{\rho}. \quad (10.37)$$

With Eq. (10.22) follows

$$-\frac{\mathbf{I}}{\rho} \nabla p = -\nabla \left(\frac{\partial I}{\partial \rho} \right)_{q_1} - \frac{q_1}{\rho} \nabla \left(\frac{\partial H}{\partial q_1} \right)_{\rho}. \quad (10.38)$$

Putting this into Eq. (10.26), you get

$$\begin{aligned} \frac{\delta H}{\delta p_{\mathbf{v}}} &= \frac{\partial \mathbf{v}}{\partial t} = -\nabla \left(\frac{\partial I}{\partial \rho} \right)_{q_1} - \frac{q_1}{\rho} \nabla \left(\frac{\partial H}{\partial q_1} \right)_{\rho} - \frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}} - \nabla \mathcal{P} - \nabla \frac{\delta K}{\delta \rho} \\ &= -\nabla \frac{\delta H}{\delta \rho} - \frac{q_1}{\rho} \nabla \frac{\delta H}{\delta q_1} - \frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}}. \end{aligned} \quad (10.39)$$

In the second line, the markings of the quantities kept constant were omitted because the definition of H makes it clear how the derivatives are to be understood. If you put the equations (10.24) - (10.25), (10.39) into Eq. (10.12), you get

$$\begin{aligned}\{F, H\} = & - \int_A \frac{\delta F}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} d^3 r - \int_A \frac{\delta F}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\ & - \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \left(\frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}} + \nabla \frac{\delta H}{\delta \rho} + \frac{q_1}{\rho} \nabla \frac{\delta H}{\delta q_1} \right) d^3 r.\end{aligned}\quad (10.40)$$

Rearrangement results

$$\begin{aligned}\{F, H\} = & - \int_A \frac{\delta F}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta \rho} d^3 r \\ & - \int_A \frac{\delta F}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) + \frac{\delta F}{\delta \mathbf{v}} \cdot \frac{q_1}{\rho} \nabla \frac{\delta H}{\delta q_1} d^3 r \\ & - \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \left(\frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r.\end{aligned}\quad (10.41)$$

They apply

$$\frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta \rho} = \nabla \cdot \left(\frac{\delta H}{\delta \rho} \frac{\delta F}{\delta \mathbf{v}} \right) - \frac{\delta H}{\delta \rho} \nabla \cdot \left(\frac{\delta F}{\delta \mathbf{v}} \right), \quad (10.42)$$

$$\frac{\delta F}{\delta \mathbf{v}} \cdot \frac{q_1}{\rho} \nabla \frac{\delta H}{\delta q_1} = \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta q_1} \frac{\delta F}{\delta \mathbf{v}} \right) - \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \right). \quad (10.43)$$

Putting this into Eq. (10.41), you get

$$\begin{aligned}\{F, H\} = & - \int_A \frac{\delta F}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \nabla \cdot \left(\frac{\delta H}{\delta \rho} \frac{\delta F}{\delta \mathbf{v}} \right) - \frac{\delta H}{\delta \rho} \nabla \cdot \left(\frac{\delta F}{\delta \mathbf{v}} \right) d^3 r \\ & - \int_A \frac{\delta F}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) + \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta q_1} \frac{\delta F}{\delta \mathbf{v}} \right) - \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \right) d^3 r \\ & - \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \left(\frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r.\end{aligned}\quad (10.44)$$

You are now leaving

$$\int_A \nabla \cdot \left(\frac{\delta H}{\delta \rho} \frac{\delta F}{\delta \mathbf{v}} \right) d^3 r = \int_A \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta q_1} \frac{\delta F}{\delta \mathbf{v}} \right) d^3 r = 0 \quad (10.45)$$

which is satisfied by Gauss's theorem if $\frac{\delta F}{\delta \mathbf{v}} \cdot \mathbf{n} = 0$ on ∂A . Under these conditions, the time evolution equation applies to any functional F in a reversible dry atmosphere

$$\begin{aligned}\frac{dF}{dt} = \{F, H\} = & - \int_A \frac{\delta F}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} - \frac{\delta H}{\delta \rho} \nabla \cdot \frac{\delta F}{\delta \mathbf{v}} d^3 r \\ & - \int_A \frac{\delta F}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) - \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \right) d^3 r \\ & - \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \left(\frac{\boldsymbol{\eta}}{\rho} \times \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r.\end{aligned}\quad (10.46)$$

This results as expected

$$\{H, H\} = 0. \quad (10.47)$$

You now define

$$\begin{aligned}
\{F, H\}_\rho &:= - \int_A \frac{\delta F}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} - \frac{\delta H}{\delta \rho} \nabla \cdot \frac{\delta F}{\delta \mathbf{v}} d^3 r = - \int_A - \frac{\delta H}{\delta \mathbf{v}} \cdot \nabla \frac{\delta F}{\delta \rho} + \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta \rho} d^3 r \\
&= - \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta \rho} - \frac{\delta H}{\delta \mathbf{v}} \cdot \nabla \frac{\delta F}{\delta \rho} d^3 r,
\end{aligned} \tag{10.48}$$

$$\begin{aligned}
\{F, H\}_{q_1} &:= - \int_A \frac{\delta F}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) - \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \right) d^3 r = - \int_A - \frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \cdot \nabla \frac{\delta F}{\delta q_1} + \frac{q_1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta q_1} d^3 r \\
&= - \int_A \frac{q_1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \cdot \nabla \frac{\delta H}{\delta q_1} - \frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \cdot \nabla \frac{\delta F}{\delta q_1} d^3 r
\end{aligned} \tag{10.49}$$

It becomes clear that each bracket can be formulated in a „scalar field x divergence“ and in a „vector field x gradient“ notation. Each of the two brackets is antisymmetric:

$$\{F, H\}_\rho = -\{H, F\}_\rho \tag{10.50}$$

$$\{F, H\}_{q_1} = -\{H, F\}_{q_1} \tag{10.51}$$

Now we define so-called *Nambu brackets* by

$$\{F, g, H\} := - \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot \left(\frac{1}{\rho} \frac{\delta g}{\delta \mathbf{v}} \times \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r = - \int_A \frac{1}{\rho} \frac{\delta F}{\delta \mathbf{v}} \cdot \left(\frac{\delta g}{\delta \mathbf{v}} \times \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r, \tag{10.52}$$

here g is a functional. For Nambu brackets applies

$$\{F, g, H\} = \{H, F, g\} = \{g, H, F\}. \tag{10.53}$$

Furthermore applies

$$\{F, g, H\} = -\{F, H, g\} = -\{g, F, H\} = -\{H, g, F\}. \tag{10.54}$$

If you put this together with the equations (10.50) - (10.51) in Eq. (10.66), you get

$$\{H, F\} = \{H, F\}_\rho + \{H, F\}_{q_1} + \{H, h_a, F\} = -\{F, H\}_\rho - \{F, H\}_{q_1} - \{F, h_a, H\} = -\{F, H\}. \tag{10.55}$$

Now define a *reduced helicity* Z (for the original definition of helicity see Eq. (15.104)).

$$Z := \frac{1}{2} \mathbf{v} \cdot \nabla \times \mathbf{v} \tag{10.56}$$

and the absolute helicity Z_a by

$$Z_a := \frac{1}{2} \mathbf{v}_a \cdot \nabla \times \mathbf{v}_a = \frac{1}{2} (\boldsymbol{\Omega} \times \mathbf{r} + \mathbf{v}) \cdot \nabla \times (\boldsymbol{\Omega} \times \mathbf{r} + \mathbf{v}), \tag{10.57}$$

this is the helicity measured in the inertial system. The corresponding functionals are given by

$$Z := \int_A \frac{1}{2} \mathbf{v} \cdot \nabla \times \mathbf{v} d^3 r, \tag{10.58}$$

$$Z_a := \int_A \frac{1}{2} \mathbf{v}_a \cdot \nabla \times \mathbf{v}_a d^3 r \tag{10.59}$$

defined. Now let $\mathbf{h} : A \rightarrow \mathbb{R}^3$ be a test function with $\mathbf{h}(\partial A) = \mathbf{0}$ and $\varepsilon > 0$. You define

$$Z'(\varepsilon) := \int_A \frac{1}{2} (\mathbf{v} + \varepsilon \mathbf{h}) \cdot \nabla \times (\mathbf{v} + \varepsilon \mathbf{h}) d^3 r = \int_A \frac{1}{2} \mathbf{v} \cdot \nabla \times \mathbf{v} d^3 r + \int_A \frac{\varepsilon}{2} \mathbf{h} \cdot \nabla \times \mathbf{v} d^3 r + \int_A \frac{\varepsilon}{2} \mathbf{v} \cdot \nabla \times \mathbf{h} d^3 r + \mathcal{O}(\varepsilon^2). \tag{10.60}$$

The equation now applies to first order in ε

$$\begin{aligned}
\frac{Z'(\varepsilon) - Z'(\circ)}{\varepsilon} &= \frac{Z'(\varepsilon) - Z}{\varepsilon} = \int_A \frac{\mathbf{1}}{2} \mathbf{h} \cdot \nabla \times \mathbf{v} d^3r + \int_A \frac{\mathbf{1}}{2} \mathbf{v} \cdot \nabla \times \mathbf{h} d^3r = \frac{\mathbf{1}}{2} \int_A \mathbf{h} \cdot \nabla \times \mathbf{v} + \mathbf{v} \cdot \nabla \times \mathbf{h} d^3r \\
&= \frac{\mathbf{1}}{2} \int_A \mathbf{v} \cdot \nabla \times \mathbf{h} - \mathbf{h} \cdot \nabla \times \mathbf{v} + \mathbf{2h} \cdot \nabla \times \mathbf{v} d^3r \stackrel{\text{Glg. (B.55)}}{=} \frac{\mathbf{1}}{2} \int_A \nabla \cdot (\mathbf{h} \times \mathbf{v}) + \mathbf{2h} \cdot \nabla \times \mathbf{v} d^3r \\
&= \int_A \mathbf{h} \cdot \nabla \times \mathbf{v} d^3r.
\end{aligned} \tag{10.61}$$

In the last step, Gauss's theorem and the fact $\mathbf{h}(\partial A) = \circ$ were used. Therefore applies

$$\frac{\delta Z}{\delta \mathbf{v}} = \nabla \times \mathbf{v} = \boldsymbol{\xi}. \tag{10.62}$$

The same applies too

$$\frac{\delta Z_a}{\delta \mathbf{v}_a} = \nabla \times \mathbf{v}_a = \boldsymbol{\eta}. \tag{10.63}$$

Due to

$$\frac{\delta Z}{\delta \mathbf{v}} = \frac{\delta H}{\delta \mathbf{v}_a} \tag{10.64}$$

also applies

$$\frac{\delta Z_a}{\delta \mathbf{v}} = \boldsymbol{\eta}. \tag{10.65}$$

Thus, one can use Eq. (10.46) in the form

$$\frac{dF}{dt} = \{F, H\} = \{F, Z_a, H + \{F, H\}_{\varrho} + \{F, H\}_{q_i}\} \tag{10.66}$$

write.

10.1.1 Semi-prognostic variable

The Poisson bracket formalism leads to a special form of pressure gradient acceleration. In addition to ϱ and q_i , this usually contains a third variable, and occasionally even a fourth or fifth. One of these variables is chosen as the so-called *semi-prognostic variable* q_z . Due to the thermal equation of state of ideal gases, this is no longer an independent prognostic variable, as the thermodynamic state would otherwise be overdetermined, but it is distinguished from other diagnostic variables because it plays a role in the evolution of forms of energy.

10.1.1.1 Conservation of energy from a Poisson bracket perspective

For energy forms F the fact $\frac{\delta F}{\delta \mathbf{v}} \parallel \mathbf{v}$ applies, so in this case applies

$$\{F, H_a, H\} = \circ \Rightarrow \{F, H\} = \{F, H\}_{\varrho} + \{F, H\}_{q_i}. \tag{10.67}$$

Follow from this

$$\begin{aligned}
 \{K, H\} &= \int_A -\frac{\delta K}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta H}{\delta \varphi} \nabla \cdot \frac{\delta K}{\delta \mathbf{v}} + \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta K}{\delta \mathbf{v}} \right) d^3 r \\
 &= \int_A -\frac{\delta K}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta H}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\
 &= \int_A \frac{\delta(H-K)}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta I'}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\
 &= \int_A \frac{\delta I'}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta I'}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r,
 \end{aligned} \tag{10.68}$$

$$\{I', H\} = \int_A -\frac{\delta I'}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} - \frac{\delta I'}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r. \tag{10.69}$$

If you add both, you get as expected

$$\{K, H\} + \{I', H\} = \{H, H\} = 0. \tag{10.70}$$

10.1.2 Potential temperature as a prognostic variable

Use the potential temperature instead of the temperature and define

$$q_1 := \tilde{\theta} = \varphi \theta, \tag{10.71}$$

follows with Eq. (9.65)

$$\begin{aligned}
 H &= H(\mathbf{v}, \varphi, q_1) = H(\mathbf{v}, \varphi, \tilde{\theta}) = \int_A \frac{1}{2} \varphi \mathbf{v}^2 + \varphi \varphi + c_d^{(v)} \frac{p(\varphi, \tilde{\theta})}{R_d} d^3 r \\
 &= \int_A \frac{1}{2} \varphi \mathbf{v}^2 + \varphi \varphi + c_d^{(v)} \frac{p_o}{R_d} \left(\frac{R_d \tilde{\theta}}{p_o} \right)^{\gamma} d^3 r = \int_A \frac{1}{2} \varphi \mathbf{v}^2 + \varphi \varphi + c_d^{(v)} \frac{p_o}{R_d} \left(\frac{R_d q_1}{p_o} \right)^{\gamma} d^3 r.
 \end{aligned} \tag{10.72}$$

The functional derivatives of this are

$$\frac{\delta H}{\delta \varphi} = \frac{1}{2} \mathbf{v}^2 + \varphi, \tag{10.73}$$

$$\frac{\delta H}{\delta q_1} = c_d^{(v)} \frac{p_o}{R_d} \frac{R_d}{p_o} \gamma \left(\frac{R_d q_1}{p_o} \right)^{\gamma-1} = c_d^{(p)} \left(\frac{R_d q_1}{p_o} \right)^{\gamma-1} = c_d^{(p)} \left(\frac{R_d q_1}{p_o} \right)^{\frac{R_d}{c_d^{(v)}}} \stackrel{\text{Glg. (9.71)}}{=} c_d^{(p)} \Pi, \tag{10.74}$$

$$\frac{\delta H}{\delta \mathbf{v}} = \varphi \mathbf{v}. \tag{10.75}$$

Now the time developments of the quantities K and I' should be examined. This includes preparation

$$\frac{\delta K}{\delta \varphi} = \frac{1}{2} \mathbf{v}^2, \quad \frac{\delta K}{\delta q_1} = 0, \quad \frac{\delta K}{\delta \mathbf{v}} = \varphi \mathbf{v}, \tag{10.76}$$

$$\frac{\delta I'}{\delta \varphi} = \varphi, \quad \frac{\delta I'}{\delta q_1} = c_d^{(p)} \Pi, \quad \frac{\delta I'}{\delta \mathbf{v}} = 0. \tag{10.77}$$

and thus receives

$$\begin{aligned}
\{K, H\} &= \int_A \frac{\delta H}{\delta \varphi} \nabla \cdot \frac{\delta K}{\delta \mathbf{v}} - \frac{\delta K}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta K}{\delta \mathbf{v}} \right) - \frac{\delta K}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\
&= \int_A \left(\frac{1}{2} \mathbf{v}^2 + \varphi \right) \nabla \cdot (\varphi \mathbf{v}) - \frac{1}{2} \mathbf{v}^2 \nabla \cdot (\varphi \mathbf{v}) + c_d^{(p)} \Pi \nabla \cdot (q_1 \mathbf{v}) d^3 r \\
&= \int_A \varphi \nabla \cdot (\varphi \mathbf{v}) + c_d^{(p)} \Pi \nabla \cdot (q_1 \mathbf{v}) d^3 r \\
&= \int_A -\varphi \mathbf{v} \cdot \nabla \varphi - c_d^{(p)} q_1 \mathbf{v} \cdot \nabla \Pi d^3 r,
\end{aligned} \tag{10.78}$$

$$\begin{aligned}
\{I', H\} &= \int_A \frac{\delta H}{\delta \varphi} \nabla \cdot \frac{\delta I'}{\delta \mathbf{v}} - \frac{\delta I'}{\delta \varphi} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta I'}{\delta \mathbf{v}} \right) - \frac{\delta I'}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\varphi} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\
&= \int_A -\varphi \nabla \cdot (\varphi \mathbf{v}) - c_d^{(p)} \Pi \nabla \cdot (q_1 \mathbf{v}) d^3 r.
\end{aligned} \tag{10.79}$$

10.1.3 Entropy density as a prognostic variable

If you use the entropy instead of the potential temperature and define

$$q_1 := \tilde{s} = \rho s, \tag{10.80}$$

follows

$$\begin{aligned}
H &= H(\mathbf{v}, \varphi, q_1) = H(\mathbf{v}, \varphi, \tilde{s}) = \int_A \frac{1}{2} \varphi \mathbf{v}^2 + \varphi \varphi + c_d^{(v)} \frac{p(\varphi, \tilde{s})}{R_d} d^3 r \\
&= \int_A \frac{1}{2} \varphi \mathbf{v}^2 + \varphi \varphi + c_d^{(v)} \frac{p(\varphi, q_1)}{R_d} d^3 r.
\end{aligned} \tag{10.81}$$

The functional derivatives of this are

$$\begin{aligned}
\frac{\delta H}{\delta \varphi} &\stackrel{\text{Glg. (5.91)}}{=} \frac{1}{2} \mathbf{v}^2 + \varphi + G, & \frac{\delta H}{\delta q_1} &\stackrel{\text{Glg. (5.91)}}{=} T, & \frac{\delta H}{\delta \mathbf{v}} &= \varphi \mathbf{v}.
\end{aligned} \tag{10.82}$$

G denotes the specific Gibbs potential. Now the time developments of the quantities K and I' are examined again. This includes preparation

$$\frac{\delta K}{\delta \varphi} = \frac{1}{2} \mathbf{v}^2, \quad \frac{\delta K}{\delta q_1} = 0, \quad \frac{\delta K}{\delta \mathbf{v}} = \varphi \mathbf{v}, \tag{10.83}$$

$$\frac{\delta I'}{\delta \varphi} = \varphi + G, \quad \frac{\delta I'}{\delta q_1} = T, \quad \frac{\delta I'}{\delta \mathbf{v}} = 0. \tag{10.84}$$

and thus receives

$$\begin{aligned}
 \{K, H\} &= \int_A \frac{\delta H}{\delta \rho} \nabla \cdot (\rho \mathbf{v}) - \frac{\delta K}{\delta \rho} \nabla \cdot (\rho \mathbf{v}) + T \nabla \cdot (q_1 \mathbf{v}) d^3 r \\
 &= \int_A (\varphi + G) \nabla \cdot (\rho \mathbf{v}) + T \nabla \cdot (q_1 \mathbf{v}) d^3 r \\
 &= \int_A -\rho \mathbf{v} \cdot \nabla (\varphi + G) - q_1 \mathbf{v} \cdot \nabla T d^3 r,
 \end{aligned} \tag{10.85}$$

$$\begin{aligned}
 \{I', H\} &= \int_A \frac{\delta H}{\delta \rho} \nabla \cdot \frac{\delta I'}{\delta \mathbf{v}} - \frac{\delta I'}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} + \frac{\delta H}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta I'}{\delta \mathbf{v}} \right) - \frac{\delta I'}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\
 &= \int_A -\frac{\delta I'}{\delta \rho} \nabla \cdot \frac{\delta H}{\delta \mathbf{v}} - \frac{\delta I'}{\delta q_1} \nabla \cdot \left(\frac{q_1}{\rho} \frac{\delta H}{\delta \mathbf{v}} \right) d^3 r \\
 &= \int_A -(\varphi + G) \nabla \cdot (\rho \mathbf{v}) - T \nabla \cdot (q_1 \mathbf{v}) d^3 r.
 \end{aligned} \tag{10.86}$$

This gives the expression for the pressure gradient acceleration

$$-\frac{1}{\rho} \nabla p = -\nabla G - s \nabla T. \tag{10.87}$$

This is also carried out

$$\begin{aligned}
 -\nabla G - s \nabla T &= -c_d^{(p)} \nabla T + T \nabla s = -c_d^{(p)} \nabla T + T c_d^{(p)} \nabla \ln(\theta) \\
 &= -c_d^{(p)} \nabla T + \frac{T}{\theta} c_d^{(p)} \nabla \theta = -c_d^{(p)} \theta \nabla \frac{T}{\theta} = -c_d^{(p)} \theta \nabla \Pi
 \end{aligned} \tag{10.88}$$

confirmed.

10.2 Irreversible dry atmosphere

This section is only formulated using the entropy formula started in Section 10.1.3. In an irreversibly dry atmosphere, two irreversible brackets are defined:

$$(F, f_R) := \left\langle \frac{\delta F}{\delta \mathbf{v}} \middle| f_R \right\rangle = \int_A \frac{\delta F}{\delta \mathbf{v}} \cdot f_R d^3 r \tag{10.89}$$

$$(F, Q) := \left\langle \frac{\delta F}{\delta \widetilde{s}} \middle| \frac{\rho \varepsilon}{T} \right\rangle = \int_A \frac{\delta F}{\delta \widetilde{s}} \frac{\rho \varepsilon}{T} d^3 r \tag{10.90}$$

According to Eq. (8.96) applies here

$$(H, f_R) + (H, Q) = 0. \tag{10.91}$$

The dynamics are then determined by

$$\frac{dF}{dt} = \{F, H\} + (F, f_R) + (F, Q). \tag{10.92}$$

10.3 Heterogeneous atmosphere

According to the findings of section 9.5.1, the replacement can be carried out in a humid atmosphere without condensates

$$\theta \rightarrow \theta_v \tag{10.93}$$

take over the reversible part of the dynamics according to Sect. 10.1.2 if one assumes that dry air and water vapor are perfect ideal gases.

10.3.1 Condensates

Condensates move at a speed $\mathbf{v}_i \neq \mathbf{v}$, which does not correspond to the wind speed because they have a superimposed fall speed. This must be taken into account in the global integral of the kinetic energy. This would generate some additional terms. However, this is not practical relative to the benefits. Instead, the existence of the condensates is linked to the dynamics with the following interventions:

- The pressure gradient acceleration is multiplied by a prefactor $\frac{\rho_h}{\rho}$, since the condensates have to be accelerated by the pressure gradient but do not generate any pressure themselves. The same applies to frictional acceleration. The Coriolis acceleration and gravity, on the other hand, are not modified in this way, since these forces also act on condensates (the fact that the Coriolis acceleration acting on condensates differs from the Coriolis acceleration acting on the gas phase due to their falling speed is ignored).
- Since the first law is formulated for the quantity $\rho_h \theta_v$, the thermal power densities must be multiplied by a prefactor $\frac{\rho_h c_h^{(v)}}{\rho c} \leq 1$.

10.4 Coupling to the radiation field

When solving the radiation transfer equation, it is assumed that the radiation field is in equilibrium with the temperature and density field at all times. The time derivatives of the radiation field are therefore neglected (quasi-stationary process). If one wanted to embed the radiation field in the Hamiltonian formalism, this would lead to equations with time derivatives for the radiation field that would have to be solved on such small time scales that this is not practical for the atmosphere.

Everything that violates adiabaticness, i.e. heat and mass flows across system boundaries, is diabatic. The power densities of heat are made up of:

- Heat conduction,
- heat transfer,
- latent heat,
- Radiation and
- Dissipation.

The swelling strengths of the mass arise from

- Diffusion,
- phase transitions,
- Collisions and
- decay,

see equations (7.23) - (7.25).

11.1 Heat conduction

Heat conduction only occurs in the gas phase and, according to Eq. (5.220) to a temperature tendency

$$\frac{\partial (\rho c_h^{(v)} T)}{\partial t} = \nabla \cdot (\rho c_h^{(v)} \kappa \nabla T) \quad (11.1)$$

with κ_h as the thermal diffusivity of moist air.

11.2 Phase transition heat

If evaporation, melting or sublimation occurs, the heat required for this is removed from the educt. If the phase transition takes place in the other direction, the heat affects the product. In Chap. 7 a distinction was made between three types of phase transitions. In the first case, new particles of class i are created, it applies

$$q'_i = c_{i,v} (\tilde{q}'_{v,i} - \tilde{q}'_{i,v}) \quad (11.2)$$

for the heat output per volume acting on component i , here $c_{i,v}$ is the phase transformation enthalpy of i into the gas phase.

In the second case, the phase transition occurs between the gas and existing particles of component i , which leads to the transformation of particles into another class of condensate j . However, the latent heat still acts on the particles of component i :¹

$$q''_i = c_{i,v} (\tilde{q}''_{v,i} - \tilde{q}''_{i,v}) \quad (11.3)$$

In the third case, condensates transform into each other. This applies to this

$$q'''_i = \sum_j c_{i,j} \tilde{q}'''_{j,i} - c_{i,j} \tilde{q}'''_{i,j}. \quad (11.4)$$

¹The heat transferred in this process within a time interval Δt is divided by mass between the two condensate classes; for Δt the heat transferred per mass approaches zero, but the converted mass also approaches zero, so that the heat acting on component j approaches zero in the second order of time.

Here $c_{i,j}$ is the phase transition enthalpy acting on i in the corresponding process. For example, if i is liquid and j is solid, then $c_{i,j} = 0$, since in this case the latent heat would act on the solid phase j as noted above. For the total source strength of heat due to phase transitions q_i applies

$$q_i = q'_i + q''_i + q'''_i. \quad (11.5)$$

It should be emphasized again at this point that there are no latent heat flows affecting the gas phase, only the condensates. The energy is then distributed via heat transfer, including to the gas phase.

11.3 Heat transfer

If the condensates have different temperatures than the moist air, this is accompanied by a *heat transfer* (diffusive heat flow through an interface). One goes from the equation

$$s = \xi \Delta T \quad (11.6)$$

where ΔT is the temperature difference between the two phases, ξ is the *heat transfer coefficient* and s is the heat flux density. For the corresponding power density q_i in the fluid, which acts on the condensate class i , one has

$$q_i = n_i A_i \xi_i (T - T_i). \quad (11.7)$$

Here n_i is the particle density of the condensates i , A_i is their surface and ξ_i is the heat transfer coefficient with respect to moist air. This applies to the air

$$q_h = \sum_i n_i A_i \xi_i (T_i - T). \quad (11.8)$$

11.4 Dissipation

In a medium with condensation products, it is assumed that the power density q_{diss} is distributed among the components according to the masses:

$$q_{\text{diss},i} = -\rho_i \mathbf{v} \cdot \mathbf{f}_R \quad (11.9)$$

The total power density then results in:

$$q_{\text{diss}} = q_h + \sum_i q_{\text{diss},i} = - \left[\rho_h + \sum_i \rho_i \right] \mathbf{v} \cdot \mathbf{f}_R = -\rho \mathbf{v} \cdot \mathbf{f}_R, \quad (11.10)$$

what again Eq. (8.66) corresponds.

11.5 Radiation transfer equation

The Poynting theorem Eq. (3.47) is a continuity equation for the radiant flux density $\mathbf{S}$. The derivation is classic, $-\mathbf{j} \cdot \mathbf{E}$ is the power that the field performs on moving charges. You can write down the equation as

$$\frac{1}{v_h} (P_{\text{Feld}} + P_{\text{Ladungen}}) = -\nabla \cdot \mathbf{S}, \quad (11.11)$$

where $P_{\text{field}} = \frac{\partial w}{\partial t}$ is the local-time derivative of the energy density and $\mathbf{j} \cdot \mathbf{E}$ is the charge carrier power. The charges are generally not free, but structured into atoms and molecules, and P_{charges} can lead to quantum mechanical excitations of a more general nature. This means you can write down the equation as

$$\frac{1}{v_h} (P_{\text{Feld}} + P_{\text{Materie}}) = -\nabla \cdot \mathbf{S}. \quad (11.12)$$

It is $P_{\text{Field}} \ll P_{\text{Matter}}$ and therefore one can get a good approximation

$$\frac{\mathbf{I}}{v_h} P_{\text{Materie}} = -\nabla \cdot \mathbf{S}. \quad (11.13)$$

set.

Planck's radiation law Eq. (5.316) was previously formulated as a function of the angular frequency ω . However, when it comes to spectra, the wavelength λ is usually used as the independent quantity. It applies

$$c = \frac{\lambda}{T} \Rightarrow \lambda = cT = \frac{2\pi c}{\frac{2\pi}{T}} = \frac{2\pi c}{\omega} \Rightarrow \omega = \frac{2\pi c}{\lambda}. \quad (11.14)$$

With the demand

$$u(\omega) d\omega \stackrel{!}{=} u(\lambda) d\lambda \quad (11.15)$$

follows

$$u(\lambda) = u(\omega(\lambda)) \left| \frac{d\omega}{d\lambda} \right| = \frac{\hbar 8\pi^3 c^3}{\pi^2 c^3 \lambda^3} \frac{\mathbf{I}}{\exp\left(\frac{\hbar 2\pi c}{k_B T \lambda}\right) - \mathbf{I}} \frac{2\pi c}{\lambda^2} = \frac{8\pi c h}{\lambda^5} \frac{\mathbf{I}}{\exp\left(\frac{hc}{k_B T \lambda}\right) - \mathbf{I}}. \quad (11.16)$$

For the spectral radiance of black body radiation, L_B follows

$$L_B(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{\mathbf{I}}{\exp\left(\frac{hc}{k_B T \lambda}\right) - \mathbf{I}}. \quad (11.17)$$

The spectral radiance in the atmosphere depends on the location, direction and wavelength, i.e. $L = L(\mathbf{r}, \lambda, \vartheta, \varphi)$. This results in the field of spectral radiation flux density $\mathbf{S}_\lambda$

$$\mathbf{S}_\lambda(\mathbf{r}, \lambda) = \int_0^{2\pi} \int_0^\pi L(\mathbf{r}, \lambda, \vartheta, \varphi) \mathbf{e}(\vartheta, \varphi) \sin(\vartheta) d\vartheta d\varphi \quad (11.18)$$

with $\mathbf{e}(\vartheta, \varphi)$ as the unit vector pointing in the direction specified by ϑ and φ .

Let $j \in \{d, v, i\}$ denote a component of air, where i stands for a condensate class. Each component has individual radiation properties and therefore has its own spectral power density q_j . It quickly becomes clear that when passing through matter, the change in spectral radiance applies

$$dL(\Omega) \propto \varrho_j, \quad dL(\Omega) \propto ds, \quad (11.19)$$

here Ω is a solid angle element. From this one can conclude:

$$dL(\Omega) = \overbrace{-\varrho_j k_j L ds}^{\text{Absorption}} + \overbrace{\varrho_j k_j L_B ds}^{\text{Emission}} + \overbrace{ds \varrho_j \int_{4\pi} s_j(\Omega', \Omega) L(\Omega') d\Omega'}^{\text{Zustreuung aus anderen Raumrichtungen}} - \overbrace{ds \varrho_j L(\Omega) \int_{4\pi} s_j(\Omega, \Omega') d\Omega'}^{\text{Wegstreuung in andere Raumrichtungen}}$$

Here k_j is the *absorption coefficient* and s_j is the *scattering cross section*. This merely describes the change in spectral radiance due to component i . To describe the actual change, one must sum over all components:

$$\begin{aligned} dL(\Omega) &= ds (L_B - L(\Omega)) \sum_j (k_j \varrho_j) + ds \sum_i \varrho_j \int_{4\pi} s_j(\Omega', \Omega) L(\Omega') d\Omega' \\ &\quad - ds \sum_j \varrho_j L(\Omega) \int_{4\pi} s_j(\Omega, \Omega') d\Omega'. \end{aligned} \quad (11.20)$$

This is the *radiation transfer equation*. The heating rate acting on component i then applies

$$q_j = \int_0^\infty (\nabla \cdot \mathbf{S}_\lambda)_j d\lambda. \quad (11.21)$$

11.6 Boundary conditions

On the surface of the earth applies

$$\mathbf{j}_v \cdot \mathbf{n} = E + S - R - C, \quad (11.22)$$

Here $\mathbf{n}$ stands for the normal vector of the earth's surface, E for the evaporation rate, S for the sublimation rate, R for the resublimation rate and C for the condensation rate, all with the dimension *mass per area and time*. This is a boundary condition on the flux density $\mathbf{j}_v$.

The boundary conditions in the radiation transfer equation are:

$$\mathbf{S}_{\text{in}} = S_o \mathbf{e}_{\text{Sonne} \rightarrow \text{Erde}} \quad (11.23)$$

at the top edge as well

$$L(\lambda, \vartheta, \varphi) = \varepsilon(\lambda, \vartheta, \varphi, T) L_B(\lambda, \vartheta, \varphi, T) \quad (11.24)$$

Furthermore is

$$\xi_{\text{SFC}}(T_{\text{SFC}} - T) \quad (11.25)$$

the heat flux density, which occurs as a boundary condition at the surface in the first law for moist air.

11.7 Compilation of the governing equations

$$\begin{aligned}
\forall (i \in \{\text{gasförmige Bestandteile der Luft}\}) \quad \frac{D\mathbf{v}_i}{Dt} &= -\frac{1}{\rho} \nabla p + \mathbf{v}_i \times \mathbf{f} + \mathbf{g} + r \Delta \mathbf{v}_g \\
\forall (i \in \{\text{Kondensatklassen}\}) \quad \mathbf{j}_i &= \rho_i \mathbf{v} - \mathbf{k}_{\rho_i} v_i \\
p &= T_g R_g \rho'_g \\
c_g^{(v)} \frac{DT}{Dt} + p \frac{D}{Dt} \left[\frac{1 - \sum_{j \in \{\text{Kondensatklassen}\}} \frac{\rho_j}{\rho'_j}}{\rho_g} \right] &= \frac{q_g}{\rho_g} \\
\frac{\partial \rho_d}{\partial t} + \nabla \cdot \mathbf{j}_d &= 0 \\
\forall (i \in \{\text{Tracerklassen}\}) \quad \frac{\partial \rho_i}{\partial t} + \nabla \cdot \mathbf{j}_i &= Q_i \\
\forall (i \in \{\text{Kondensatklassen}\}) \quad c_i^{(v)} \frac{DT}{Dt} &= \frac{q_i}{\rho_i} \\
dL(\Omega) &= ds(L_B - L(\Omega)) \sum_{j \in \{d,v,i\}} (k_j \rho_j) \\
&+ ds \sum_{j \in \{d,v,i\}} \rho_j \int_{4\pi} s_j(\Omega', \Omega) L(\Omega') d\Omega' \\
&- ds \sum_{j \in \{d,v,i\}} \rho_j L(\Omega) \int_{4\pi} s_j(\Omega, \Omega') d\Omega'
\end{aligned}$$

Randbedingungen

$$\begin{aligned}
\mathbf{v} \cdot \mathbf{n} &= 0 \text{ am Oberrand} \\
\rho_i &= 0 \text{ am Oberrand} \\
\mathbf{v} \cdot \mathbf{n} &= 0 \text{ am Unterrand} \\
\mathcal{S}_{\text{in}} &= \mathcal{S}_o \mathbf{e}_{\text{Sonne} \rightarrow \text{Erde}} \text{ am Oberrand} \\
\mathbf{j}_v \cdot \mathbf{n} &= E + S - R - C \text{ am Unterrand} \\
L(\mathcal{I}, \mathcal{J}, \varphi, T) &= \varepsilon(\mathcal{I}, \mathcal{J}, \varphi, T) L_B(\mathcal{I}, \mathcal{J}, \varphi, T) \text{ am Oberrand} \\
\tau_{\text{SFC}} (T_{\text{SFC}} - T) &= \text{Wärmedurchgang am Unterrand}
\end{aligned}$$

Not only is the determinism of these equations mathematically unclear, they are also incomplete because, as equations of statistical physics, they contain higher statistical moments. These are usually small, but due to the nonlinearity, the smallest inaccuracies lead to a major change in the solution after a time $t > t_{\text{crit}}$. A non-statistical prediction is therefore in principle only possible for a limited period of time.

Part III
dynamics

12 GENERALIZED VERTICAL COORDINATES

A generalized vertical coordinate μ is defined by a transformation $\mu \leftrightarrow z$. This illustration is i. A. depends on the horizontal coordinates: $z = z(\varphi, \lambda, \mu)$. For a scalar field ψ is written in geographical coordinates with geodetic or generalized vertical coordinates

$$\psi(\varphi, \lambda, z(\varphi, \lambda, \mu)) = \tilde{\psi}(\varphi, \lambda, \mu), \quad (12.1)$$

so follows for the gradients in these coordinates

$$\nabla \psi = \begin{pmatrix} \frac{\partial \psi}{\partial \varphi} \\ \frac{\partial \psi}{\partial \lambda} \\ \frac{\partial \psi}{\partial z} \end{pmatrix}, \quad (12.2)$$

$$\nabla \tilde{\psi} = \begin{pmatrix} \frac{\partial \tilde{\psi}}{\partial \varphi} \\ \frac{\partial \tilde{\psi}}{\partial \lambda} \\ \frac{\partial \tilde{\psi}}{\partial \mu} \end{pmatrix}. \quad (12.3)$$

It applies

$$\frac{\partial \tilde{\psi}}{\partial \lambda} = \frac{d}{d\lambda} \psi(\varphi, \lambda, z(\varphi, \lambda, \mu)) = \nabla \psi \cdot \begin{pmatrix} \frac{d\varphi}{d\lambda} \\ \frac{d\lambda}{d\lambda} \\ \frac{dz}{d\lambda} \end{pmatrix} = \nabla \psi \cdot \begin{pmatrix} 0 \\ 1 \\ \frac{\partial z}{\partial \lambda} \end{pmatrix} = \frac{\partial \psi}{\partial \lambda} + \frac{\partial z}{\partial \lambda} \frac{\partial \psi}{\partial z}. \quad (12.4)$$

The derivatives with respect to λ are proportional to the derivatives with respect to x . This follows

$$\frac{\partial \tilde{\psi}}{\partial x} = \frac{\partial \psi}{\partial x} + \frac{\partial z}{\partial x} \frac{\partial \psi}{\partial z}. \quad (12.5)$$

If you ignore the difference between ψ and $\tilde{\psi}$ in the notation and instead mark variables that are kept constant with indices, you get

$$\left(\frac{\partial \psi}{\partial x} \right)_{\mu} = \left(\frac{\partial \psi}{\partial x} \right)_z + \left(\frac{\partial z}{\partial x} \right)_{\mu} \frac{\partial \psi}{\partial z}. \quad (12.6)$$

z and μ are interchangeable in the derivation, so the same applies

$$\left(\frac{\partial \psi}{\partial x} \right)_z = \left(\frac{\partial \psi}{\partial x} \right)_{\mu} + \left(\frac{\partial \mu}{\partial x} \right)_z \frac{\partial \psi}{\partial \mu}. \quad (12.7)$$

Partial derivatives $\frac{\partial}{\partial x}, \frac{\partial}{\partial z}$ occur in the governing equations; up to now, z was used as the vertical coordinate. If you want to transform to a generalized coordinate μ , you use the chain rule and set Eq. (12.6) at:

$$\frac{\partial \psi}{\partial z} = \frac{\partial \mu}{\partial z} \frac{\partial \psi}{\partial \mu} \quad (12.8)$$

$$\left(\frac{\partial \psi}{\partial x} \right)_z = \left(\frac{\partial \psi}{\partial x} \right)_{\mu} - \left(\frac{\partial z}{\partial x} \right)_{\mu} \frac{\partial \mu}{\partial z} \frac{\partial \psi}{\partial \mu} \quad (12.9)$$

Analogously also in the y direction. The material derivative $\frac{D}{Dt}$ is independent of the vertical coordinate. However, the horizontal material derivative $\frac{D_h}{Dt}$ (see equation (B.12)) depends on the coordinate system. z is not distinguished in the above derivation, so z can be replaced by any vertical coordinate r .

12.1 p system

In the p-system, the pressure p is used as the vertical coordinate, which is possible with hydrostatics ($\frac{\partial p}{\partial z} = -g\rho \neq 0$, see section 13.7). For the *total derivative* in the p-system then applies

$$\frac{D\psi}{Dt} = \frac{\partial\psi}{\partial t} + u\frac{\partial\psi}{\partial x} + v\frac{\partial\psi}{\partial y} + \omega\frac{\partial\psi}{\partial p}. \quad (12.10)$$

Here $\omega := \frac{Dp}{Dt}$ is the vertical velocity in the p-system. In Section 13.7 the governing equations are transformed into the p-system.

12.2 θ -system

In a thermally stable stratified atmosphere, θ can be used as a generalized vertical coordinate. In addition, hydrostatics is assumed here. This is called θ -system or also as *isentropic coordinates*. If you write down the equations (12.8) - (12.9) with $\mu = \theta$, it follows

$$\frac{\partial\psi}{\partial z} = \frac{\partial\theta}{\partial z} \frac{\partial\psi}{\partial\theta}, \quad (12.11)$$

$$\left(\frac{\partial\psi}{\partial x}\right)_z = \left(\frac{\partial\psi}{\partial x}\right)_\theta - \left(\frac{\partial z}{\partial x}\right)_\theta \frac{\partial\theta}{\partial z} \frac{\partial\psi}{\partial\theta} = \left(\frac{\partial\psi}{\partial x}\right)_\theta + \varrho \left(\frac{\partial\varphi}{\partial x}\right)_\theta \frac{\partial\theta}{\partial p} \frac{\partial\psi}{\partial\theta}, \quad (12.12)$$

$$\left(\frac{\partial\psi}{\partial y}\right)_z = \left(\frac{\partial\psi}{\partial y}\right)_\theta - \left(\frac{\partial z}{\partial y}\right)_\theta \frac{\partial\theta}{\partial z} \frac{\partial\psi}{\partial\theta} = \left(\frac{\partial\psi}{\partial y}\right)_\theta + \varrho \left(\frac{\partial\varphi}{\partial y}\right)_\theta \frac{\partial\theta}{\partial p} \frac{\partial\psi}{\partial\theta}. \quad (12.13)$$

In the case $\psi = p$ it follows

$$\left(\frac{\partial p}{\partial x}\right)_z = \left(\frac{\partial p}{\partial x}\right)_\theta - \left(\frac{\partial z}{\partial x}\right)_\theta \frac{\partial\theta}{\partial z} \frac{\partial p}{\partial\theta} = \left(\frac{\partial p}{\partial x}\right)_\theta + \varrho \left(\frac{\partial\varphi}{\partial x}\right)_\theta. \quad (12.14)$$

It applies

$$\begin{aligned} p &= \varrho R_d \theta \left(\frac{p}{p_\circ}\right)^{\frac{R_d}{c(p)}} \\ \Rightarrow \left(\frac{\partial p}{\partial x}\right)_\theta &= R_d \theta \left(\frac{p}{p_\circ}\right)^{\frac{R_d}{c(p)}} \left(\frac{\partial\varrho}{\partial x}\right)_\theta + \varrho R_d \theta \frac{1}{p_\circ^{\frac{R_d}{c(p)}}} \frac{R_d}{c(p)} p^{\frac{R_d}{c(p)}-1} \left(\frac{\partial p}{\partial x}\right)_\theta \\ &= R_d T \left(\frac{\partial\varrho}{\partial x}\right)_\theta + \varrho R_d \theta \left(\frac{p}{p_\circ}\right)^{\frac{R_d}{c(p)}} \frac{R_d}{c_p p} \left(\frac{\partial p}{\partial x}\right)_\theta \\ &= R_d T \left(\frac{\partial\varrho}{\partial x}\right)_\theta + \varrho R_d T \frac{R_d}{c^{(p)} \varrho R_d T} \left(\frac{\partial p}{\partial x}\right)_\theta \\ &= R_d T \left(\frac{\partial\varrho}{\partial x}\right)_\theta + \frac{R_d}{c^{(p)}} \left(\frac{\partial p}{\partial x}\right)_\theta \\ \Rightarrow \left(\frac{\partial p}{\partial x}\right)_\theta &= \frac{c^{(p)} R_d T}{c^{(V)}} \left(\frac{\partial\varrho}{\partial x}\right)_\theta = \frac{c^{(p)}}{c^{(V)}} T \left(\frac{\partial}{\partial x} \left(\frac{p}{T}\right)\right)_\theta \\ &= \frac{c^{(p)}}{c^{(V)}} T \left(\frac{1}{T} \frac{\partial p}{\partial x} - \frac{p}{T^2} \frac{\partial T}{\partial x}\right) = \frac{c^{(p)}}{c^{(V)}} \left(\frac{\partial p}{\partial x}\right)_\theta - \frac{c^{(p)}}{c^{(V)}} \frac{p}{T} \left(\frac{\partial T}{\partial x}\right)_\theta \\ &= \frac{c^{(p)}}{c^{(V)}} \left(\frac{\partial p}{\partial x}\right)_\theta - \frac{c^{(p)}}{c^{(V)}} \varrho R_d \left(\frac{\partial T}{\partial x}\right)_\theta \\ \Rightarrow \frac{R_d}{c^{(V)}} \left(\frac{\partial p}{\partial x}\right)_\theta &= \frac{c^{(p)}}{c^{(V)}} \varrho R_d \left(\frac{\partial T}{\partial x}\right)_\theta \Rightarrow \left(\frac{\partial p}{\partial x}\right)_\theta = c^{(p)} \varrho \left(\frac{\partial T}{\partial x}\right)_\theta. \end{aligned} \quad (12.15)$$

Thus you get

$$\frac{1}{\rho} \left(\frac{\partial p}{\partial x} \right)_z = \frac{\partial}{\partial x} \left(c^{(p)} T + \varphi \right), \quad (12.16)$$

where on the right-hand side the partial derivative is carried out in the θ -system. You define

$$M := c^{(p)} T + \varphi \quad (12.17)$$

as the *Montgomery potential*.

12.3 σ_z -System

With h as *orography* and H as the upper edge of the atmosphere, one defines the *orographic coordinate* σ_z by

$$\sigma_z := \frac{z - h}{H - h} \Leftrightarrow z = h + \sigma_z (H - h), \quad (12.18)$$

follow from this

$$\frac{\partial \sigma_z}{\partial z} = \frac{1}{H - h}, \quad (12.19)$$

$$\left(\frac{\partial z}{\partial x} \right)_{\sigma_z} = (1 - \sigma_z) \frac{\partial h}{\partial x}, \quad (12.20)$$

$$\left(\frac{\partial z}{\partial x} \right)_{\sigma_z} \frac{\partial \sigma_z}{\partial z} = \frac{1 - \sigma_z}{H - h} \frac{\partial h}{\partial x}. \quad (12.21)$$

12.4 σ_p -system

Using p_S as the surface pressure and p_T as the pressure at the top of the atmosphere, one defines another orographic coordinate σ_p by

$$\sigma_p := \frac{p - p_T}{p_S - p_T} \Leftrightarrow p = p_T + \sigma_p (p_S - p_T), \quad (12.22)$$

follow from this

$$\frac{\partial \sigma_p}{\partial p} = \frac{1}{p_S - p_T}, \quad (12.23)$$

$$\left(\frac{\partial p}{\partial x} \right)_{\sigma_p} = \sigma_p \frac{\partial p_S}{\partial x}, \quad (12.24)$$

$$\left(\frac{\partial p}{\partial x} \right)_{\sigma_p} \frac{\partial \sigma_p}{\partial z} = \frac{\sigma_p}{p_S - p_T} \frac{\partial p_S}{\partial x}. \quad (12.25)$$

13 IMPORTANT APPROXIMATIONS

In meteorology and oceanography there are many difficult approximations with detailed and complex assumptions. This chapter explains the most common lists of them, starting with the less rigorous ones.

13.1 General

13.1.1 Filtering

Approximations are often made to the governing equations that are physically contradictory or contradict the definitions. Humidity definitely plays a role in the dynamics, but cyclogenesis (i.e. the formation of low pressure areas) can also be observed in a dry atmosphere. This is called *filtering*: Moisture is not necessary for the formation of low pressure areas because low pressure areas still form in a dry atmosphere and are therefore not filtered. If you want to investigate a phenomenon, you first always choose the simplest possible system of equations.

13.1.2 Dimensionless metrics

In order to be able to compare different terms in the governing equations, dimensionless key figures are introduced.

Nonlinearity is particularly problematic in the theoretical treatment of hydrodynamics. A large part of this lies in the momentum advection $(\mathbf{v} \cdot \nabla) \mathbf{v}$. These terms make a decisive contribution to the interaction of the scales (spectral components) and to the creation of instabilities. Friction, on the other hand, is a stabilizing influence. The so-called *Reynolds number* N_{Re} is therefore defined as the ratio of these two terms:

$$N_{\text{Re}} := \frac{U^2}{L} \frac{L^2}{rU} = \frac{UL}{r} \quad (13.1)$$

The larger the Reynolds number is, the more unstable and turbulent the flow is. On the synoptic scale applies

$$N_{\text{Re}} \sim \frac{10^1 10^6}{10^{-5}} = 10^{12}. \quad (13.2)$$

Synoptic currents are therefore very unstable.

The *Rossby number* N_{Ro} is defined as the ratio of advective terms to the Coriolis force, i.e

$$N_{\text{Ro}} := \frac{U^2}{LfU} = \frac{U}{Lf}. \quad (13.3)$$

13.2 Spherical geopotential approximation

Horizontal pressure gradients are four orders of magnitude smaller than vertical ones (see section 13.7), so it is practical to align one axis of the coordinate system with gravity so that it does not affect the horizontal equations of motion. First of all, you can simply use spherical coordinates for this; the orography can be interpreted as the height of the earth's surface above the sphere. However, the Earth is more of an ellipsoid than a sphere. A first approach to this could be to absorb the Earth's more ellipsoidal shape into the orography and continue to use spherical coordinates. The following applies to the angle φ that the ellipsoid includes with a spherical surface

$$\tan(\varphi) \approx \frac{\tilde{f}}{\pi/2} \approx 0,2\%. \quad (13.4)$$

Assuming that the gravity is perpendicular to the ellipsoid, it has a horizontal component in spherical coordinates of the order of magnitude 10^{-2} m/s^2 , which is an order of magnitude larger than the horizontal pressure gradient. Overlaying the horizontal dynamics with such a large force is disadvantageous. So if you want to take the eccentricity of the gravity field into account, you should choose non-spherical coordinates.

However, if one calculates these effects into g_z in terms of magnitude and uses a spherical approximation of the gravity field, one speaks of the *spherical geopotential approximation (SGA)*. This means

$$g_x = 0, \quad (13.5)$$

$$g_y = 0. \quad (13.6)$$

Furthermore, one defines

$$\mathbf{g} := -g_z. \quad (13.7)$$

Thus, the equation system Equations (8.104) - (8.105) under the SGA becomes

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} - \frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} - f'w + fv + F_{R,x}, \quad (13.8)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} + \frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} - fu + F_{R,y}, \quad (13.9)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} - \frac{u^2 + v^2}{a+z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g + f'u + F_{R,z}. \quad (13.10)$$

$\mathbf{g}$ must be rotation-free as a gradient field,

$$\nabla \times \mathbf{g} = \mathbf{o}. \quad (13.11)$$

According to Eq. (B.114) applies

$$\begin{aligned} \mathbf{o} = \nabla \times \mathbf{g} &= -\frac{g_y}{r} \mathbf{i} + \frac{g_x \tan(\varphi)}{r} \mathbf{k} + \frac{g_x}{r} \mathbf{j} + \mathbf{k} \left(-\frac{\partial g_x}{\partial y} + \frac{\partial g_y}{\partial x} \right) - \mathbf{j} \left(\frac{\partial g_z}{\partial x} - \frac{\partial g_x}{\partial r} \right) + \mathbf{i} \left(-\frac{\partial g_y}{\partial r} + \frac{\partial g_z}{\partial y} \right) \\ &\stackrel{g_x=g_y=\mathbf{o}}{=} -\mathbf{j} \frac{\partial g_z}{\partial x} + \mathbf{i} \frac{\partial g_z}{\partial y}. \end{aligned} \quad (13.12)$$

Thus, in the SGA

$$\frac{\partial g_z}{\partial x} = \frac{\partial g_z}{\partial y} = \mathbf{o}. \quad (13.13)$$

So g can only be a function of height,

$$g = g(z). \quad (13.14)$$

The SGA is a relatively weak approximation, which greatly simplifies the system of equations. It is therefore almost always appropriate for analytical considerations. They can be given up for models, see section D.3.4.

13.3 Shallow atmosphere

The so-called *shallow-atmosphere* approximation is [31, 39]

$$\sqrt{g} = r^2 \cos(\varphi) \rightarrow a^2 \cos(\varphi) \quad (13.15)$$

for the functional determinant of the *geographic coordinates*, where a is a constant value for the radius. Putting this into Eq. (B.98), you get

$$\begin{aligned}
\nabla \times \mathbf{v} &= \frac{\mathbf{1}}{a^2 \sin(\theta)} \left[\mathbf{e}_r \left(\frac{\partial (a \sin(\theta) \tilde{v}_\varphi)}{\partial \theta} - \frac{\partial (a \tilde{v}_\theta)}{\partial \varphi} \right) + a \mathbf{e}_\theta \left(\frac{\partial \tilde{v}_r}{\partial \varphi} - \frac{\partial (a \sin(\theta) \tilde{v}_\varphi)}{\partial r} \right) \right. \\
&\quad \left. + a \sin(\theta) \mathbf{e}_\varphi \left(\frac{\partial (a \tilde{v}_\theta)}{\partial r} - \frac{\partial \tilde{v}_r}{\partial \theta} \right) \right] \\
&= \frac{\tilde{v}_\varphi}{a \tan(\theta)} \mathbf{e}_r + \mathbf{e}_r \left(\frac{\mathbf{1}}{a} \frac{\partial \tilde{v}_\varphi}{\partial \theta} - \frac{\mathbf{1}}{a \sin(\theta)} \frac{\partial \tilde{v}_\theta}{\partial \varphi} \right) \\
&\quad + \mathbf{e}_\theta \left(\frac{\mathbf{1}}{a \sin(\theta)} \frac{\partial \tilde{v}_r}{\partial \varphi} - \frac{\partial \tilde{v}_\varphi}{\partial r} \right) + \mathbf{e}_\varphi \left(\frac{\partial \tilde{v}_\theta}{\partial r} - \frac{\mathbf{1}}{a} \frac{\partial \tilde{v}_r}{\partial \theta} \right). \tag{13.16}
\end{aligned}$$

This means that Eq. (B.115) in the shallow atmosphere the form

$$\nabla \times \mathbf{v} = \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) \mathbf{i} + \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) \mathbf{j} + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \mathbf{k} + \frac{u \tan(\varphi)}{a} \mathbf{k}. \tag{13.17}$$

accepts. In the shallow atmosphere, the speed resulting from the earth's rotation applies

$$\begin{aligned}
\mathbf{v}_i &= \boldsymbol{\Omega} \times \mathbf{r} = \begin{pmatrix} 0 \\ 0 \\ \Omega \end{pmatrix} \times a \begin{pmatrix} \cos(\varphi) \cos(\mathcal{I}) \\ \cos(\varphi) \sin(\mathcal{I}) \\ \sin(\varphi) \end{pmatrix} = \Omega a \begin{pmatrix} -\cos(\varphi) \sin(\mathcal{I}) \\ \cos(\varphi) \cos(\mathcal{I}) \\ 0 \end{pmatrix} = \Omega a \cos(\varphi) \begin{pmatrix} -\sin(\mathcal{I}) \\ \cos(\mathcal{I}) \\ 0 \end{pmatrix} \\
&= \Omega a \cos(\varphi) \mathbf{i}. \tag{13.18}
\end{aligned}$$

With Eq. (13.17) is obtained

$$\begin{aligned}
\nabla \times \mathbf{v}_i &= \left(-\frac{\partial (\Omega a \cos(\varphi))}{\partial y} + \Omega a \cos(\varphi) \frac{\tan(\varphi)}{a} \right) \mathbf{k} \\
&= \left(-\frac{\partial (\Omega \cos(\varphi))}{\partial \varphi} + \Omega \sin(\varphi) \right) \mathbf{k} = \Omega \sin(\varphi) \mathbf{k} \tag{13.19}
\end{aligned}$$

Therefore, the shallow atmosphere approximation implies the so-called *traditional approximation*

$\mathbf{f}' = \mathbf{0}. \quad (\text{traditionelle Approximation}) \tag{13.20}$

Eq. (13.17) implies with Eq. (B.130) that in momentum advection the terms $\propto uw/r, vw/r, u^2/r, v^2/r$ must be neglected.

If you put Eq. (13.15) in Eq. (B.90), you get

$$\begin{aligned}
\nabla \cdot \mathbf{v} &= \frac{\mathbf{1}}{a^2 \sin(\theta)} \left(\frac{\partial (v^{(r)} a^2 \sin(\theta))}{\partial r} + \frac{\partial (v^{(\theta)} a^2 \sin(\theta))}{\partial \theta} + \frac{\partial (v^{(\varphi)} a^2 \sin(\theta))}{\partial \varphi} \right) \\
&= \frac{\partial v^{(r)}}{\partial r} + \frac{\partial v^{(\theta)}}{\partial \theta} + \frac{\partial v^{(\varphi)}}{\partial \varphi} + \cot(\theta) v^{(\theta)} \\
&= \frac{\partial \tilde{v}^{(r)}}{\partial r} + \frac{\mathbf{1}}{r} \frac{\partial \tilde{v}^{(\theta)}}{\partial \theta} + \frac{\mathbf{1}}{r \sin(\theta)} \frac{\partial \tilde{v}^{(\varphi)}}{\partial \varphi} + \frac{\cot(\theta)}{a} \tilde{v}^{(\theta)}. \tag{13.21}
\end{aligned}$$

This means that Eq. (B.112) in the shallow atmosphere the form

$$\nabla \cdot \mathbf{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} - \frac{v \tan(\varphi)}{a} \tag{13.22}$$

accepts. Since the density of the atmosphere is neglected when calculating $\mathbf{g}$, the following applies with the SGA

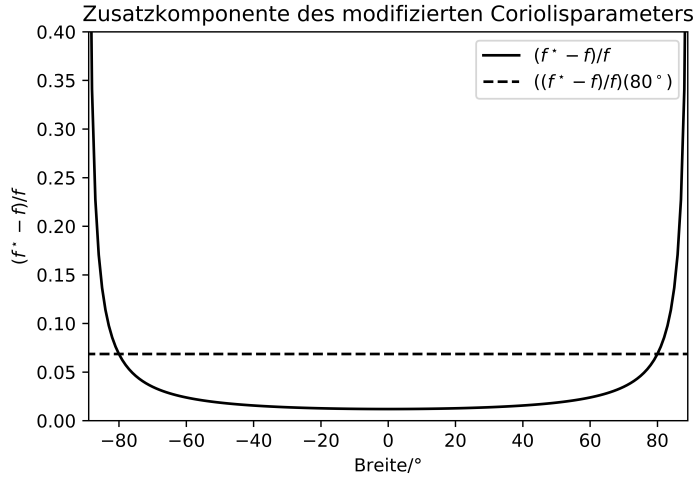


Figure 13.1: The additional component of f^* as a function of width. The value at $\varphi = \pm 85^\circ$ is also entered. A wind speed of $u = 10$ m/s was assumed.

$$\nabla \cdot \mathbf{g} = -\frac{dg}{dz} = 0, \quad (13.23)$$

which implies that g must be independent of height in the shallow atmosphere,

$$g = g_0. \quad (13.24)$$

The implications of Eq. (13.15) are summarized as follows

1. in differential operators, $\frac{1}{r}$ must be replaced by $\frac{1}{a}$,
2. the traditional approximation $f' = 0$ must be done,
3. all metric terms that do not contain $\tan(\varphi)$ must be neglected (in divergence, vorticity and momentum advection),
4. the gravity must be independent of height, $g \rightarrow g_0 = \text{homogeneous}$.

The momentum equation of the shallow atmosphere is therefore:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - \frac{uv \tan(\varphi)}{a} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + fv + F_{R,x}, \quad (13.25)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{u^2 \tan(\varphi)}{a} = -\frac{1}{\rho} \frac{\partial p}{\partial y} - fu + F_{R,y}, \quad (13.26)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g_0 + F_{R,z}. \quad (13.27)$$

13.3.1 Modified Coriolis parameter

All approximations made so far are globally applicable. This is no longer the case with the approximation made in this section. One defines the modified Coriolis parameter f^* by

$$f^* := f \left(\mathbf{1} + \frac{u}{2a\omega \cos(\varphi)} \right). \quad (13.28)$$

Unlike f , f^* also depends on the velocity field and no longer just describes the Coriolis force. This means that the equations (13.25) - (13.26) can be written down shorter than

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + f^* v + F_{R,x}, \quad (13.29)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} - f^* u + F_{R,y}. \quad (13.30)$$

For most dynamic considerations one can assume $f^* = f$, at least up to latitudes of 80 degrees. This is illustrated in Fig. 13.1. This gives the following simplified horizontal equations of motion:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + f v + F_{R,x} \quad (13.31)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} - f u + F_{R,y} \quad (13.32)$$

13.4 Pseudo-incompressible approximation

The so-called *pseudo-incompressible approximation* was presented in [8]. In order to justify them, one first considers the equations of the shallow atmosphere in the form in Sect. 10.1.2

$$\frac{Du}{Dt} = -c^{(p)} \theta \frac{\partial \Pi}{\partial x} + f v, \quad (13.33)$$

$$\frac{Dv}{Dt} = -c^{(p)} \theta \frac{\partial \Pi}{\partial y} - f u, \quad (13.34)$$

$$\frac{Dw}{Dt} = -c^{(p)} \theta \frac{\partial \Pi}{\partial z} - g, \quad (13.35)$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}, \quad (13.36)$$

$$\frac{D\Pi}{Dt} \stackrel{\text{Glg. (9.79)}}{=} -\frac{R_d \Pi}{c^{(V)}} \nabla \cdot \mathbf{v}. \quad (13.37)$$

Only Eq. is now modified. (13.37). To do this, a background state $(\bar{\Pi}(z), \bar{\theta}(z))$ is introduced; deviations from this are indicated as usual with primed values. This allows Eq. (13.37) assuming $\Pi' \ll \bar{\Pi}$ in the form

$$\frac{D\Pi'}{Dt} + w \frac{d\bar{\Pi}}{dz} + \frac{R_d \bar{\Pi}}{c^{(V)}} \nabla \cdot \mathbf{v} = 0 \quad (13.38)$$

$$\Leftrightarrow \frac{c^{(V)}}{R_d \bar{\Pi}} \frac{D\Pi'}{Dt} + \frac{c^{(V)}}{R_d \bar{\Pi}} w \frac{d\bar{\Pi}}{dz} + \nabla \cdot \mathbf{v} = 0 \quad (13.39)$$

note down. The pseudo-incompressible approximation is now based on, in Eq. (13.39) to neglect the term $\frac{c^{(V)}}{R_d \bar{\Pi}} \frac{D\Pi'}{Dt}$, i.e. from

$$\frac{c^{(V)}}{R_d \bar{\Pi}} w \frac{d\bar{\Pi}}{dz} + \nabla \cdot \mathbf{v} = 0 \quad (13.40)$$

to go out. The background state satisfies the equation of state in the form Eq. (9.71):

$$\bar{\Pi} = \left(\frac{R_d \bar{\varrho} \bar{\theta}}{p_o} \right)^{R_d / c^{(V)}} \quad (13.41)$$

This follows from the chain rule

$$\frac{d\bar{\Pi}}{dz} = \bar{\Pi} \frac{R_d}{c^{(V)} \bar{\varrho} \bar{\theta}} \frac{d(\bar{\varrho} \bar{\theta})}{dz}. \quad (13.42)$$

Putting this into Eq. (13.40), you get

$$w \frac{d(\bar{\varrho} \bar{\Pi})}{dz} + \bar{\varrho} \bar{\theta} \nabla \cdot \mathbf{v} = 0 \quad (13.43)$$

This leads to the compact formulation

$$\nabla \cdot (\bar{\varrho} \bar{\theta} \mathbf{v}) = 0 \quad (13.44)$$

the pseudo-incompressible approximation.

13.5 Anelastic approximation

In the so-called *anelastic approximation* the thermodynamic quantities are written in the form

$$\varrho(\varphi, \lambda, z, t) = \varrho_o(z) + \varrho'(\varphi, \lambda, z, t), \quad (13.45)$$

$$p(\varphi, \lambda, z, t) = p_o(z) + p'(\varphi, \lambda, z, t), \quad (13.46)$$

$$\theta(\varphi, \lambda, z, t) = \theta_o + \theta'(\varphi, \lambda, z, t). \quad (13.47)$$

The background state $(\varrho_o, p_o, \theta_o)$ is isentropic and hydrostatically balanced,

$$\frac{dp_o}{dz} = -g\varrho_o. \quad (13.48)$$

The unapproximated reversible equations are

$$\varrho \frac{D\mathbf{v}}{Dt} = -\nabla p - \varrho \mathbf{f} \times \mathbf{v} + \varrho \mathbf{g}, \quad (13.49)$$

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \mathbf{v}) = 0, \quad (13.50)$$

$$\frac{D\theta}{Dt} = 0. \quad (13.51)$$

If you insert the equations (13.45) - (13.47) here, you get

$$(\varrho_o + \varrho') \frac{D\mathbf{v}}{Dt} = -\nabla(p_o + p') - (\varrho_o + \varrho') \mathbf{f} \times \mathbf{v} + (\varrho_o + \varrho') \mathbf{g}, \quad (13.52)$$

$$\frac{\partial \varrho'}{\partial t} + \nabla \cdot [(\varrho_o + \varrho') \mathbf{v}] = 0, \quad (13.53)$$

$$\frac{D\theta'}{Dt} = 0. \quad (13.54)$$

The anelastic system of equations, like the incompressible one, is often used to study atmospheric deep convection.

13.5.1 Horizontal momentum equation

If you replace the density in the prefactor of the acceleration (including the Coriolis acceleration) by its mean value, you get

$$\begin{aligned}
 \varrho_{\circ} \frac{D\mathbf{v}}{Dt} &= -\nabla (p_{\circ} + p') - \varrho_{\circ} \mathbf{f} \times \mathbf{v} + (\varrho_{\circ} + \varrho') \mathbf{g} \\
 \Leftrightarrow \frac{D\mathbf{v}}{Dt} &= -\frac{\mathbf{I}}{\varrho_{\circ}} \nabla (p_{\circ} + p') - \mathbf{f} \times \mathbf{v} + \frac{\varrho_{\circ} + \varrho'}{\varrho_{\circ}} \mathbf{g} \\
 \Leftrightarrow \frac{D\mathbf{v}}{Dt} &= -\nabla \Phi - \mathbf{f} \times \mathbf{v} + \frac{\varrho_{\circ} + \varrho'}{\varrho_{\circ}} \mathbf{g}
 \end{aligned} \tag{13.55}$$

with

$$\Phi := \frac{p'}{\varrho_{\circ}} \tag{13.56}$$

With the shallow atmosphere approximation one obtains the components of the horizontal momentum equation in the form

$$\frac{Du}{Dt} = -\frac{\partial \Phi}{\partial x} + fv, \tag{13.57}$$

$$\frac{Dv}{Dt} = -\frac{\partial \Phi}{\partial y} - fu. \tag{13.58}$$

13.5.2 Vertical momentum equation

If you project Eq. (13.55) on $\mathbf{k}$, one obtains

$$\begin{aligned}
 \frac{Dw}{Dt} &= -\frac{\mathbf{I}}{\varrho_{\circ}} \frac{\partial (p_{\circ} + p')}{\partial z} - \frac{\varrho_{\circ} + \varrho'}{\varrho_{\circ}} g \\
 \Leftrightarrow \frac{Dw}{Dt} &= -\frac{\mathbf{I}}{\varrho_{\circ}} \frac{\partial p_{\circ}}{\partial z} - g - \frac{\mathbf{I}}{\varrho_{\circ}} \frac{\partial p'}{\partial z} - \frac{\varrho'}{\varrho_{\circ}} g \\
 \Leftrightarrow \frac{Dw}{Dt} &\stackrel{\text{Gl. (13.48)}}{=} -\frac{\mathbf{I}}{\varrho_{\circ}} \frac{\partial p'}{\partial z} - \frac{\varrho'}{\varrho_{\circ}} g \\
 \Leftrightarrow \frac{Dw}{Dt} &= -\frac{\partial \Phi}{\partial z} - \frac{\Phi}{\varrho_{\circ}} \frac{d\varrho_{\circ}}{dz} - \frac{\varrho'}{\varrho_{\circ}} g \\
 \Leftrightarrow \frac{Dw}{Dt} &= -\frac{\partial \Phi}{\partial z} - \frac{p'}{\varrho_{\circ}^2} \frac{d\varrho_{\circ}}{dz} - \frac{\varrho'}{\varrho_{\circ}} g.
 \end{aligned} \tag{13.59}$$

For the background temperature $T_{\circ} = T_{\circ}(z)$ as a function of height applies

$$T_{\circ}(z) = \theta_{\circ} \left(\frac{p_{\circ}}{p_{\text{ref}}} \right)^{R_d/c^{(p)}}. \tag{13.60}$$

For the background density $\varrho_{\circ} = \varrho_{\circ}(z)$ applies with the thermal equation of state of ideal gases

$$\varrho_{\circ}(z) = \frac{p_{\circ}}{R_d T_{\circ}} = \frac{p_{\circ}}{R_d \theta_{\circ}} \left(\frac{p_{\text{ref}}}{p_{\circ}} \right)^{R_d/c^{(p)}}. \tag{13.61}$$

From this it follows

$$\frac{d\varrho_{\circ}}{dz} = \varrho_{\circ} \frac{1 - \frac{R_d}{c^{(p)}}}{p_{\circ}} \frac{dp_{\circ}}{dz} = -\varrho_{\circ} \frac{1 - \frac{R_d}{c^{(p)}}}{p_{\circ}} g\varrho_{\circ} = -\frac{c^{(p)} - c^{(p)} + c^{(V)}}{c^{(p)} p_{\circ}} g\varrho_{\circ}^2 = -\frac{c^{(V)}}{c^{(p)} p_{\circ}} g\varrho_{\circ}^2 = -\frac{g\varrho_{\circ}^2}{\kappa p_{\circ}}. \quad (13.62)$$

Putting this into Eq. (13.59), you get

$$\frac{Dw}{Dt} = -\frac{\partial\Phi}{\partial z} + \frac{gp'}{\kappa p_{\circ}} - \frac{\varrho'}{\varrho_{\circ}} g = -\frac{\partial\Phi}{\partial z} + g \left(\frac{p'}{\kappa p_{\circ}} - \frac{\varrho'}{\varrho_{\circ}} \right). \quad (13.63)$$

From Eq. (13.61) follows

$$\theta(\varrho, p) = \frac{p}{R_d \varrho} \left(\frac{p_{\text{ref}}}{p} \right)^{R_d/c^{(p)}}. \quad (13.64)$$

If you expand this to first order around $(\varrho_{\circ}, p_{\circ})$, you get

$$\theta \approx \theta_{\circ} \left(1 - \frac{\varrho'}{\varrho_{\circ}} + \frac{p'}{\kappa p_{\circ}} \right) \Rightarrow \theta' \approx \theta_{\circ} \left(-\frac{\varrho'}{\varrho_{\circ}} + \frac{p'}{\kappa p_{\circ}} \right). \quad (13.65)$$

This means that the approximately sign is ignored

$$g \left(\frac{p'}{\kappa p_{\circ}} - \frac{\varrho'}{\varrho_{\circ}} \right) = g \frac{\theta'}{\theta_{\circ}}. \quad (13.66)$$

Define the buoyancy b by

$$b := g \frac{\theta'}{\theta_{\circ}}, \quad (13.67)$$

this is the vertical momentum equation of the anelastic approximation

$$\frac{Dw}{Dt} = -\frac{\partial\Phi}{\partial z} + b. \quad (13.68)$$

13.5.3 Temperature equation

The buoyancy b is only a function of the potential temperature θ , so it follows from Eq. (13.51)

$$\frac{Db}{Dt} = 0. \quad (13.69)$$

13.5.4 Continuity equation

If you put Eq. (13.45) into the continuity equation, you get

$$\frac{\partial\varrho'}{\partial t} + \nabla \cdot [(\varrho_{\circ} + \varrho') \mathbf{v}] = 0. \quad (13.70)$$

If you neglect the fluctuation ϱ' , you get

$$\nabla \cdot (\varrho_{\circ} \mathbf{v}) = 0. \quad (13.71)$$

13.5.5 Compilation

The anelastic system of equations is summarized as follows

$$\frac{Du}{Dt} = -\frac{\partial \Phi}{\partial x} + fv, \quad (13.72)$$

$$\frac{Dv}{Dt} = -\frac{\partial \Phi}{\partial y} - fu, \quad (13.73)$$

$$\frac{Dw}{Dt} = -\frac{\partial \Phi}{\partial z} + b, \quad (13.74)$$

$$\frac{Db}{Dt} = 0, \quad (13.75)$$

$$\nabla \cdot (\rho_o \mathbf{v}) = 0. \quad (13.76)$$

13.6 Boussinesq approximation

In [33] the so-called *Boussinesq approximation* was derived for an ideal gas. However, nowadays it is mainly applied to the ocean, so the derivation in [33] is generalized here for a general fluid.

Let ψ be one of the thermodynamic state variables. Note for these

$$\psi = \psi(\varphi, \lambda, z) = \psi_m + \psi_o(z) + \psi'(\varphi, \lambda, z), \quad (13.77)$$

where ψ_m is the mean of ψ , ψ_o is the hydrostatic stratification in the absence of motion and accelerations and ψ' is the variation caused by motion. Define the scale height corresponding to ψ D_ψ by

$$D_\psi := \left| \frac{1}{\psi_m} \frac{d\psi_o}{dz} \right|^{-1}. \quad (13.78)$$

The fluid has thickness h . The first part of the so-called *Boussinesq approximation*

$$h \ll (D_\psi)_{\min}, \quad (13.79)$$

where $(D_\psi)_{\min}$ denotes the minimum scale height of all thermodynamic state variables. This implies

$$\left| \frac{\psi_o}{\psi_m} \right| \ll 1 \quad (13.80)$$

for all thermodynamic variables. The second part of the Boussinesq approximation is

$$|\rho'| \leq O(\rho_o). \quad (13.81)$$

The Boussinesq approximation is justified in the ocean, but in the atmosphere only for shallow systems.

At this point we assume a homogeneous system. In this case one can write the thermal equation of state in the form

$$\rho = \rho(p, T) \quad (13.82)$$

note down. This can be developed into a Taylor series around the development point $(p, T)^T = (p_m, T_m)^T$ ¹

¹If you define ρ_m, p_m, T_m as the mean of the respective quantities, due to the nonlinearity of the equation of state, in general $\rho_m \neq \rho(p_m, T_m)$ applies. Therefore, it makes sense to define $\rho_m := \rho(p_m, T_m)$.

$$\begin{aligned}
\varrho(p, T) = \varrho_m & \left[1 - a_m (T - T_m) + K_m (p - p_m) + \frac{1}{2} \left(\frac{1}{\varrho} \frac{\partial^2 \varrho}{\partial T^2} \right)_m (T - T_m)^2 \right. \\
& + \frac{1}{2} \left(\frac{1}{\varrho} \frac{\partial^2 \varrho}{\partial p^2} \right)_m (p - p_m)^2 + \left(\frac{1}{\varrho} \frac{\partial^2 \varrho}{\partial T \partial p} \right)_m (T - T_m) (p - p_m) \\
& \left. + O[(T - T_m)^3, (p - p_m)^3] \right]
\end{aligned} \tag{13.83}$$

The definitions were

$$a_m := - \left[\frac{1}{\varrho} \left(\frac{\partial \varrho}{\partial T} \right)_p \right]_m \quad (\text{thermischer Expansionskoeffizient}), \tag{13.84}$$

$$K_m := \left[\frac{1}{\varrho} \left(\frac{\partial \varrho}{\partial p} \right)_T \right]_m \quad (\text{Kompressibilität}) \tag{13.85}$$

used. For ideal gases, $\varrho = \frac{p}{R_s T}$

$$a_m = - \left[\frac{1}{\varrho} \left(\frac{\partial \varrho}{\partial T} \right)_p \right]_m = \frac{p_m}{R_s \varrho_m T_m^2} = \frac{\varrho_m R_s T_m}{R_s \varrho_m T_m^2} = \frac{1}{T_m}, \tag{13.86}$$

$$K_m = \left[\frac{1}{\varrho} \left(\frac{\partial \varrho}{\partial p} \right)_T \right]_m = \frac{1}{\varrho_m} \frac{1}{R_s T_m} = \frac{1}{p_m}. \tag{13.87}$$

For fluids you can

$$a_m \ll - \frac{1}{\varrho_m} \frac{-\varrho_m}{T_m} = \frac{1}{T_m}, \quad K_m \ll \frac{1}{\varrho_m} \frac{\varrho_m}{p_m} = \frac{1}{p_m} \tag{13.88}$$

estimate. Putting this into Eq. (13.83) also for the second derivatives, which is obtained by neglecting the third and higher order terms

$$\frac{\varrho - \varrho_m}{\varrho_m} \ll - \frac{T - T_m}{T_m} + \frac{p - p_m}{p_m} \pm \frac{(T - T_m)^2}{T_m^2} \pm \frac{(p - p_m)^2}{p_m^2}. \tag{13.89}$$

Based on equations (13.80) and (13.81) one can do the right side

$$- \frac{T - T_m}{T_m} + \frac{p - p_m}{p_m} \pm \frac{(T - T_m)^2}{T_m^2} \pm \frac{(p - p_m)^2}{p_m^2} \approx - \frac{T - T_m}{T_m} + \frac{p - p_m}{p_m} \tag{13.90}$$

approach. It therefore applies, neglecting the approximate sign (in the first order in the perturbations $\mathcal{Y} - \mathcal{Y}_m$ of the thermodynamic variable $\mathcal{Y}$)

$$\frac{\varrho - \varrho_m}{\varrho_m} = -a_m (T - T_m) + K_m (p - p_m). \tag{13.91}$$

This implies

$$\varrho_o = \varrho_m (-a_m T_o + K_m p_o), \tag{13.92}$$

$$\varrho' = \varrho_m (-a_m T' + K_m p'). \tag{13.93}$$

13.6.1 Momentum equation

The basic hydrostatic equation (13.122) is

$$\frac{dp_o}{dz} = -g\varrho_m - g\varrho_o. \tag{13.94}$$

Plugging this into the momentum equation you get

$$\begin{aligned}
 \varrho \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} &= -\nabla p' - \frac{dp_o}{dz} \mathbf{k} - g \varrho \mathbf{k} - \varrho \mathbf{f} \times \mathbf{v} + \varrho \mathbf{f}_R \\
 &= -\nabla p' - \frac{dp_o}{dz} \mathbf{k} - g \varrho_m \mathbf{k} - g \varrho_o \mathbf{k} - g \varrho' \mathbf{k} - \varrho \mathbf{f} \times \mathbf{v} + \varrho \mathbf{f}_R \\
 &= -\nabla p' - g \varrho' \mathbf{k} - \varrho \mathbf{f} \times \mathbf{v} + \varrho \mathbf{f}_R.
 \end{aligned} \tag{13.95}$$

Dividing this by ϱ_m gives

$$\frac{\varrho}{\varrho_m} \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = -\frac{\mathbf{I}}{\varrho_m} \nabla p' - g \frac{\varrho'}{\varrho_m} \mathbf{k} - \frac{\varrho}{\varrho_m} \mathbf{f} \times \mathbf{v} + \frac{\varrho}{\varrho_m} \mathbf{f}_R. \tag{13.96}$$

Due to Eq. (13.80) you can

$$\frac{\varrho}{\varrho_m} \approx \mathbf{I} \tag{13.97}$$

approach. This leads to

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = -\frac{\mathbf{I}}{\varrho_m} \nabla p' - g \frac{\varrho'}{\varrho_m} \mathbf{k} - \mathbf{f} \times \mathbf{v} + \mathbf{f}_R. \tag{13.98}$$

The continuity equation is:

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \varrho = -\varrho \nabla \cdot \mathbf{v}. \tag{13.99}$$

Dividing this by ϱ_m gives

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \frac{\varrho - \varrho_m}{\varrho_m} = -\frac{\varrho}{\varrho_m} \nabla \cdot \mathbf{v}. \tag{13.100}$$

If you put Eq. (13.80), you get

$$\nabla \cdot \mathbf{v} = 0 \Leftrightarrow \frac{D\varrho}{Dt} = 0. \tag{13.101}$$

So, under the Boussinesq approximation, the continuity equation simplifies to its incompressible form.

One can use the momentum equation Eq. (13.98) simplify a bit. The vertical component of this equation is

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) w = -\frac{\mathbf{I}}{\varrho_m} \frac{\partial p'}{\partial z} - g \frac{\varrho'}{\varrho_m} - (\mathbf{f} \times \mathbf{v}) \cdot \mathbf{k} + \mathbf{f}_R \cdot \mathbf{k}. \tag{13.102}$$

For pressure gradient and gravity one obtains using Eq. (13.93)

$$\begin{aligned}
 -\frac{\mathbf{I}}{\varrho_m} \frac{\partial p'}{\partial z} - g \frac{\varrho'}{\varrho_m} &= -\frac{\mathbf{I}}{\varrho_m} \frac{\partial p'}{\partial z} - g (-a_m T' + K_m p') = -\frac{\mathbf{I}}{\varrho_m} \frac{\partial p'}{\partial z} - g K_m p' + g a_m T' \\
 &= -\frac{\mathbf{I}}{\varrho_m} \left(\frac{\partial p'}{\partial z} + g \varrho_m K_m p' \right) + g a_m T' = -\frac{\mathbf{I}}{\varrho_m} \left(\frac{\partial p'}{\partial z} + \frac{p'}{H} \right) + g a_m T'
 \end{aligned} \tag{13.103}$$

with

$$H := \frac{\mathbf{I}}{g \varrho_m K_m}. \quad (13.104)$$

With Eq. (13.88) you can

$$H = \frac{\mathbf{I}}{g \varrho_m} \frac{\mathbf{I}}{K_m} \gg \frac{\mathbf{I}}{g \varrho_m} p_m =: H' \quad (13.105)$$

estimate. H' is the thickness of a fluid of homogeneous density ϱ_m , which rests hydrostatically in the gravity field g and in which the pressure increases linearly from top to bottom from zero to p_m . One can

$$H' \sim \frac{h}{2} \quad (13.106)$$

estimate, so it also applies

$$H \gg h. \quad (13.107)$$

This means that in Eq. (13.103)

$$\frac{\partial p'}{\partial z} + \frac{p'}{H} \approx \frac{\partial p'}{\partial z} \quad (13.108)$$

can approach. This leads to a simplified form of Eq. (13.98):

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = -\frac{\mathbf{I}}{\varrho_m} \nabla p' + g a_m T' \mathbf{k} - \mathbf{f} \times \mathbf{v} + \mathbf{f}_R \quad (13.109)$$

In the ideal gas with Eq. (13.86)

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} = -\frac{\mathbf{I}}{\varrho_m} \nabla p' + g \frac{T'}{T_m} \mathbf{k} - \mathbf{f} \times \mathbf{v} + \mathbf{f}_R. \quad (13.110)$$

13.6.2 Temperature equation

If you multiply Eq. (9.10) with density ϱ is obtained

$$\varrho c^{(V)} \frac{DT}{Dt} - \frac{p}{\varrho} \frac{D\varrho}{Dt} = q^{(V)}, \quad (13.111)$$

where $q^{(V)}$ is the thermal power density. Due to Eq. (13.77) applies

$$\frac{DT}{Dt} = \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T'. \quad (13.112)$$

Putting this into Eq. (13.111), you get

$$\varrho_m c^{(V)} \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) - \frac{p}{\varrho} \frac{D\varrho}{Dt} = q^{(V)}, \quad (13.113)$$

where in the prefactor of the temperature tendency the density ϱ was replaced by the mean density ϱ_m . The compression term can be found in the first order in the deviations from the average values

$$-\frac{p}{\varrho} \frac{D\varrho}{Dt} \approx -\frac{p_m}{\varrho_m} \frac{D\varrho}{Dt} = -\frac{p_m}{\varrho_m} \left(\frac{\partial \varrho}{\partial t} + \mathbf{v} \cdot \nabla \varrho \right) \quad (13.114)$$

simplify. With Eq. (13.91) follows, ignoring the approximately sign

$$-\frac{p}{\rho} \frac{D\rho}{Dt} \approx -\frac{p_m}{\rho_m} \left(\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho \right) = -p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) [-a_m (T - T_m) + K_m (p - p_m)]. \quad (13.115)$$

In order to eliminate the time dependence of the pressure, one approaches further

$$\begin{aligned} -\frac{p}{\rho} \frac{D\rho}{Dt} &\approx -p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) [-a_m (T - T_m) + K_m (p - p_m)] \\ &= -p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) [-a_m (T_o + T') + K_m p_o] \\ &= p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) a_m T' + p_m w a_m \frac{dT_o}{dz} - p_m K_m w \frac{dp_o}{dz}. \end{aligned} \quad (13.116)$$

According to Eq. (13.94) applies to the first order in the deviation from the mean density

$$\frac{dp_o}{dz} \approx -g \rho_m. \quad (13.117)$$

This means that the approximately sign is ignored

$$\begin{aligned} -\frac{p}{\rho} \frac{D\rho}{Dt} &= p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) a_m T' + p_m w a_m \frac{dT_o}{dz} - p_m K_m w \frac{dp_o}{dz} \\ &= p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) a_m T' + p_m w a_m \frac{dT_o}{dz} + p_m K_m w g \rho_m. \end{aligned} \quad (13.118)$$

Putting this into Eq. (13.113), you get

$$\begin{aligned} \rho_m c^{(V)} \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) - \frac{p}{\rho} \frac{D\rho}{Dt} &= q^{(V)} \\ \rho_m c^{(V)} \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) + p_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) a_m T' + p_m w a_m \frac{dT_o}{dz} + p_m K_m w g \rho_m &= q^{(V)} \\ \left(\rho_m c^{(V)} + p_m a_m \right) \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) + w \left(p_m a_m + \rho_m c^{(V)} \right) \frac{dT_o}{dz} + p_m K_m w g \rho_m &= q^{(V)} \end{aligned} \quad (13.119)$$

This is the temperature equation of the Boussinesq approximation:

$$\boxed{\left(c^{(V)} + \frac{p_m a_m}{\rho_m} \right) \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) + w \left[\left(\frac{p_m a_m}{\rho_m} + c^{(V)} \right) \frac{dT_o}{dz} + p_m K_m g \right] = \frac{q^{(V)}}{\rho_m}} \quad (13.120)$$

For the ideal gas, the following equations apply (13.86) - (13.87)

$$\begin{aligned} \left(c^{(V)} + R_s \right) \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) + w \left[\left(R_s + c^{(V)} \right) \frac{dT_o}{dz} + g \right] &= \frac{q^{(V)}}{\rho_m} \\ \Leftrightarrow c^{(p)} \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) + w c^{(p)} \left(\frac{dT_o}{dz} + g \right) &= \frac{q^{(V)}}{\rho_m} \\ \Leftrightarrow \left(\frac{\partial T'}{\partial t} + \mathbf{v} \cdot \nabla T' \right) + w \left(\frac{dT_o}{dz} + \frac{g}{c^{(p)}} \right) &= \frac{q^{(V)}}{c^{(p)} \rho_m}. \end{aligned} \quad (13.121)$$

The pseudo-incompressible, anelastic and Boussinesq approximations are summarized under the term *soundproof* because they filter sound waves.

13.7 Hydrostatics

The pressure gradient and gravity are of the order of 10 m/s^2 , while the vertical acceleration is of the order of 10^{-7} m/s^2 . The equation

$$0 = -\frac{1}{\rho} \nabla p + \mathbf{g} \Leftrightarrow \nabla p = \rho \mathbf{g} \quad \begin{array}{c} \text{radialsymmetrisches} \\ \text{Schwerefeld} \end{array} \Rightarrow \frac{\partial p}{\partial z} = -g\rho \quad (13.122)$$

is therefore valid on the synoptic scale in an excellent approximation, this is the *hydrostatic basic equation*.

Another formulation of this equation is $\frac{Dw}{Dt} = 0$. The particles therefore have a constant vertical speed. This must be zero, otherwise it will be the rule that a particle disappears into the ground or space. So the implication applies

$$\frac{\mathbf{g}}{g} \cdot \nabla p = \rho \mathbf{g} \Rightarrow w = 0. \quad (13.123)$$

Nevertheless, it makes sense to allow a vertical velocity in hydrostatic equation systems. Although this is physically contradictory, it is not mathematically contradictory, since the system of equations cannot know anything about the above conclusion. The vertical movements of such a system arise from the continuity equation.

The basic hydrostatic equation makes it possible to use the pressure p not as a dependent but as an independent coordinate (vertical coordinate). If you transform from $p(\Phi)$ to $\Phi(p)$, this is the basic hydrostatic equation

$$\frac{\partial \Phi}{\partial p} = -a \quad (13.124)$$

with $a := \frac{1}{\rho}$ as the specific volume. The equation of state follows $a = \frac{R_d T}{p}$ in a dry atmosphere. That's why $\frac{\partial \Phi}{\partial p}$ is often simply referred to as „temperature“. It can be seen that the layer thickness is proportional to the temperature of the layer. The three-dimensional geopotential field is an expression of the ground pressure and the temperature of the air masses.

13.7.1 Continuity equation

The continuity equation is general

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (13.125)$$

If one inserts the basic hydrostatic equation $\rho = -\frac{1}{g} \frac{\partial p}{\partial z}$, it follows

$$\begin{aligned} & \frac{\partial^2 p}{\partial z \partial t} + \nabla \cdot \left(\frac{\partial p}{\partial z} \mathbf{v} \right) = 0 \\ \Leftrightarrow & \frac{\partial^2 p}{\partial z \partial t} + \mathbf{v} \cdot \nabla \left(\frac{\partial p}{\partial z} \right) + \frac{\partial p}{\partial z} \nabla \cdot \mathbf{v} = \frac{\partial^2 p}{\partial z \partial t} + \frac{\partial}{\partial z} (\mathbf{v} \cdot \nabla p) - \nabla p \cdot \frac{\partial \mathbf{v}}{\partial z} + \frac{\partial p}{\partial z} \nabla \cdot \mathbf{v} \\ & = \frac{\partial \omega}{\partial z} - \nabla_h p \cdot \frac{\partial \mathbf{v}_h}{\partial z} + \frac{\partial p}{\partial z} \nabla \cdot \mathbf{v}_h = 0. \end{aligned} \quad (13.126)$$

A small transformation term was neglected, see Eq. (B.112). According to the chain rule, $\frac{\partial}{\partial z} = \frac{\partial p}{\partial z} \frac{\partial}{\partial p}$. This follows

$$\frac{\partial \omega}{\partial p} + \nabla \cdot \mathbf{v}_h - \nabla_h p \cdot \frac{\partial \mathbf{v}_h}{\partial p} = 0. \quad (13.127)$$

If you use Eq. (12.7), you get

$$\left(\frac{\partial u}{\partial x} \right)_z = \left(\frac{\partial u}{\partial x} \right)_p + \frac{\partial u}{\partial p} \left(\frac{\partial p}{\partial x} \right)_z \Leftrightarrow \left(\frac{\partial u}{\partial x} \right)_z - \frac{\partial u}{\partial p} \left(\frac{\partial p}{\partial x} \right)_z = \left(\frac{\partial u}{\partial x} \right)_p \quad (13.128)$$

and analogously for v . Unspecified partial derivatives have so far been derivatives in the z system. Now derivatives are used in the p -system:

$$\frac{\partial \omega}{\partial p} + \nabla \cdot \mathbf{v}_h = 0. \quad (13.129)$$

In the p -system, the continuity equation is reduced to a purely diagnostic equation, which formally corresponds to the continuity equation for an incompressible fluid in the z -system. If you scale this equation with the values from tab. 1.2, it follows in SI units

- $\nabla \cdot \mathbf{v}_h \sim 10^{-5}$
- $\frac{\partial \omega}{\partial p} \sim 10^{-6}$.

So the divergence of the horizontal wind is actually an order of magnitude smaller than the synoptic-scale vorticity.

13.7.2 Horizontal momentum equation

If you want to transform the equations of motion for flat geofluids (13.31) - (13.32), only the total derivatives in the p -system have to be noted on the left side. The pressure gradient takes a little more work. With Eq. (12.7) and the hydrostatic approximation follows

$$\left(\frac{\partial p}{\partial x} \right)_p = 0 = \left(\frac{\partial p}{\partial x} \right)_z + \left(\frac{\partial z}{\partial x} \right)_p \frac{\partial p}{\partial z} = \left(\frac{\partial p}{\partial x} \right)_z - g \rho \left(\frac{\partial z}{\partial x} \right)_p. \quad (13.130)$$

So it applies

$$\frac{1}{\rho} \left(\frac{\partial p}{\partial x} \right)_z = g \left(\frac{\partial z}{\partial x} \right)_p = \left(\frac{\partial \Phi}{\partial x} \right)_p \quad (13.131)$$

and analogously in the y direction. This means that the horizontal momentum equations in the p -system become

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \omega \frac{\partial u}{\partial p} = - \frac{\partial \Phi}{\partial x} + f v + F_{R,x}, \quad (13.132)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \omega \frac{\partial v}{\partial p} = - \frac{\partial \Phi}{\partial y} - f u + F_{R,y}. \quad (13.133)$$

13.7.3 Temperature equation

If you derive the equation of state $pa = R_d T$ in time, it follows

$$\begin{aligned} \frac{D(pa)}{Dt} &= \frac{D(R_d T)}{Dt} \\ \Rightarrow \omega a + p \frac{Da}{Dt} &= R_d \frac{DT}{Dt}. \end{aligned} \quad (13.134)$$

From Eq. (9.11) follows ignoring the mass source density

$$p \frac{Da}{Dt} = -c^{(V)} \frac{DT}{Dt} + a q_T^{(V)}. \quad (13.135)$$

Thus you get

$$\begin{aligned} \omega a - c^{(V)} \frac{DT}{Dt} + a q_T^{(V)} &= R_d \frac{DT}{Dt} \Leftrightarrow -\omega a + \left(R_d + c^{(V)} \right) \frac{DT}{Dt} = c^{(p)} \frac{DT}{Dt} - a \omega = a q_T^{(V)} \\ \frac{D_h T}{Dt} - \omega \left(\frac{a}{c^{(p)}} - \frac{\partial T}{\partial p} \right) &= \frac{a}{c^{(p)}} q_T^{(V)}. \end{aligned} \quad (13.136)$$

With the equation of state follows

$$\frac{a}{c^{(p)}} - \frac{\partial T}{\partial p} = \frac{R_d T}{c^{(p)} p} - \frac{\partial T}{\partial p} =: S_p, \quad (13.137)$$

this defines the stability parameter S_p . You receive

$$\frac{D_h T}{Dt} - S_p \omega = \frac{a}{c^{(p)}} q_T^{(V)} \quad (13.138)$$

This should now be rewritten as an equation for the evolution of $\Phi = \Phi(\varphi, \lambda, p, t)$. From Eq. (13.124) follows

$$\frac{\partial \Phi}{\partial p} = -\frac{R_d T}{p} \Rightarrow T = -\frac{p}{R_d} \frac{\partial \Phi}{\partial p}. \quad (13.139)$$

This is now put into Eq. (13.138), it follows

$$\begin{aligned} \frac{D_h}{Dt} \left(-\frac{p}{R_d} \frac{\partial \Phi}{\partial p} \right) - S_p \omega &= \frac{a}{c^{(p)}} q_T^{(V)} \\ \Rightarrow \frac{D_h}{Dt} \left(\frac{p}{R_d} \frac{\partial \Phi}{\partial p} \right) + S_p \omega &= -\frac{a}{c^{(p)}} q_T^{(V)} \\ \Rightarrow \frac{D_h}{Dt} \left(\frac{\partial \Phi}{\partial p} \right) + \frac{R_d S_p}{p} \omega &= -\frac{R_d a}{p c^{(p)}} q_T^{(V)} \\ \Rightarrow \left(\frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \right) \left(\frac{\partial \Phi}{\partial p} \right) + \frac{R_d S_p}{p} \omega &= -\frac{R_d a}{p c^{(p)}} q_T^{(V)}. \end{aligned} \quad (13.140)$$

The stability parameter S_p is related to the vertical gradient of potential temperature:

$$S_p = \frac{R_d T}{c^{(p)} p} - \frac{\partial T}{\partial p} = -\frac{T}{\theta} \left(\frac{\partial T}{\partial p} - T \frac{1}{p} \frac{R_d}{c^{(p)}} \right) \left(\frac{p_o}{p} \right)^{\frac{R_d}{c^{(p)}}} = -\frac{T}{\theta} \frac{\partial}{\partial p} \left[T \left(\frac{p_o}{p} \right)^{\frac{R_d}{c^{(p)}}} \right] = -\frac{T}{\theta} \frac{\partial \theta}{\partial p} \quad (13.141)$$

Now define the *static stability parameter* σ by

$$\sigma := \frac{R_d S_p}{p} \stackrel{\text{Gl.g. (13.141)}}{=} -\frac{R_d}{p} \frac{T}{\theta} \frac{\partial \theta}{\partial p} = -\frac{a}{\theta} \frac{\partial \theta}{\partial p}. \quad (13.142)$$

This depends on Eq. (13.122) about

$$\sigma = -\frac{a}{\theta} \frac{\partial z}{\partial p} \frac{\partial \theta}{\partial z} = \frac{a^2}{g \theta} \frac{\partial \theta}{\partial z} = \frac{a^2}{g^2} \frac{g}{\theta} \frac{\partial \theta}{\partial z} = \left(\frac{a}{g} N \right)^2 \quad (13.143)$$

with the Brunt-Väisälä frequency N . You receive

$$\Rightarrow \left(\frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \right) \frac{\partial \Phi}{\partial p} + \frac{a^2}{g^2} N^2 \omega = \frac{a}{c(p)} q_T^{(V)}. \quad (13.144)$$

13.7.4 Summary

The state of a dry hydrostatic atmosphere is determined by the fields $(u, v, \Phi)^T$, where all fields depend on $(\varphi, \lambda, p, t)^T$. The governing equations are as follows:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \omega \frac{\partial u}{\partial p} = -\frac{\partial \Phi}{\partial x} + f v + F_{R,x}, \quad (13.145)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \omega \frac{\partial v}{\partial p} = -\frac{\partial \Phi}{\partial y} - f u + F_{R,y}, \quad (13.146)$$

$$\frac{\partial^2 \Phi}{\partial p \partial t} + \left(u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \right) \frac{\partial \Phi}{\partial p} + \frac{a^2}{g^2} N^2 \omega = -\frac{R_d a}{p c(p)} q_T^{(V)}, \quad (13.147)$$

$$\frac{\partial \omega}{\partial p} = -\nabla \cdot \mathbf{v}_h. \quad (13.148)$$

As you can see, ω is a diagnostic quantity. a can be calculated from Φ using Eq. (13.124) can be determined, then the temperature can also be calculated diagnostically via $T = \frac{p a}{R_d}$.

13.7.5 Hydrostatic background condition

Even if one does not make the hydrostatic assumption, one can introduce a ground state $\{\bar{a}, \bar{p}\}$ with $a := \frac{1}{\rho}$ as the specific volume, the Eq. (13.122) is fulfilled, and the actual quantities $\{a, p\}$ are to be noted as an overlay of the ground state with deviations $\{a', p'\}$, i.e

$$a = \bar{a} + a', \quad (13.149)$$

$$p = \bar{p} + p'. \quad (13.150)$$

Then applies

$$-a \nabla p + \mathbf{g} = -a' \nabla \bar{p} - \bar{a} \nabla p' - a' \nabla p' = -a' \nabla p - \bar{a} \nabla p' = -a \nabla p' - a' \nabla \bar{p}. \quad (13.151)$$

The Earth's gravity field has a complicated shape that can be approached in different stages. First of all, it is assumed that the gravity field is radially symmetric with a homogeneous magnitude of the gravity vector. If you use the geopotential height $\Phi = gz$ instead of the geometric height z (this is the energy per mass that is necessary to bring a particle from sea level to the height z), the basic hydrostatic equation with the chain rule is

$$\frac{\partial p}{\partial \Phi} = \frac{\partial p}{\partial z} \frac{\partial z}{\partial \Phi} = -\rho. \quad (13.152)$$

The SI unit of geopotential is m^2/s^2 . A geopotential meter gpm is defined by

$$1 \text{ gpm} := 9,8 \text{ m}^2/\text{s}^2, \quad (13.153)$$

so that

$$\frac{z}{\text{m}} = \frac{\varphi/g}{\text{m}} \approx \frac{\varphi}{\text{gpm}} \quad (13.154)$$

applies. If you want to take into account the height dependence of gravitational acceleration, you first use the formula for the gravitational potential

$$\Phi_g(r) = -\frac{\Phi_o a}{r} + \Phi_o \quad (13.155)$$

with $\Phi_o := GM/a$ with G as Newton's gravitational constant and M as Earth's mass. This is the formula for the gravity field of a planet with a radially symmetric mass distribution; it results from the formula for a point mass using Gauss's theorem. At $r = a$ the potential is normalized to zero. From this it follows

$$g = \frac{\Phi_o a}{r^2} = g_o \frac{a^2}{r^2} \quad (13.156)$$

with $g_o := \frac{\Phi_o}{a}$. In this approximation one requires that the generalized vertical coordinate geopotential height z_g holds

$$g_o z_g \stackrel{!}{=} \Phi_g(a+z) = -\frac{\Phi_o a}{a+z} + \Phi_o \Rightarrow z_g = -\frac{a^2}{a+z} + a = \frac{-a^2 + a^2 + za}{a+z} = \frac{z}{1 + \frac{z}{a}}. \quad (13.157)$$

It still follows from this

$$\begin{aligned} \frac{\partial p}{\partial z} &= \frac{z_g}{z} \frac{\partial p}{\partial z_g} = \left(\frac{1}{1 + \frac{z}{a}} - \frac{z}{a} \frac{1}{\left(1 + \frac{z}{a}\right)^2} \right) \frac{\partial p}{\partial z_g} = \frac{1}{\left(1 + \frac{z}{a}\right)^2} \frac{\partial p}{\partial z_g} = \frac{a^2}{r^2} \frac{\partial p}{\partial z_g} = -g_\rho = -g_o \frac{a^2}{r^2} \rho \\ \Rightarrow \frac{\partial p}{\partial z_g} &= -g_o \rho. \end{aligned} \quad (13.158)$$

13.8 Barotropy

Barotropy is when the contour areas of the pressure field and the density field are the same. In a dry atmosphere this is equivalent to the fact that the temperature surfaces and the pressure surfaces are equal. In reality, the baroclinity angle, which describes the angle between ∇_ρ and ∇p , is small. However, the existing baroclinicity is very important for atmospheric dynamics and barotropy has far-reaching limiting implications.

Deriving the x component of Eq. (13.132) assuming barotropy to p , one obtains

$$\frac{\partial}{\partial p} \frac{Du}{Dt} = -\frac{\partial}{\partial p} \frac{\partial \Phi}{\partial x} + f \frac{\partial v}{\partial p} = -\frac{\partial}{\partial x} \frac{\partial \Phi}{\partial p} + f \frac{\partial v}{\partial p} = f \frac{\partial v}{\partial p}. \quad (13.159)$$

It also applies

$$\frac{\partial}{\partial p} \frac{Du}{Dt} = \frac{\partial}{\partial p} \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \omega \frac{\partial u}{\partial p} \right), \quad (13.160)$$

it follows from this

$$\frac{\partial}{\partial t} \frac{\partial u}{\partial p} = \frac{\partial}{\partial p} \frac{\partial u}{\partial t} = f \frac{\partial v}{\partial p} - \frac{\partial}{\partial p} \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \omega \frac{\partial u}{\partial p} \right). \quad (13.161)$$

From this equation you can see that if the vertical shear disappears globally for one point in time, it will do so for all points in time. If the vertical shear disappears, the horizontal divergence and thus according to Eq. (13.129) $\frac{\partial \omega}{\partial p}$ constant height. The vertical velocity field in the p-system $\omega = \omega(p)$ is in this case a straight line and a diagnostic quantity.

13.8.1 Shallow water equations

The simplest system of equations in geofluid dynamics with time derivatives is that of *shallow water equations* (SWEs). To derive this, one starts from the equations (13.31) - (13.32) and assumes a homogeneous density and also ignores the friction. This makes the continuity equation:

$$\nabla \cdot \mathbf{v} = 0. \quad (13.162)$$

The fluid still has a surface where $p = 0$. Let the depth of the medium be $h = h(x, y, t)$ and the ground have the z coordinate $b = b(x, y)$. This is obtained by integrating the basic hydrostatic equation

$$p(z) = -(0 - p(z)) = -(p(b+h) - p(z)) = - \int_z^{b+h} \frac{\partial p}{\partial z} dz = g\rho \int_z^{b+h} dz = (b+h-z)g\rho. \quad (13.163)$$

Thus follows

$$\frac{\partial p}{\partial x} = g\rho \frac{\partial}{\partial x} (b+h) \quad (13.164)$$

and analogously in the y direction. If the vertical shear of the horizontal movement $\left(\frac{\partial u}{\partial z}, \frac{\partial v}{\partial z}\right)^T$ disappears globally at any point in time, the local time tendency of the vertical shear also disappears. The velocity field is therefore independent of height at all times. This is now assumed. This means that the terms of vertical velocity advection disappear. Now one can trivially integrate the continuity equation:

$$h\nabla \cdot \mathbf{v} = \int_b^{b+h} \nabla \cdot \mathbf{v} dz = - \int_b^{b+h} \frac{\partial w}{\partial z} dz = -w(b+h) + w(b) \quad (13.165)$$

The assumption that the horizontal velocity is not sheared and that the integration Eq. (13.165) gives the shallow water equations their name. At great depths, this can clearly no longer be assumed. In Section 16.5.2 we go beyond this assumption. When dealing with waves, one can use the shallow water equations if

$$\text{Wellenlänge} \gg \text{Tiefe}, \quad (13.166)$$

$$\text{Wellenhöhe} \ll \text{Tiefe} \quad (13.167)$$

apply, which can be the case for the tide (except in marginal seas) and the swell on the open sea.

At depth b the kinematic boundary condition applies:

$$w(b) = \frac{dz}{dt}(b) = \frac{db}{dt} = \mathbf{v} \cdot \nabla_h b \quad (13.168)$$

On the surface applies

$$w(b+h) = \frac{D}{Dt}(b+h) = \frac{\partial h}{\partial t} + \mathbf{v}_h \cdot \nabla_h (b+h). \quad (13.169)$$

Putting this into Eq. (13.165), you get

$$h\nabla_h \cdot \mathbf{v} = -\frac{\partial h}{\partial t} - \mathbf{v} \cdot \nabla_h h. \quad (13.170)$$

This results in the following system of equations:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -g\nabla_h (h+b) - f(y) \mathbf{k} \times \mathbf{v} \quad (13.171)$$

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\mathbf{v}) = 0 \quad (13.172)$$

13.8.1.1 Linearization

Assuming a homogeneous subsurface b and an average depth D on which a fault d is superimposed, and neglecting all nonlinear terms, it follows

$$\frac{\partial \mathbf{v}}{\partial t} = -g\nabla d - f\mathbf{k} \times \mathbf{v}, \quad (13.173)$$

$$\frac{\partial d}{\partial t} + D\nabla \cdot \mathbf{v} = 0. \quad (13.174)$$

13.9 Developments of the Coriolis parameter in plane geometry

For the Coriolis parameter f as a function of the width φ holds

$$f(\varphi) = 2\omega \sin(\varphi). \quad (13.175)$$

If you Taylor-expand this at a width φ_o , you get

$$\begin{aligned} f(\varphi) &= f(\varphi_o) + f'(\varphi_o)(\varphi - \varphi_o) + \frac{1}{2}f''(\varphi_o)(\varphi - \varphi_o)^2 + \frac{1}{6}f'''(\varphi_o)(\varphi - \varphi_o)^3 + \mathcal{O}[(\varphi - \varphi_o)^4] \\ &= f(\varphi_o) \left[1 + \cot(\varphi_o)(\varphi - \varphi_o) - \frac{1}{2}(\varphi - \varphi_o)^2 - \frac{1}{6}\cot(\varphi_o)(\varphi - \varphi_o)^3 \right], \end{aligned} \quad (13.176)$$

whereby the fourth and higher order terms were no longer noted. With

$$y := r(\varphi - \varphi_o) \quad (13.177)$$

with r as the distance from the center of the earth this can be written as

$$f(\varphi) = f(\varphi_o) \left[1 + \cot(\varphi_o) \frac{y}{r} - \frac{y^2}{2r^2} - \frac{y^3}{6r^3} \cot(\varphi_o) \right] \quad (13.178)$$

note down. The *Rossby parameter* is defined by

$$\beta(\varphi_o) := \cot(\varphi_o) \frac{f(\varphi_o)}{r} = \frac{2\omega \cos(\varphi_o)}{r} = \frac{d\varphi}{dy} \frac{df}{d\varphi} = \frac{df}{dy}. \quad (13.179)$$

The approximations to be derived now assume a zonal channel of meridional extent $2B$, which is centered at the width φ_o . The curvature terms are neglected, which is why we speak of planes.

13.9.1 f-plane

This is where the approximation is made

$$f(\varphi) \approx f(\varphi_o). \quad (13.180)$$

According to Eq. (13.178) is this justified if

$$B \ll r \tan(\varphi_o), \quad B \ll \sqrt{2}r \quad (13.181)$$

apply. The so-called *f-sphere* assumes a globally homogeneous Coriolis parameter, which is not suitable for operational predictions.

13.9.2 β -plane

This is where the approximation is set

$$f(\varphi) \approx f(\varphi_o) + \beta y \quad (13.182)$$

to. According to Eq. (13.178) is this justified if

$$B \ll 2r \cot(\varphi_o), \quad B \ll \sqrt{6}r \quad (13.183)$$

Term	Magnitude in SI
$\frac{\partial u}{\partial t}$	10^{-4}
$u \frac{\partial u}{\partial x}$	10^{-4}
fv	10^{-3}
$\frac{1}{\rho} \frac{\partial p}{\partial x}$	10^{-3}

Table 13.1: Scaling the horizontal momentum equation on the synoptic scale.

apply.

13.10 Equilibrium winds

13.10.1 Geostrophy

For the Rossby number N_{Ro} applies

$$N_{Ro} = \frac{U}{Lf} \sim 10^{-1} \quad (13.184)$$

on the synoptic scale. In the first order, there is a balance of forces consisting of the Coriolis force and the pressure gradient force. This is the geostrophic approximation. The corresponding wind field $\mathbf{v}_h = (u_g, v_g)^T$ is obtained by setting the acceleration equal to zero in the horizontal equations of motion (13.132) - (13.133).

$$0 = -\frac{\partial \Phi}{\partial x} + fv_g, \quad 0 = -\frac{\partial \Phi}{\partial y} - fu_g \quad (13.185)$$

If you adjust this according to the wind speed, you get:

$$v_g = \frac{1}{f} \frac{\partial \Phi}{\partial x}, \quad u_g = -\frac{1}{f} \frac{\partial \Phi}{\partial y}. \quad (13.186)$$

So the geostrophic wind is

$$\mathbf{v}_{h,g} = \frac{1}{f} \begin{pmatrix} -\frac{\partial \Phi}{\partial y} \\ \frac{\partial \Phi}{\partial x} \end{pmatrix} = \mathbf{k} \times \frac{1}{f} \nabla \Phi. \quad (13.187)$$

The geostrophic wind speed decreases as the latitude increases; at the equator it approaches infinity. It must therefore be questioned up to which latitudes geostrophy is a good approximation. This question will be examined in more detail in Section 13.9.2.

If you form the dot product with the gradient of the geopotential, it follows

$$\nabla \Phi \cdot \mathbf{v}_{h,g} = 0, \quad (13.188)$$

the geostrophic wind is perpendicular to the geopotential gradient. Therefore, the geostrophic wind is isohypse-parallel. In geostrophy, the local temporal tendency of the horizontal wind arises purely from advection. Further important implications of the geostrophic assumption are discussed in Sect. 13.9.

If one forms the divergence of Eq. (13.187), you get

$$\nabla \cdot \mathbf{v}_{h,g} = -\frac{1}{f} \frac{\partial^2 \Phi}{\partial x \partial y} + \frac{1}{f} \frac{\partial^2 \Phi}{\partial y \partial x} - \frac{\beta}{f^2} \frac{\partial \Phi}{\partial x} - \frac{v \tan(\varphi)}{r} = -\frac{\beta}{f^2} \frac{\partial \Phi}{\partial x} = -\frac{\beta}{f} v - \frac{v \tan(\varphi)}{r}. \quad (13.189)$$

Using the scales from tab. 1.3 follows

$$\mathcal{O}(\nabla \cdot \mathbf{v}_{h,g}) = \frac{10^{-11}}{10^{-4}} 10^1 \frac{1}{s} = 10^{-6} \frac{1}{s} \quad (13.190)$$

for medium and high latitudes. This is about an order of magnitude smaller than the synoptic-scale divergence, so the geostrophic wind can be viewed as almost divergence-free outside the tropics, but this no longer applies at lower latitudes. The geostrophic approximation is therefore not applicable globally, especially for models.

The *thermal wind* refers to the change of the geostrophic wind with height due to baroclinity. From Eq. (13.187) follows

$$\frac{\partial \mathbf{v}_{h,g}}{\partial p} = \mathbf{k} \times \frac{1}{f} \nabla \frac{\partial \Phi}{\partial p} = -\frac{R_d}{pf} \mathbf{k} \times \nabla T. \quad (13.191)$$

The vertical shear of the geostrophic wind results from the baroclinicity of the atmosphere. One also speaks of *vertical shear of the geostrophic wind due to horizontal temperature gradients*, where *horizontal* here refers to the pressure area. Eq. (13.191) is the *thermal wind equation*.

Let $p_1 < p_2$ be two pressure levels, then by integrating Eq. (13.191)

$$\begin{aligned} \mathbf{v}_{h,g}(p_2) - \mathbf{v}_{h,g}(p_1) &= \int_{p_1}^{p_2} -\frac{R_d}{pf} \mathbf{k} \times \nabla T dp \\ \Rightarrow \mathbf{v}_{h,g}(p_1) &= \mathbf{v}_{h,g}(p_2) + \int_{p_1}^{p_2} \frac{R_d}{pf} \mathbf{k} \times \nabla T dp = \mathbf{v}_{h,g}(p_2) + \frac{R_d}{f} \int_{p_1}^{p_2} \frac{1}{p} \mathbf{k} \times \nabla T dp \\ &= \mathbf{v}_{h,g}(p_2) + \frac{R_d}{f} \ln\left(\frac{p_2}{p_1}\right) \mathbf{k} \times \nabla \bar{T}(p_1, p_2) \end{aligned} \quad (13.192)$$

with a weighted layer average temperature

$$\bar{T}(p_1, p_2) = \frac{\int_{p_1}^{p_2} \frac{1}{p} T dp}{\int_{p_1}^{p_2} \frac{1}{p} dp}. \quad (13.193)$$

13.10.2 Gradient wind

With the *gradient wind* it is assumed that the Coriolis force and the pressure gradient together produce the centripetal force that is necessary to move a fluid particle along a trajectory with radius $R > 0$, i.e

$$\frac{V^2}{R} = \left| |f| V - \frac{1}{\rho} |\nabla_h p| \right|. \quad (13.194)$$

In the cyclonic case, the expression between the outer magnitude signs is negative, i.e

$$\begin{aligned} \frac{V^2}{R} &= \frac{1}{\rho} |\nabla_h p| - |f| V \\ \Leftrightarrow V^2 + |f| VR - R \frac{1}{\rho} |\nabla_h p| &= 0 \\ \Leftrightarrow \frac{V^2}{R} &= -\frac{1}{\rho} |\nabla_h p| + |f| V \\ \Leftrightarrow V &= -\frac{|f|R}{2} \pm \sqrt{\frac{f^2 R^2}{4} + R \frac{1}{\rho} |\nabla_h p|}. \end{aligned} \quad (13.195)$$

Because $V = |\mathbf{v}_h| > 0$ only the positive sign comes into question. In this case the wind speed is lower than the geostrophic wind speed, one speaks of *subgeostrophic wind*. The same applies in the anticyclonic case

$$\begin{aligned}
\frac{V^2}{R} &= -\frac{1}{\rho} |\nabla_h p| + |f| V \\
\Leftrightarrow V^2 - |f| VR + R \frac{1}{\rho} |\nabla_h p| &= 0 \\
\Leftrightarrow \frac{V^2}{R} &= -\frac{1}{\rho} |\nabla_h p| + |f| V \\
\Leftrightarrow V &= \frac{|f| R}{2} \pm \sqrt{\frac{f^2 R^2}{4} - R \frac{1}{\rho} |\nabla_h p|}.
\end{aligned} \tag{13.196}$$

In this case the wind is *supergeostrophic*. Only the negative sign comes into play here, since in the limit case $|\nabla_h p| = 0$ no wind $V = R|f|$ should blow. The expression under the root is positive, so

$$|\nabla_h p| \leq \frac{\rho f^2 R}{4}. \tag{13.197}$$

Anticyclones have a weaker gradient near the core; there is no such limitation for cyclones. This is because

$$\frac{\rho f^2 R}{4} \sim 10 \frac{\text{hPa}}{1000 \text{ km}} \tag{13.198}$$

actually significant on the synoptic scale.

13.10.3 Frictional wind

If you take a pressure gradient acceleration

$$P := \frac{1}{\rho} |\nabla p| \tag{13.199}$$

which points in the y -direction and additionally a friction force $-\mu \mathbf{v}_h$ and sets the acceleration equal to zero, you get

$$0 = fV \sin(\psi) - \mu V \cos(\psi) \xrightarrow{\psi \in [0, \pi/2]} \psi = \arctan\left(\frac{\mu}{f}\right), \tag{13.200}$$

$$0 = P - fV \cos(\psi) - \mu V \sin(\psi) \Rightarrow V = \frac{P}{f \cos(\psi) + \mu \sin(\psi)}, \tag{13.201}$$

where ψ is the angle at which the wind intersects the isobar. This is called *frictional wind*. The frictional wind therefore leads to overisobaric transport and thus counteracts the formation of extremes in the ground pressure field or promotes their dissipation. The annihilation effect on a low is estimated with $R \sim 500 \text{ km}$ and $\psi \sim 30^\circ$ from by

$$\frac{\partial p}{\partial t} \sim \frac{g}{\pi r^2} \frac{dm}{dt} \sim \frac{g}{\pi r^2} 2\pi r H \rho V \frac{1}{2} = \frac{g V H \rho}{r} \sim 4 \text{ hPa/hr} \tag{13.202}$$

where the boundary layer height was estimated to be $H = 500 \text{ m}$. The frictional wind dissipates a cyclone within hours, so it is a relevant effect on the synoptic scale. Divergences above the friction layer were not taken into account, and ψ was assumed to be independent of height within the boundary layer. In reality, of course, this is not the case, but ψ decreases with height, which leads to the formation of a spiral-like wind field, the so-called *Ekman spiral*.

13.10.4 Euler wind

The *Euler wind* is the increase in wind under the effect of a pressure gradient and the absence of Coriolis acceleration, i.e

$$\mathbf{v}_h = -t \frac{\mathbf{I}}{\rho} \nabla p. \quad (13.203)$$

13.10.5 Cyclostrophic wind

The *cyclostrophic wind* is given when a pressure gradient applies a centripetal force:

$$\left| \frac{\partial p}{\partial r} \right| = \frac{\rho V^2}{|R|} \quad (13.204)$$

It applies in *Tornados* and *Dust Devils*.

13.11 Quasigeostrophy

Here we start from the hydrostatic adiabatic equation system, which was summarized in Sect. 13.7:

$$\frac{D_h \mathbf{v}_h}{Dt} + \omega \frac{\partial \mathbf{v}_h}{\partial p} = -f \mathbf{k} \times \mathbf{v}_h - \nabla \Phi, \quad (13.205)$$

$$\frac{\partial \Phi}{\partial p} = -a, \quad (13.206)$$

$$\frac{\partial^2 \Phi}{\partial p \partial t} + \left(u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \right) \frac{\partial \Phi}{\partial p} + \sigma \omega = 0, \quad (13.207)$$

$$\nabla \cdot \mathbf{v}_h + \frac{\partial \omega}{\partial p} = 0, \quad (13.208)$$

$$pa = R_d T. \quad (13.209)$$

Now some simplifications need to be made first. The goal is the *quasigeostrophic system of equations*. This concept is applied exclusively to channels in the extratropics that are narrow enough for the β plane. One also approximates the Coriolis parameter f

$$f = f_o + \beta (y - y_o) \stackrel{y_o \equiv 0}{=} f_o + \beta y, \quad (13.210)$$

see section 13.9. Then Eq. applies to the geostrophic wind. (13.187)

$$\mathbf{v}_{h,g} = \mathbf{k} \times \frac{\mathbf{I}}{f} \nabla \Phi = \mathbf{k} \times \frac{\mathbf{I}}{f_o} \nabla \Phi - \mathbf{k} \times \frac{\beta y}{f_o^2} \nabla \Phi + \mathcal{O}(f'') \stackrel{\text{in 0. Ordnung}}{\rightarrow} \mathbf{v}_{h,g} = \mathbf{k} \times \frac{\mathbf{I}}{f_o} \nabla \Phi. \quad (13.211)$$

From this one can derive the thermal wind

$$\frac{\partial \mathbf{v}_{h,g}}{\partial p} = -\frac{\mathbf{I}}{f_o} \mathbf{k} \times \nabla a. \quad (13.212)$$

The relative vorticity ζ is now approximately replaced by the relative vorticity of the geostrophic wind ζ_g , which according to Eq. (15.86) approximately

$$\zeta_g = \frac{\mathbf{I}}{f_o} \Delta \Phi. \quad (13.213)$$

is given. The absolute vorticity is approximated from this

$$\eta_g := f + \zeta_g = f_o + \beta y + \zeta_g. \quad (13.214)$$

With Eq. (13.221) one now simplifies the material derivation to

$$\begin{aligned}
\frac{D}{Dt} &= \frac{D_h}{Dt} + \omega \frac{\partial}{\partial p} = \frac{\partial}{\partial t} + \mathbf{v}_h \cdot \nabla_h + \omega \frac{\partial}{\partial p} \\
&\rightarrow \frac{D^{(g)}}{Dt} := \frac{D_h^{(g)}}{Dt} + \omega \frac{\partial}{\partial p} = \frac{\partial}{\partial t} + \mathbf{v}_{h,g} \cdot \nabla_h + \omega \frac{\partial}{\partial p}.
\end{aligned} \tag{13.215}$$

This follows for the first law

$$\frac{\partial}{\partial t} \left(\frac{\partial \Phi}{\partial p} \right) = -\mathbf{v}_{h,g} \cdot \nabla_h \left(\frac{\partial \Phi}{\partial p} \right) - \sigma \omega. \tag{13.216}$$

The vorticity equation Eq. (15.85) is repeated here:

$$\frac{\partial \zeta}{\partial t} = -v_l \beta - (f + \zeta) \nabla \cdot \mathbf{v}_h - \mathbf{v}_h \cdot \nabla \zeta - \omega \frac{\partial \zeta}{\partial p} + \mathbf{k} \cdot \left[\frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega \right] \tag{13.217}$$

According to Sect. 13.10.1, the geostrophic wind is an order of magnitude larger than the ageostrophic component, so one can calculate the horizontal advection with $\mathbf{v}_{h,g}$ and replace ζ by ζ_g :

$$\frac{\partial \zeta_g}{\partial t} = -v_{gl} \beta - (f + \zeta_g) \nabla \cdot \mathbf{v}_h - \mathbf{v}_{h,g} \cdot \nabla \zeta_g - \omega \frac{\partial \zeta_g}{\partial p} + \mathbf{k} \cdot \left[\frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega \right] \tag{13.218}$$

The values in tab. 1.3 also result in SI units

- $\frac{\partial \zeta_g}{\partial t} \sim 10^{-10},$
- $\omega \frac{\partial \zeta_g}{\partial p} \sim 10^{-11},$
- $\mathbf{k} \cdot \left[\frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega \right] \sim 10^{-11}.$

Consequently, the rotation term and the vertical advection can also be neglected, as can the relative versus absolute vorticity in the rotation term, which leads to the so-called *quasigeostrophic vorticity equation* with $f \approx f_0$

$$\frac{\partial \zeta_g}{\partial t} = -\mathbf{v}_{h,g} \cdot \nabla (\zeta_g + f) - f_0 \nabla \cdot \mathbf{v}_h = -\mathbf{v}_{h,g} \cdot \nabla (\zeta_g + f) + f_0 \frac{\partial \omega}{\partial p}. \tag{13.219}$$

At this point, a current function is introduced to simplify things

$$\psi := \frac{\Phi}{f_0} \tag{13.220}$$

one, so follow

$$\mathbf{v}_{h,g} = \mathbf{k} \times \nabla \psi, \tag{13.221}$$

$$\zeta_g = \Delta_h \psi. \tag{13.222}$$

From this it follows for the vorticity equation Eq. (13.219) and the First Law Eq. (3.12)

$$\Delta \frac{\partial \psi}{\partial t} = -\mathbf{v}_{h,g} \cdot \nabla (\Delta \psi + f) + f_0 \frac{\partial \omega}{\partial p}, \tag{13.223}$$

$$\begin{aligned}
\frac{\partial}{\partial t} \left(\frac{\partial \psi}{\partial p} \right) &= -\mathbf{v}_{h,g} \cdot \nabla \left(\frac{\partial \psi}{\partial p} \right) - \frac{\sigma}{f_0} \omega \\
\Rightarrow \frac{f_0}{\sigma} \frac{\partial^2}{\partial p^2} \left(\frac{\partial \psi}{\partial t} \right) &= -\frac{f_0}{\sigma} \mathbf{v}_h \cdot \nabla \left(\frac{\partial^2 \psi}{\partial p^2} \right) - f_0 \frac{\partial \omega}{\partial p}
\end{aligned} \tag{13.224}$$

The last implication neglected the p-dependence on σ and will continue to do so. Since σ is related to stratification, this is a bad assumption, as of course in reality stratification is highly location dependent within the troposphere.

Nevertheless, this assumption can be made here because the relevant phenomena are not filtered by this assumption. Furthermore, it was

$$\frac{\partial \mathbf{v}_{h,g}}{\partial p} \cdot \nabla \left(\frac{\partial \psi}{\partial p} \right) \stackrel{\text{Glg. (13.221)}}{=} \left(\mathbf{k} \times \nabla \frac{\partial \psi}{\partial p} \right) \cdot \nabla \left(\frac{\partial \psi}{\partial p} \right) = 0 \quad (13.225)$$

used. Now the two equations are added

$$\frac{\partial}{\partial t} \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) + \mathbf{v}_{h,g} \cdot \nabla \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) = 0. \quad (13.226)$$

The size

$$q_g := f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \quad (13.227)$$

is called *quasigeostrophic potential vorticity* or also *pseudopotential vorticity*, so Eq. (13.226) as

$$\frac{D_h^{(g)}}{Dt} q_g = 0 \quad (13.228)$$

note down. This is the so-called *tendency equation*. ω can be diagnosed from this by first applying the horizontal Laplace operator Δ_h to Equation. (13.216) to:

$$\Delta \frac{\partial}{\partial p} \frac{\partial \psi}{\partial t} = -\Delta_h \left[\mathbf{v}_{h,g} \cdot \nabla \left(\frac{\partial \psi}{\partial p} \right) \right] - \frac{\sigma}{f_o} \Delta \omega. \quad (13.229)$$

Now Eq. (13.219) differentiated according to p :

$$\frac{\partial}{\partial p} \Delta \frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial p} \left[\mathbf{v}_{h,g} \cdot \nabla (\Delta \psi + f) \right] + f_o \frac{\partial^2 \omega}{\partial p^2} \quad (13.230)$$

Now subtract Eq. (13.229) from (13.230) and gets

$$0 = \Delta \left[\mathbf{v}_{h,g} \cdot \nabla \left(\frac{\partial \psi}{\partial p} \right) \right] + \frac{\sigma}{f_o} \Delta \omega - \frac{\partial}{\partial p} \left[\mathbf{v}_{h,g} \cdot \nabla (\Delta \psi + f) \right] + f_o \frac{\partial^2 \omega}{\partial p^2}$$

$$\Rightarrow \left[\Delta + \frac{f_o}{\sigma} \frac{\partial^2}{\partial p^2} \right] \omega = \frac{f_o}{\sigma} \frac{\partial}{\partial p} \left[\mathbf{v}_{h,g} \cdot \nabla (\Delta \psi + f) \right] + \frac{f_o}{\sigma} \Delta \left[\mathbf{v}_{h,g} \cdot \nabla \left(\frac{\partial \psi}{\partial p} \right) \right]. \quad (13.231)$$

This is the ω -*equation*. This formalism is not globally applicable due to the linear expansion of f contained therein; the performance lies in the fact that it can be used to understand baroclinic Rossby waves and baroclinic instabilities within zonal channels of limited extent in the extratropics, which is the theoretical basis of *cyclogenesis*.

13.12 Semigeostrophy

The semigeostrophic assumption is a relaxation of the quasigeostrophic assumption. In contrast to this, it leads to a globally applicable system of equations. As part of the solution spectrum, surfaces in the space of particular baroclinicity, so-called *fronts*, are obtained.

The starting point is the hydrostatic equation system derived in Section 13.7, which is noted again here:

$$\frac{\partial u}{\partial t} - \mathbf{v}_h \cdot \nabla u - \omega \frac{\partial u}{\partial p} - fv + \frac{\partial \Phi}{\partial x} = 0 \quad (13.232)$$

$$\frac{\partial v}{\partial t} - \mathbf{v}_h \cdot \nabla v - \omega \frac{\partial v}{\partial p} + fu + \frac{\partial \Phi}{\partial y} = 0 \quad (13.233)$$

$$\frac{\partial^2 \Phi}{\partial t \partial p} + \mathbf{v}_h \cdot \nabla \frac{\partial \Phi}{\partial p} + \frac{1}{\rho^2 g^2} N^2 \omega = 0 \quad (13.234)$$

$$\frac{\partial \omega}{\partial p} + \nabla \cdot \mathbf{v}_h = 0, \quad (13.235)$$

$$\frac{\partial \Phi}{\partial p} + \frac{1}{\rho} = 0. \quad (13.236)$$

Diabatic terms were omitted.

In the semigeostrophic approximation only the horizontal momentum equation is modified. is a basic requirement

$$N_{\text{Ro}} = \frac{U}{Lf} \ll 1, \quad (13.237)$$

so that the material acceleration is small compared to the Coriolis acceleration [19]. N_{Ro} is the value in Eq. (13.3) defined Rossby number.

The semi-geostrophic system of equations is thus summarized as:

$$\frac{\partial u_g}{\partial t} + \mathbf{v}_h \cdot \nabla u_g - \omega \frac{\partial u_g}{\partial p} - fv + \frac{\partial \Phi}{\partial x} = 0, \quad (13.238)$$

$$\frac{\partial v_g}{\partial t} + \mathbf{v}_h \cdot \nabla v_g - \omega \frac{\partial v_g}{\partial p} + fu + \frac{\partial \Phi}{\partial y} = 0, \quad (13.239)$$

$$\frac{\partial \theta}{\partial t} + \mathbf{v}_h \cdot \nabla \theta - \omega \frac{\partial \theta}{\partial p} = 0, \quad (13.240)$$

$$\frac{\partial^2 \Phi}{\partial t \partial p} + \mathbf{v}_h \cdot \nabla \frac{\partial \Phi}{\partial p} + \frac{1}{\rho^2 g^2} N^2 \omega = 0, \quad (13.241)$$

$$\frac{\partial \omega}{\partial p} + \nabla \cdot \mathbf{v}_h = 0, \quad (13.242)$$

$$\frac{\partial \Phi}{\partial p} + \frac{1}{\rho} = 0. \quad (13.243)$$

This is a system of equations for the prognostic variables u , v , ω , Φ , θ . Note that u_g and v_g are diagnostic variables, although they have fixed time derivatives.

14.1 Momentum and angular momentum

For the total momentum $\mathbf{P}$ of the atmosphere applies

$$\mathbf{P} = \int_A \rho \mathbf{v} d^3r. \quad (14.1)$$

According to Newton's Second Axiom only the external forces have to be taken into account for the time derivative of this quantity:

$$\frac{d\mathbf{P}}{dt} = \int_A \rho \mathbf{f}_{\text{ext}} d^3r. \quad (14.2)$$

$\mathbf{P}$ is therefore never conserved, since external forces always act at least through the surface and gravity.

For the total angular momentum $\mathbf{L}$ of the atmosphere applies

$$\mathbf{L} = \int_A \mathbf{r} \times \rho \mathbf{v} d^3r \Rightarrow \frac{d\mathbf{L}}{dt} = \int_A \mathbf{r} \times \rho \mathbf{f}_{\text{ext}} d^3r. \quad (14.3)$$

The angular momentum is conserved exactly when all external forces act on the radial axis, i.e. only in stationary coordinates over a planet with radially symmetrical mass distribution inside.

14.2 entropy

The total entropy S of an atmosphere has all but one constant

$$S = \int_A \tilde{s} d^3r \quad (14.4)$$

with $\tilde{s}$ as in Eq. (9.33) is defined. The prognostic equation of this quantity is Eq. (9.34):

$$\frac{\partial \tilde{s}}{\partial t} + \nabla \cdot (\tilde{s} \mathbf{v}) = c^{(V)} \frac{\rho}{T} q_T \quad (14.5)$$

Global integration delivers

$$\frac{dS}{dt} = \int_A c^{(V)} \frac{\rho}{T} q_T d^3r. \quad (14.6)$$

This integral is nonnegative because the heat flow is positive in colder areas and negative in warmer areas. Therefore applies

$$\frac{dS}{dt} \geq 0. \quad (14.7)$$

In an ideal adiabatic single-phase atmosphere, the processes are reversible.

14.3 energy

14.3.1 Total energy

The prognostic equation of the specific kinetic energy $k = \frac{1}{2} \mathbf{v}^2$ is obtained by multiplying the momentum equation in the form Eq. (8.101) from the left with $\mathbf{v}$:

$$\frac{Dk}{Dt} = \frac{\partial k}{\partial t} + \mathbf{v} \cdot \nabla k = -\frac{1}{\rho} \mathbf{v} \cdot \nabla p - wg + \mathbf{v} \cdot \mathbf{f}_R. \quad (14.8)$$

If you multiply this equation by ρ and add the product of the continuity equation by k , you get

$$\frac{DK}{Dt} = \frac{\partial K}{\partial t} + \mathbf{v} \cdot \nabla K = -\mathbf{v} \cdot \nabla p - \rho wg - K \nabla \cdot \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{f}_R \quad (14.9)$$

as a prognostic equation for the kinetic energy density $K = \frac{1}{2} \rho \mathbf{v}^2$. The prognostic equation for the specific geopotential energy φ is obtained

$$\frac{D\varphi}{Dt} = \mathbf{v} \cdot \nabla \varphi = wg. \quad (14.10)$$

If you multiply this equation by ρ and add the product of the continuity equation by φ , you get

$$\frac{DP}{Dt} = \frac{\partial P}{\partial t} + \mathbf{v} \cdot \nabla P = \rho wg - P \nabla \cdot \mathbf{v} \quad (14.11)$$

as a prognostic equation for the geopotential energy density $P = \rho \varphi$. The prognostic equation for the specific internal energy is $i = c^{(V)} T$

$$\frac{Di}{Dt} = \frac{\partial i}{\partial t} + \mathbf{v} \cdot \nabla i = -p \frac{Da}{Dt} + \varepsilon = -p a \nabla \cdot \mathbf{v} + \varepsilon. \quad (14.12)$$

If you multiply this equation by ρ and add the product of the continuity equation by i , you get

$$\frac{D\tilde{I}}{Dt} = \frac{\partial \tilde{I}}{\partial t} + \mathbf{v} \cdot \nabla \tilde{I} = -\left(p + \tilde{I}\right) \nabla \cdot \mathbf{v} + \rho \varepsilon \quad (14.13)$$

as a prognostic equation for the internal energy density $\tilde{I} := \rho i$. The energy density e is the sum of kinetic, potential and internal energy per volume,

$$e = K + P + \tilde{I}. \quad (14.14)$$

The total derivation of this is obtained by summing the equations just derived (14.9) - (14.13):

$$\begin{aligned} \frac{DK}{Dt} &= \frac{\partial K}{\partial t} + \mathbf{v} \cdot \nabla K = \frac{\partial K}{\partial t} + \mathbf{v} \cdot \nabla K = -\mathbf{v} \cdot \nabla p - \rho wg - K \nabla \cdot \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{f}_R \\ + \frac{DP}{Dt} &= \frac{\partial P}{\partial t} + \mathbf{v} \cdot \nabla P = \frac{\partial P}{\partial t} + \mathbf{v} \cdot \nabla P = \rho wg - P \nabla \cdot \mathbf{v} \\ + \frac{D\tilde{I}}{Dt} &= \frac{\partial \tilde{I}}{\partial t} + \mathbf{v} \cdot \nabla \tilde{I} = \frac{\partial \tilde{I}}{\partial t} + \mathbf{v} \cdot \nabla \tilde{I} = -p \nabla \cdot \mathbf{v} - \tilde{I} \nabla \cdot \mathbf{v} + \varepsilon \end{aligned}$$

$$\frac{\partial}{\partial t} (K + P + \tilde{I}) + \mathbf{v} \cdot \nabla (K + P + \tilde{I}) = -\left(K + P + \tilde{I}\right) \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla p - p \nabla \cdot \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{f}_R + \varepsilon \quad (14.15)$$

The terms marked **blue** are the gravity terms, these cancel each other out: if gravity produces kinetic energy, this comes at the expense of potential energy. Thus you get

$$\frac{\partial e}{\partial t} + \mathbf{v} \cdot \nabla e = -e \nabla \cdot \mathbf{v} - \nabla \cdot (p \mathbf{v}) + \rho \mathbf{v} \cdot \mathbf{f}_R + \varepsilon. \quad (14.16)$$

This follows

$$\frac{\partial e}{\partial t} = -\nabla \cdot (p\mathbf{v}) - \nabla \cdot (e\mathbf{v}) \Leftrightarrow \frac{\partial e}{\partial t} + \nabla \cdot (e\mathbf{v}) = -\nabla \cdot (p\mathbf{v}) + \rho\mathbf{v} \cdot \mathbf{f}_R + \varepsilon. \quad (14.17)$$

This is also referred to as the *Poynting theorem of meteorology* in analogy to the Poynting theorem of ED Eq. (3.47). As a special case of Eq. (14.16) is obtained for stationary flows of incompressible ideal media

$$\nabla \cdot \mathbf{v} = 0, \quad (14.18)$$

$$\frac{Dp}{Dt} = \mathbf{v} \cdot \nabla p \quad (14.19)$$

the equation

$$\frac{D}{Dt} (K + P + p) = 0, \quad (14.20)$$

which is called *Bernoulli equation*. Other forms of this statement are:

$$\frac{1}{2}\rho\mathbf{v}^2 + \rho gz + p = \text{const. entlang Stromlinien}, \quad (14.21)$$

$$\frac{1}{2}\mathbf{v} + gz + \frac{p}{\rho} = \text{const. entlang Stromlinien}. \quad (14.22)$$

The total energy E of the atmosphere is A

$$E = \int_A e d^3r. \quad (14.23)$$

If one assumes A to be constant, Gauss's theorem applies

$$\frac{dE}{dt} = \int_A \frac{\partial e}{\partial t} d^3r = \int_A -\nabla \cdot [(e + p)\mathbf{v}] + \rho\mathbf{v} \cdot \mathbf{f}_R + \varepsilon d^3r. \quad (14.24)$$

Due to Eq. (8.96) applies

$$\int_A \rho\mathbf{v} \cdot \mathbf{f}_R + \varepsilon d^3r = 0. \quad (14.25)$$

Thus follows

$$\frac{dE}{dt} = - \int_O (e + p) \mathbf{v} \cdot d\mathbf{n} - \int_v (e + p) \mathbf{v} \cdot d\mathbf{n}, \quad (14.26)$$

Here O is the top of the atmosphere and U is the earth's surface. So with the kinematic boundary condition applies:

$$E = \text{const.} \quad (14.27)$$

14.3.2 forms of energy

For the time derivative of the internal energy of a single-phase atmosphere, Eq. (14.13)

$$\frac{d}{dt} \int_A \tilde{I} d^3r = \frac{d}{dt} \int_A -p \nabla \cdot \mathbf{v} - \rho\mathbf{v} \cdot \mathbf{f}_R d^3r = \int_A \mathbf{v} \cdot \nabla p - \rho\mathbf{v} \cdot \mathbf{f}_R d^3r. \quad (14.28)$$

The enthalpy balance is obtained by multiplying this equation by the adiabatic exponent $\kappa = \frac{c^{(p)}}{c^{(V)}}$. Analogously one obtains for the kinetic or potential energy

$$\frac{d}{dt} \int_A K d^3r \stackrel{\text{Glg. (14.9)}}{=} \int_A -\mathbf{v} \cdot \nabla p - \varrho w g + \varrho \mathbf{v} \cdot \mathbf{f}_R d^3r, \quad (14.29)$$

$$\frac{d}{dt} \int_A P d^3r \stackrel{\text{Glg. (14.11)}}{=} \int_A \varrho w g d^3r. \quad (14.30)$$

Thus follows

$$\frac{d}{dt} \int_A \tilde{I} + P d^3r = D - C, \quad (14.31)$$

$$\frac{d}{dt} \int_A K d^3r = C - D \quad (14.32)$$

with the *adiabatic conversion*

$$C := \int_A -\mathbf{v} \cdot \nabla p - \varrho w g d^3r \quad (14.33)$$

and the dissipation

$$D := \int_A -\varrho \mathbf{v} \cdot \mathbf{f}_R d^3r \stackrel{\text{Glg. (8.87)}}{\geq} 0. \quad (14.34)$$

The adiabatic conversion stands for the conversion of potential and internal energy into kinetic energy. This is done by the pressure gradient and gravity doing work. The assignment can therefore be made in the momentum equation

$$\underbrace{\overbrace{\frac{\partial \mathbf{v}}{\partial t}}^{\text{lokalzeitl. \u00c4nderung}} = \underbrace{-\overbrace{(\mathbf{v} \cdot \nabla) \mathbf{v} - \mathbf{f} \times \mathbf{v}}^{\text{Advektion}} - \underbrace{\frac{1}{\varrho} \nabla p + \mathbf{g}}_{\text{adiabatische Konversion}}}_{\text{reversibel}} + \underbrace{\mathbf{f}_R}_{\text{Dissipation}}}_{\text{irreversibel}} \quad (14.35)$$

or

$$\underbrace{\overbrace{\frac{\partial \mathbf{v}}{\partial t}}^{\text{lokalzeitl. \u00c4nderung}} = \underbrace{\mathbf{v} \times \boldsymbol{\eta} - \nabla k}_{\text{reversibel}} - \underbrace{\frac{1}{\varrho} \nabla p - \nabla \varphi}_{\text{adiabatische Konversion}} + \underbrace{\mathbf{f}_R}_{\text{Dissipation}}}_{\text{irreversibel}} \quad (14.36)$$

make.

14.4 APE

14.4.1 Forms of energy in a hydrostatic atmosphere

The kinetic energy KE of a column of air in a hydrostatic atmosphere is by

$$\text{KE} = \int_0^\infty \frac{1}{2} \varrho \mathbf{v}_h^2 dz = \int_{p(0)}^{p(\infty)} \frac{1}{2} \varrho \mathbf{v}_h^2 \frac{\partial z}{\partial \varrho} dp \stackrel{\partial z / \partial \varrho = -1 / (g \varrho)}{=} -\frac{1}{g} \int_{p_S}^0 \frac{1}{2} \mathbf{v}_h^2 dp = \frac{1}{g} \int_0^{p_S} \frac{1}{2} \mathbf{v}_h^2 dp \quad (14.37)$$

given, where p_S is the pressure at the earth's surface. The same applies to internal energy

$$\text{IE} = \int_0^\infty \rho c^{(V)} T dz = \frac{1}{g} \int_0^{p_S} c^{(V)} T dp. \quad (14.38)$$

For the potential energy PE one obtains with partial integration

$$\begin{aligned} \text{PE} &= \int_0^\infty \rho g z dz = \int_0^{p_S} z(p) dp = \int_0^{p_S} \mathbf{1} \cdot z(p) dp = [pz(p)]_0^{p_S} - \int_0^{p_S} p \frac{\partial z}{\partial p} dp \\ &= p_S z_S + \frac{1}{g} \int_0^{p_S} \frac{p}{\rho} dp = p_S z_S + \frac{1}{g} \int_0^{p_S} R_d T dp \end{aligned} \quad (14.39)$$

with z_S as orography. One defines the *total potential energy* TPE by

$$\text{TPE} := \text{PE} + \text{IE}. \quad (14.40)$$

This form of energy is often simply referred to as „potential energy“ It applies

$$\begin{aligned} \text{TPE} &= p_S z_S + g^{-1} \int_0^{p_S} (c^{(V)} + R_d) T dp = p_S z_S + g^{-1} \int_0^{p_S} h dp \\ &= p_S z_S + \frac{c^{(p)}}{g} \int_0^{p_S} \theta \left(\frac{p}{p_0} \right)^{R_d/c^{(p)}} dp \end{aligned} \quad (14.41)$$

with $h = c^{(p)} T$ as enthalpy. You estimate

$$\frac{\text{KE}}{\text{IE}} \sim \frac{\bar{v}_h^2}{2c^{(V)} \bar{T}} \sim 0,03 \%. \quad (14.42)$$

So there is much more internal than kinetic energy in the atmosphere.

14.4.2 Definition and properties of APE

Since the gravity potential could also be shifted by an arbitrary constant, the concept of *available potential energy* APE is introduced. To do this, first transform Eq. (14.41) into the θ -System:

$$\text{TPE} = p_S z_S + \frac{c^{(p)}}{g p_0^{R_d/c^{(p)}}} \int_\infty^{\theta_S} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta \quad (14.43)$$

Using partial integration one obtains

$$\begin{aligned} &\int_\infty^{\theta_S} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta = \left[\theta p^{1+\frac{R_d}{c^{(p)}}} \right]_\infty^{\theta_S} - \int_\infty^{\theta_S} p(\theta) \frac{d}{d\theta} \left(\theta p(\theta)^{R_d/c^{(p)}} \right) d\theta \\ \Rightarrow &\int_\infty^{\theta_S} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta = \theta_S p_S^{1+\frac{R_d}{c^{(p)}}} - \int_\infty^{\theta_S} p(\theta) \left(p(\theta)^{R_d/c^{(p)}} + \theta \frac{R_d}{c^{(p)}} \frac{\partial p}{\partial \theta} p(\theta)^{R_d/c^{(p)}-1} \right) d\theta \\ \Rightarrow &\int_\infty^{\theta_S} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta = \theta_S p_S^{1+\frac{R_d}{c^{(p)}}} - \int_\infty^{\theta_S} p(\theta)^{1+\frac{R_d}{c^{(p)}}} + \frac{R_d}{c^{(p)}} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta \end{aligned}$$

$$\begin{aligned}
&\Rightarrow \frac{c^{(p)} + R_d}{c^{(p)}} \int_{\infty}^{\theta_S} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta = \theta_S p_S^{1+\frac{R_d}{c^{(p)}}} - \int_{\infty}^{\theta_S} p(\theta)^{1+\frac{R_d}{c^{(p)}}} d\theta \\
&\Rightarrow \int_{\infty}^{\theta_S} \theta p(\theta)^{R_d/c^{(p)}} \frac{\partial p}{\partial \theta} d\theta = \frac{c^{(p)}}{c^{(p)} + R_d} \theta_S p_S^{1+\frac{R_d}{c^{(p)}}} + \frac{c^{(p)}}{c^{(p)} + R_d} \int_{\theta_S}^{\infty} p(\theta)^{1+\frac{R_d}{c^{(p)}}} d\theta \\
&\Rightarrow \text{TPE} = p_S z_S + \frac{c^{(p)2} \theta_S p_S^{1+\frac{R_d}{c^{(p)}}}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} + \frac{c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_{\theta_S}^{\infty} p(\theta)^{1+\frac{R_d}{c^{(p)}}} d\theta.
\end{aligned} \tag{14.44}$$

To obtain the total potential energy contained in an atmosphere over an area A , one calculates

$$\begin{aligned}
\int_A \text{TPE} dA &= \int_A p_S z_S dA + \frac{c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_A \theta_S p_S^{1+\frac{R_d}{c^{(p)}}} dA + \frac{c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_A \int_{\theta_S}^{\infty} p(\theta)^{1+\frac{R_d}{c^{(p)}}} d\theta dA \\
&= A \overline{p_S z_S} + \frac{A c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \overline{\theta_S p_S^{1+\frac{R_d}{c^{(p)}}}} + \frac{c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_{\theta_S}^{\infty} \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} d\theta \\
&\approx A \overline{p_S z_S} + \frac{A c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \overline{\theta_S p_S^{1+\frac{R_d}{c^{(p)}}}} + \frac{A c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_{\overline{\theta_S}}^{\infty} \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} d\theta.
\end{aligned} \tag{14.45}$$

According to Eq. (14.41) is

$$\int_A \text{TPE} + \text{KE} dA \tag{14.46}$$

conservative if there is no mass flow across the lateral edges of A . The APE is the fraction of the TPE that could be converted into kinetic energy, i.e

$$\boxed{\text{APE} := \int_A \text{TPE} - \text{TPE}_{\min} dA,} \tag{14.47}$$

where is meant the minimum potential energy of all hydrostatic states that can be reached from the initial state by adiabatic rearrangement without producing overadiabatic gradients. Here, the particles move along the isentropes and after such a rearrangement, all state variables only depend on the vertical coordinate, since otherwise pressure gradients would exist that would work towards this (the Coriolis force does no work, therefore has no energetic relevance and therefore does not have to be taken into account for this consideration). If you designate the fields of the state of minimum potential energy by primed quantities, you can make a note

$$\int_A \text{TPE}_{\min} dA \approx A \overline{p'(z_S) z_S} + \frac{A c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \overline{\theta'(z_S) p'(z_S)^{1+\frac{R_d}{c^{(p)}}}} + \frac{A c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_{\overline{\theta_S}}^{\infty} \overline{p'(\theta)^{1+\frac{R_d}{c^{(p)}}}} d\theta. \tag{14.48}$$

The first two terms on the right-hand sides of the equations (14.45) and (14.48) refer exclusively to the surface; their difference is abbreviated as C . This gives you

$$\text{APE} \approx C + \frac{A c^{(p)2}}{g p_o^{R_d/c^{(p)}} (c^{(p)} + R_d)} \int_{\overline{\theta_S}}^{\infty} \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} - \overline{p'(\theta)^{1+\frac{R_d}{c^{(p)}}}} d\theta. \tag{14.49}$$

The mass M over the isentrope θ is conservative, so

$$\overline{p'(\theta)} = p'(\theta) = \overline{p(\theta)} \Rightarrow \overline{p'(\theta)^{1+\frac{R_d}{c^{(p)}}}} = \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}}, \tag{14.50}$$

from which follows

$$\begin{aligned}
\text{APE} &\approx C + \frac{Ac^{(p)^2}}{gp_{\circ}^{R_d/c^{(p)}}(c^{(p)} + R_d)} \int_{\bar{\theta}_S}^{\infty} \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} - \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} d\theta \\
&= C + \frac{Ac^{(p)}}{gp_{\circ}^{R_d/c^{(p)}}\left(1 + \frac{R_d}{c^{(p)}}\right)} \int_{\bar{\theta}_S}^{\infty} \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} - \overline{p(\theta)^{1+\frac{R_d}{c^{(p)}}}} d\theta \\
&= C + \frac{A}{\Gamma_d p_{\circ}^{\mathcal{X}}(1 + \mathcal{X})} \int_{\bar{\theta}_S}^{\infty} \overline{p(\theta)^{1+\mathcal{X}}} - \overline{p(\theta)^{1+\mathcal{X}}} d\theta
\end{aligned} \tag{14.51}$$

with the dry adiabatic temperature gradient $\Gamma_d = g/c^{(p)}$ and the abbreviation $\mathcal{X} := \frac{R_d}{c^{(p)}}$. One notes $p = \bar{p} + p'$, so the Taylor expansion applies

$$p^{1+\mathcal{X}} = \bar{p}^{1+\mathcal{X}} + (1 + \mathcal{X}) \bar{p}^{\mathcal{X}} p' + \frac{1}{2} \mathcal{X} (1 + \mathcal{X}) \bar{p}^{\mathcal{X}-1} p'^2 + \dots \tag{14.52}$$

From this it follows

$$\begin{aligned}
p^{1+\mathcal{X}} - \bar{p}^{1+\mathcal{X}} &= (1 + \mathcal{X}) \bar{p}^{\mathcal{X}} p' + \frac{1}{2} \mathcal{X} (1 + \mathcal{X}) \bar{p}^{\mathcal{X}-1} p'^2 + \dots \\
\Leftrightarrow \overline{p^{1+\mathcal{X}}} - \bar{p}^{1+\mathcal{X}} &= (1 + \mathcal{X}) \bar{p}^{\mathcal{X}} \overline{p'} + \frac{1}{2} \mathcal{X} (1 + \mathcal{X}) \bar{p}^{\mathcal{X}-1} \overline{p'^2} + \dots \\
\Leftrightarrow \overline{p^{1+\mathcal{X}}} - \bar{p}^{1+\mathcal{X}} &= \frac{1}{2} \mathcal{X} (1 + \mathcal{X}) \bar{p}^{\mathcal{X}-1} \overline{p'^2} + \dots
\end{aligned} \tag{14.53}$$

So you get

$$\text{APE} \approx C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{\theta}_S}^{\infty} \bar{p}^{1+\mathcal{X}} \overline{\left(\frac{p'}{\bar{p}}\right)^2} d\theta. \tag{14.54}$$

Now this is transformed back into the p-system. For this you use

$$p = p(\theta(p)) \approx \bar{p}(\theta(p)) \Rightarrow p' \approx \theta' \frac{\partial \bar{p}}{\partial \theta}. \tag{14.55}$$

Thus you get

$$\begin{aligned}
\text{APE} &\approx C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{\theta}_S}^{\infty} \bar{p}^{\mathcal{X}-1} \overline{\left(\theta' \frac{\partial \bar{p}}{\partial \theta}\right)^2} d\theta = C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{\theta}_S}^{\infty} \bar{p}^{\mathcal{X}-1} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^2 dp \\
&= C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{p}(\bar{\theta}_S)}^{\bar{p}(\infty)} \bar{p}^{\mathcal{X}-1} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^2 \frac{\partial \theta}{\partial \bar{p}} dp = C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{p}_S}^{\circ} \bar{p}^{\mathcal{X}-1} \overline{\theta'^2} \frac{\partial \bar{p}}{\partial \theta} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^2 \frac{\partial \theta}{\partial \bar{p}} dp \\
&= C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{p}_S}^{\circ} \bar{p}^{\mathcal{X}-1} \overline{\theta'^2} \frac{\partial \bar{p}}{\partial \theta} dp \approx C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{p}_S}^{\circ} \bar{p}^{\mathcal{X}-1} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^{-1} dp \\
&= C + \frac{A\mathcal{X}}{2\Gamma_d p_{\circ}^{\mathcal{X}}} \int_{\bar{p}_S}^{\circ} \bar{p}^{\mathcal{X}} \frac{1}{\bar{p}} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^{-1} dp = C + \frac{A\mathcal{X}}{2\Gamma_d} \int_{\bar{p}_S}^{\circ} \left(\frac{\bar{p}}{p_{\circ}}\right)^{\mathcal{X}} \frac{1}{\bar{p}} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^{-1} dp \\
&\approx C + \frac{A\mathcal{X}}{2\Gamma_d} \int_{\bar{p}_S}^{\circ} \frac{\bar{T}}{\bar{\theta}} \frac{1}{\bar{p}} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^{-1} dp = C + \frac{A\mathcal{X}}{2\Gamma_d} \int_{\bar{p}_S}^{\circ} \frac{\bar{T}}{\bar{p}} \overline{\theta'^2} \left(\frac{\partial \bar{p}}{\partial \theta}\right)^{-1} dp.
\end{aligned} \tag{14.56}$$

With

$$\theta' = \frac{\partial \theta}{\partial T} T' = \frac{\theta}{T} T' \approx \frac{\bar{\theta}}{\bar{T}} T' \tag{14.57}$$

you can further transform this to

$$\begin{aligned}
 \text{APE} &\approx C + \frac{A\chi}{2\Gamma_d} \int_{\bar{p}_s}^o \frac{1}{\bar{p}} \overline{\bar{\theta} T \left(\frac{T'}{\bar{T}} \right)^2} \left(\frac{\partial \bar{\theta}}{\partial p} \right)^{-1} dp \\
 &= C + \frac{A}{2} \int_{\bar{p}_s}^o \frac{\chi^{\bar{\theta}}}{\Gamma_d \bar{p}} \left(\frac{\partial \bar{\theta}}{\partial p} \right)^{-1} \overline{\bar{T} \left(\frac{T'}{\bar{T}} \right)^2} dp = C - \frac{A}{2} \int_o^{\bar{p}_s} \frac{\chi^{\bar{\theta}}}{\Gamma_d \bar{p}} \left(\frac{\partial \bar{\theta}}{\partial p} \right)^{-1} \overline{\bar{T} \left(\frac{T'}{\bar{T}} \right)^2} dp.
 \end{aligned} \tag{14.58}$$

According to Eq. (9.48) applies

$$\frac{\Gamma_d \bar{p}}{\chi^{\bar{\theta}}} \frac{\partial \bar{\theta}}{\partial p} \approx \frac{\overline{\Gamma_d p}}{\overline{\chi^{\bar{\theta}}}} \frac{\partial \bar{\theta}}{\partial p} = -(\Gamma_d - \bar{\Gamma}), \tag{14.59}$$

it follows from this

$$\text{APE} \approx C + \frac{A}{2} \int_o^{\bar{p}_s} \frac{\bar{T}}{\Gamma_d - \bar{\Gamma}} \overline{\left(\frac{T'}{\bar{T}} \right)^2} dp. \tag{14.60}$$

14.4.3 Estimation

If one takes a climatological value $\bar{\Gamma} \approx \frac{2}{3}\Gamma_d$ and neglects C to make an estimate, it follows

$$\text{APE} \approx \frac{3Ac^{(p)}}{2g} \int_{\bar{p}_s}^o \bar{T} \overline{\left(\frac{T'}{\bar{T}} \right)^2} dp. \tag{14.61}$$

For A you choose the entire earth's surface and set $T' \sim 15$ K, $\bar{T} \sim 270$ K, then follow

$$\frac{\text{APE}/A}{\text{KE}} \sim \frac{3\overline{T'^2}c^{(p)}}{\bar{T}v_h^2} \sim 25. \tag{14.62}$$

It remains an open question in this section why most of the available potential energy is not converted into kinetic energy.

15 VORTICITY AND DIVERGENCE

Let an arbitrary vector field $\mathbf{v}$ be given. The approach

$$\mathbf{v} = \Delta \mathbf{w} \quad (15.1)$$

with the boundary conditions

$$\lim_{|\mathbf{r}| \rightarrow \infty} \mathbf{w} = \mathbf{o} \quad (15.2)$$

with a vector field $\mathbf{v}$ is clearly solvable for continuous $\mathbf{v}$, namely there are three independent *Poisson equations*

$$v_i = \Delta w_i. \quad (15.3)$$

According to Eq. (B.54) applies

$$\Delta \mathbf{w} = \nabla (\nabla \cdot \mathbf{w}) - \nabla \times (\nabla \times \mathbf{w}). \quad (15.4)$$

You define

$$\mathcal{X} := \nabla \cdot \mathbf{w} \quad (15.5)$$

as *velocity potential*, further one defines

$$\mathbf{A} := -\nabla \times \mathbf{w} \quad (15.6)$$

as vector potential, then applies

$$\mathbf{v} = \nabla \mathcal{X} + \nabla \times \mathbf{A}. \quad (15.7)$$

So you have a *unique* decomposition

$$\mathbf{v} = \mathbf{v}_{\text{nonrot}} + \mathbf{v}_{\text{nondiv}}, \quad \nabla \times \mathbf{v}_{\text{nonrot}} = \mathbf{o}, \quad \nabla \cdot \mathbf{v}_{\text{nondiv}} = \mathbf{o} \quad (15.8)$$

made. The fact that this is always possible is the *principal theorem of vector analysis*. $\mathcal{X}$ and $\mathbf{A}$ have a total of four components, but the wind field only has three. Therefore one can set another linear condition, here will

$$\nabla \cdot \mathbf{A} = \mathbf{o} \quad (15.9)$$

chosen, it follows

$$\nabla \times \mathbf{v} = \Delta \mathbf{A}. \quad (15.10)$$

If you only look at the horizontal wind field

$$\mathbf{v}_h := \mathbf{v} - w \mathbf{k}, \quad (15.11)$$

of course this also applies. Instead of the condition $\nabla \cdot \mathbf{A} \stackrel{!}{=} \mathbf{o}$, one places the algebraic condition on the vector potential

$$\mathbf{A} \stackrel{!}{=} (\mathbf{k} \cdot \mathbf{A}) \mathbf{k} \quad (15.12)$$

and defines a *current function* $\psi = \psi(\varphi, \lambda) := -\mathbf{k} \cdot \mathbf{A}$. Then applies

$$\mathbf{v}_{h, \text{nondiv}} = \nabla \times [-\mathbf{k} \psi] \stackrel{\text{Glg. (B.51)}}{=} \mathbf{k} \times \nabla \psi. \quad (15.13)$$

Expected to be checked

$$\nabla \cdot (\mathbf{k} \times \nabla \psi) \stackrel{\text{Glg. (B.55)}}{=} \nabla \psi \cdot (\nabla \times \mathbf{k}) - \mathbf{k} \cdot (\nabla \times \nabla \psi) = 0. \quad (15.14)$$

You define

$$\boldsymbol{\xi} := \nabla \times \mathbf{v}. \quad (15.15)$$

It applies

$$\zeta := \mathbf{k} \cdot (\nabla \times \mathbf{v}_h) = \mathbf{k} \cdot [\nabla \times (\mathbf{k} \times \nabla \psi)] \stackrel{\text{Glg. (B.53)}}{=} \Delta \psi. \quad (15.16)$$

The divergence still applies

$$\nabla \cdot \mathbf{v}_h = \Delta \chi. \quad (15.17)$$

Note that ζ is not the magnitude of $\boldsymbol{\xi}$, but the z-component of it.

15.1 Vorticity

The rotating base of the global coordinates is denoted by $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$, so the velocity field is written as

$$\mathbf{v} = u_x \mathbf{e}_x + u_y \mathbf{e}_y + u_z \mathbf{e}_z. \quad (15.18)$$

You write

$$\mathbf{U}' = \boldsymbol{\omega} \times \mathbf{r} + \mathbf{v}, \quad (15.19)$$

so $\mathbf{U}'$ is the field of particle velocities in coordinates at rest. It is composed of the proportion of the Earth's rotation $\boldsymbol{\omega} \times \mathbf{r}$ and the wind field $\mathbf{v}$ measured relative to the rotating Earth. This follows

$$\boldsymbol{\eta} := \nabla \times \mathbf{v}' = \nabla \times \mathbf{v} + \nabla \times (\boldsymbol{\omega} \times \mathbf{r}) = \boldsymbol{\xi} + \mathbf{f}, \quad (15.20)$$

it was

$$\nabla \times (\boldsymbol{\omega} \times \mathbf{r}) \stackrel{\text{Glg. (B.53)}}{=} \boldsymbol{\omega} (\nabla \cdot \mathbf{r}) - (\boldsymbol{\omega} \cdot \nabla) \mathbf{r} = 3\boldsymbol{\omega} - \left(\boldsymbol{\omega} \frac{\partial}{\partial z} \right) \mathbf{r} = 3\boldsymbol{\omega} - \boldsymbol{\omega} = 2\boldsymbol{\omega} = \mathbf{f} \quad (15.21)$$

used. The absolute vorticity $\boldsymbol{\eta}$ is defined by the vertical component of the rotation of $\mathbf{v}'$. This is obtained as the dot product of $\nabla \times \mathbf{v}'$ with the vertical unit vector $\mathbf{k}$:

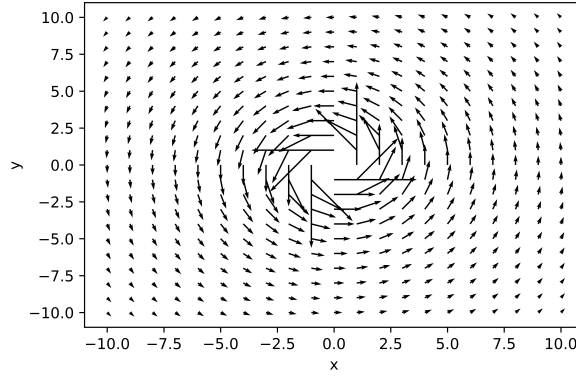
$$\eta := \mathbf{k} \cdot (\nabla \times \mathbf{v}) + \mathbf{k} \cdot \mathbf{f} = \zeta + f \quad (15.22)$$

Recall that the Coriolis parameter is the vertical component of the Coriolis vector, not its magnitude. The portion of the absolute vorticity that is caused by the Earth's rotation is also referred to as *planetary vorticity*, while the portion that is caused by the wind field measured in rotating coordinates is referred to as *relative vorticity*.

The vorticity also has a clear meaning that is not initially as obvious as that of the divergence. Two examples are considered here.

- Take the field $\mathbf{v} = (y, 0, 0)^T$. The streamlines of this field are not curved. Nevertheless, $\nabla \times \mathbf{v} = (0, 0, -1)^T \neq 0$.
- Take the field $\mathbf{v} = \frac{1}{x^2 + y^2} (-y, x, 0)^T$. The field looks very much like a rotating field (see Fig. 15.1). Trotzdem gilt

$$\begin{aligned} \nabla \times \mathbf{v} &= \left(\frac{\partial}{\partial x} \frac{x}{x^2 + y^2} + \frac{\partial}{\partial y} \frac{y}{x^2 + y^2} \right) \mathbf{e}_z \\ &= \left(\frac{1}{x^2 + y^2} - x^2 x \frac{1}{(x^2 + y^2)^2} + \frac{1}{x^2 + y^2} - y^2 y \frac{1}{(x^2 + y^2)^2} \right) \mathbf{e}_z = 0. \end{aligned} \quad (15.23)$$

Figure 15.1: The vorticity of this vector field $\mathbf{v}$ is zero.

To understand the true meaning of vorticity, it is best to imagine a 2D vector field $\mathbf{v}_h = (u, v)^T$ (in Cartesian coordinates). Take a rectangle $[-a, a] \times [-b, b]$. Let $\mathbf{s}$ be a curve that encloses this set in the positive mathematical sense of rotation. Then approximately with (u, v) as the vector at the origin

$$\begin{aligned} \int_{\mathbf{s}} \mathbf{v}_h \cdot d\mathbf{s} &\approx \mathbf{z}a \left(u - b \frac{\partial u}{\partial y} \right) + \mathbf{z}b \left(v + a \frac{\partial v}{\partial x} \right) - \mathbf{z}a \left(u + b \frac{\partial u}{\partial y} \right) - \mathbf{z}b \left(v - a \frac{\partial v}{\partial x} \right) \\ &= -\mathbf{z}ba \frac{\partial u}{\partial y} + \mathbf{z}ba \frac{\partial v}{\partial x} - \mathbf{z}ab \frac{\partial u}{\partial y} + \mathbf{z}ba \frac{\partial v}{\partial x} = -4ba \frac{\partial u}{\partial y} + 4ab \frac{\partial v}{\partial x} = 4ab \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right). \end{aligned} \quad (15.24)$$

The area of the surface is $4ab$. If we consider the circulation of the vector field around a particle, then forms

$$\lim_{a, b \rightarrow 0} \frac{\int_{\mathbf{s}} \mathbf{v}_h \cdot d\mathbf{s}}{4ab} = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}, \quad (15.25)$$

This results in the definition of the z component of the vortex strength. The components of the rotation therefore indicate how the flow flows around a small area in a plane perpendicular to the respective component. So there is a connection between circulation and vorticity. In integral form, this is the statement of *Stokes Theorem*:

$$\int_A \nabla \times \mathbf{v} \cdot d\mathbf{f} = \int_{\partial A} \mathbf{v} \cdot d\mathbf{s}. \quad (15.26)$$

Just like the above consideration, Stokes' theorem links the vectorial curve integral along the edge of a surface with the vortex strength within the surface. A further illustration of vorticity is shown in the coming section.

15.1.1 Shear and curvature vorticity

Define o.b.d. A. in plane geometry, a right-handed orthonormal base $\mathbf{s}, \mathbf{n}, \mathbf{k}$, where $\mathbf{s}$ is parallel to the horizontal wind at the origin. This applies

$$\mathbf{v} = \begin{pmatrix} V \cos(\beta) \\ V \sin(\beta) \\ w \end{pmatrix} \quad (15.27)$$

with the horizontal wind speed V and the vertical wind w . Here β is the horizontal wind direction relative to $\mathbf{s}$. This follows for the vorticity

$$\zeta = \frac{\partial}{\partial s} V \sin(\beta) - \frac{\partial}{\partial n} V \cos(\beta) = \sin(\beta) \frac{\partial V}{\partial s} + V \frac{\partial \beta}{\partial s} \cos(\beta) - \cos(\beta) \frac{\partial V}{\partial n} + V \sin(\beta) \frac{\partial \beta}{\partial n}. \quad (15.28)$$

At the coordinate origin $\beta = 0$, so there you have

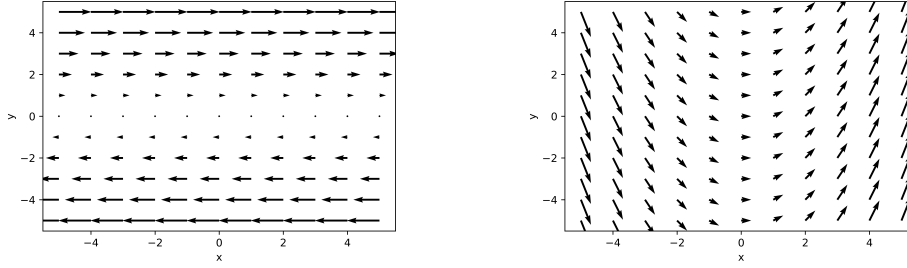


Figure 15.2: Shear vorticity (left) and curvature vorticity (right).

$$\zeta = V \frac{\partial \beta}{\partial s} - \frac{\partial V}{\partial n}. \quad (15.29)$$

The first term $V \frac{\partial \beta}{\partial s}$ is called curvature vorticity. It is greater than zero if the streamline is curved to the left, equal to zero if the streamline is straight, and less than zero if the streamline is curved to the right. The term $-\frac{\partial V}{\partial n}$ is called shear vorticity. It is greater than zero if the wind speed increases to the right of the wind direction. In particular, one sees that a flow field with curved streamlines can be rotation-free and one with straight streamlines can be rotation-affected.

15.1.2 circulation rate

Let A be an arbitrarily shaped surface in space, then the circulation S of the wind field $\mathbf{v}$ around A at time t is defined by

$$S(t) := \int_{\partial A} \mathbf{v} \cdot d\mathbf{s} = \int_0^1 \mathbf{v}(\mathbf{r}(\tau), t) \cdot \frac{d\mathbf{r}}{d\tau} d\tau, \quad (15.30)$$

where $\mathbf{r}(\tau)$ is a function defined on the interval $[0, 1]$ that traverses the boundary of A . If the surface A moves with the wind field, the circulation S also changes by A , i.e

$$\frac{DS}{Dt} = \frac{D}{Dt} \int_0^1 \mathbf{v}(\mathbf{r}(\tau), t) \cdot \frac{d\mathbf{r}}{d\tau} d\tau = \int_0^1 \frac{D\mathbf{v}}{Dt} \cdot \frac{d\mathbf{r}}{d\tau} d\tau + \int_0^1 \mathbf{v} \cdot \frac{D}{Dt} \left(\frac{d\mathbf{r}}{d\tau} \right) d\tau. \quad (15.31)$$

In order to determine the second integral in more detail, one prepares

$$\begin{aligned} \frac{d\mathbf{r}}{d\tau} &= \lim_{\Delta \rightarrow 0} \frac{\mathbf{r}(\tau + \Delta) - \mathbf{r}(\tau)}{\Delta} \\ \Rightarrow \frac{D}{Dt} \frac{d\mathbf{r}}{d\tau} &= \lim_{\Delta \rightarrow 0} \frac{\frac{D\mathbf{r}}{Dt}(\tau + \Delta) - \frac{D\mathbf{r}}{Dt}(\tau)}{\Delta} = \lim_{\Delta \rightarrow 0} \frac{\mathbf{v}(\mathbf{r}(\tau + \Delta)) - \mathbf{v}(\mathbf{r}(\tau))}{\Delta} \\ &= \left(\frac{d\mathbf{r}}{d\tau} \cdot \nabla \right) \mathbf{v} \end{aligned} \quad (15.32)$$

firmly. Define $\mathbf{v}(\tau) := \mathbf{v}(\mathbf{r}(\tau), t)$, then holds

$$\left(\frac{d\mathbf{r}}{d\tau} \cdot \nabla \right) \mathbf{v} = \frac{d\mathbf{v}}{d\tau}, \quad (15.33)$$

with what you

$$\int_0^1 \mathbf{v} \cdot \frac{D}{Dt} \left(\frac{d\mathbf{r}}{d\tau} \right) d\tau = \int_0^1 \mathbf{v} \cdot \frac{d\mathbf{v}}{d\tau} d\tau = \frac{1}{2} [\mathbf{v}^2]_0^1 = 0 \quad (15.34)$$

because due to the closedness of the curve $\mathbf{v}(0) = \mathbf{v}(1)$. Using Stokes' theorem follows

$$\frac{DS}{Dt} = \int_A \nabla \times \mathbf{F} \cdot d\mathbf{n}, \quad (15.35)$$

where $\mathbf{F}$ is the sum of all acting forces. So conservative forces do not change the circulation. With

$$\nabla \times \left(-\frac{\mathbf{I}}{\rho} \nabla p \right) \stackrel{\text{Glg. (B.51)}}{=} \frac{\mathbf{I}}{\rho^2} \nabla \rho \times \nabla p, \quad (15.36)$$

$$\nabla \times \mathbf{v} \times \mathbf{f} \stackrel{\text{Glg. (B.53)}}{=} (\mathbf{f} \cdot \nabla) \mathbf{v} - \mathbf{f} \nabla \cdot \mathbf{v} \quad (15.37)$$

follows

$$\frac{DS}{Dt} = \int_A \left(\frac{\mathbf{I}}{\rho^2} \nabla \rho \times \nabla p + (\mathbf{f} \cdot \nabla) \mathbf{v} - \mathbf{f} \nabla \cdot \mathbf{v} + \nabla \times \mathbf{f}_R \right) \cdot d\mathbf{n}. \quad (15.38)$$

In IS this applies in barotropic ideal media

$$\frac{DS}{Dt} = 0 \Leftrightarrow S = \text{const.} \quad (15.39)$$

15.1.3 Vorticity equation

The momentum equation Eq. (8.101) is

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{\mathbf{I}}{\rho} \nabla p + \mathbf{v} \times \boldsymbol{\eta} - \nabla k + \mathbf{g} + \mathbf{f}_R. \quad (15.40)$$

Now you apply the operator $\nabla \times$ to the individual terms:

$$\nabla \times \frac{\partial \mathbf{v}}{\partial t} \stackrel{\text{Glg. (B.50)}}{=} \frac{\partial}{\partial t} (\nabla \times \mathbf{v}) \quad (15.41)$$

$$\nabla \times \left(-\frac{\mathbf{I}}{\rho} \nabla p \right) = -\nabla \times \left(\frac{\mathbf{I}}{\rho} \nabla p \right) \stackrel{\text{Glg. (B.51)}}{=} -\frac{\mathbf{I}}{\rho^2} \nabla p \times \nabla \rho \quad (15.42)$$

$$\nabla \times (\mathbf{v} \times \boldsymbol{\eta}) \stackrel{\text{Glg. (B.53)}}{=} (\mathbf{v} \cdot \nabla) \boldsymbol{\eta} - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + (\boldsymbol{\eta} \cdot \nabla) \mathbf{v} \quad (15.43)$$

$$\nabla \times \nabla k \stackrel{\text{Glg. (B.47)}}{=} 0 \quad (15.44)$$

$$\nabla \times \mathbf{g} = \nabla \times (-\nabla \Phi) \stackrel{\text{Glg. (B.47)}}{=} 0 \quad (15.45)$$

Therefore applies

$$\frac{\partial}{\partial t} (\nabla \times \mathbf{v}) = \frac{\mathbf{I}}{\rho^2} \nabla \rho \times \nabla p - (\mathbf{v} \cdot \nabla) \boldsymbol{\eta} - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + (\boldsymbol{\eta} \cdot \nabla) \mathbf{v} + \nabla \times \mathbf{f}_R. \quad (15.46)$$

15.1.3.1 Formulation in geographical coordinates

By projecting onto the local perpendicular one obtains

$$\begin{aligned}
\frac{\partial \zeta}{\partial t} &= \mathbf{k} \cdot \left[\frac{1}{\rho^2} \nabla_{\rho} \times \nabla p - (\mathbf{v} \cdot \nabla) \boldsymbol{\eta} - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + (\boldsymbol{\eta} \cdot \nabla) \mathbf{v} + \nabla \times \mathbf{f}_R \right] \\
\Leftrightarrow \frac{\partial \zeta}{\partial t} &= \mathbf{k} \cdot \left[\frac{1}{\rho^2} \nabla_{\rho} \times \nabla p - \boldsymbol{\eta} \nabla \cdot \mathbf{v} - (\mathbf{v} \cdot \nabla) \boldsymbol{\eta} + (\boldsymbol{\eta} \cdot \nabla) \mathbf{v} + \nabla \times \mathbf{f}_R \right] \\
\Leftrightarrow \frac{\partial \zeta}{\partial t} &= \mathbf{k} \cdot \left[\frac{1}{\rho^2} \nabla_{\rho} \times \nabla p - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + (\boldsymbol{\eta} \cdot \nabla) \mathbf{v} - (\mathbf{v} \cdot \nabla) \boldsymbol{\eta} + \nabla \times \mathbf{f}_R \right] \\
\Rightarrow \frac{\partial \zeta}{\partial t} &= \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p) - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + \mathbf{k} \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{v}] - \mathbf{k} \cdot [(\mathbf{v} \cdot \nabla) \boldsymbol{\eta}] + \mathbf{k} \cdot \nabla \times \mathbf{f}_R.
\end{aligned} \tag{15.47}$$

One first calculates with Eq. (B.58)

$$\begin{aligned}
(\boldsymbol{\eta} \cdot \nabla) w &= (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \mathbf{k}) = \mathbf{k} \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{v}] + \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{k}] \\
&\Rightarrow \mathbf{k} \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{v}] = (\boldsymbol{\eta} \cdot \nabla) w - \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{k}],
\end{aligned} \tag{15.48}$$

$$\begin{aligned}
\mathbf{v} \cdot \nabla \boldsymbol{\eta} &= (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \mathbf{k}) = \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \mathbf{k}] + \mathbf{k} \cdot [(\mathbf{v} \cdot \nabla) \boldsymbol{\eta}] \\
&\Rightarrow \mathbf{k} \cdot [(\mathbf{v} \cdot \nabla) \boldsymbol{\eta}] = \mathbf{v} \cdot \nabla \boldsymbol{\eta} - \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \mathbf{k}].
\end{aligned} \tag{15.49}$$

Therefore applies

$$\frac{\partial \zeta}{\partial t} = \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p) - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + (\boldsymbol{\eta} \cdot \nabla) w - \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{k}] - \mathbf{v} \cdot \nabla \boldsymbol{\eta} + \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \mathbf{k}] + \mathbf{k} \cdot \nabla \times \mathbf{f}_R. \tag{15.50}$$

The findings in Section B.2.1 apply

$$\frac{\partial \mathbf{k}}{\partial x} = \frac{\mathbf{i}}{r}, \quad \frac{\partial \mathbf{k}}{\partial y} = \frac{\mathbf{j}}{r}, \quad \frac{\partial \mathbf{k}}{\partial z} = \mathbf{o}. \tag{15.51}$$

Thus follows

$$\begin{aligned}
\frac{\partial \zeta}{\partial t} &= \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p) - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + \boldsymbol{\eta} \cdot \nabla w - \mathbf{v} \cdot \left(\eta_x \frac{\partial \mathbf{k}}{\partial x} + \eta_y \frac{\partial \mathbf{k}}{\partial y} \right) - \mathbf{v} \cdot \nabla \boldsymbol{\eta} + \boldsymbol{\eta} \cdot \left(u \frac{\partial \mathbf{k}}{\partial x} + v \frac{\partial \mathbf{k}}{\partial y} \right) + \mathbf{k} \cdot \nabla \times \mathbf{f}_R \\
\Leftrightarrow \frac{\partial \zeta}{\partial t} &= \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p) - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + \boldsymbol{\eta} \cdot \nabla w - \frac{u \eta_x}{r} - \frac{v \eta_y}{r} - \mathbf{v} \cdot \nabla \boldsymbol{\eta} + \frac{\eta_x u}{r} + \frac{\eta_y v}{r} + \mathbf{k} \cdot \nabla \times \mathbf{f}_R.
\end{aligned} \tag{15.52}$$

The terms marked in color cancel each other out. Therefore applies

$$\frac{\partial \zeta}{\partial t} = \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p) - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + \boldsymbol{\eta} \cdot \nabla w - \mathbf{v} \cdot \nabla \boldsymbol{\eta} + \mathbf{k} \cdot \nabla \times \mathbf{f}_R. \tag{15.53}$$

The vorticity equation is finally:

$$\boxed{\boxed{\frac{\partial \zeta}{\partial t} = -\mathbf{v} \cdot \nabla \boldsymbol{\eta} - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + \boldsymbol{\eta} \cdot \nabla w + \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p) + \mathbf{k} \cdot \nabla \times \mathbf{f}_R.}} \tag{15.54}$$

15.1.3.2 Interpretation of the terms

If you neglect the friction, you get

$$\frac{\partial \zeta}{\partial t} = -\mathbf{v} \cdot \nabla \boldsymbol{\eta} - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + \boldsymbol{\eta} \cdot \nabla w + \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla_{\rho} \times \nabla p). \tag{15.55}$$

If one assumes a flat geofluid and introduces a horizontal wind vector $\mathbf{v}_h$, it follows

$$\begin{aligned}
\frac{\partial \zeta}{\partial t} &= -\mathbf{v} \cdot \nabla \eta - \eta \nabla \cdot \mathbf{v}_h - \eta \frac{\partial w}{\partial z} + \boldsymbol{\eta}_h \cdot \nabla_h w + \eta \frac{\partial w}{\partial z} + \frac{1}{\rho^2} \mathbf{k} \cdot (\nabla \rho \times \nabla p) \\
&= \underbrace{-\mathbf{v} \cdot \nabla \eta - \eta \nabla \cdot \mathbf{v}_h + \boldsymbol{\eta}_h \cdot \nabla_h w}_{\text{Advektion}} + \underbrace{\frac{1}{\rho^2} \mathbf{k} \cdot (\nabla \rho \times \nabla p)}_{\text{Solenoidterm}}.
\end{aligned} \tag{15.56}$$

The so-called *solenoid term* arises from the rotation of the pressure gradient acceleration. The rotation of ∇p is zero. A closed line integral over $-\nabla p \cdot d\mathbf{n}$ therefore disappears. However, due to the location dependence of the density, $\int_{\partial\Omega \subseteq \mathbb{R}^3} -\frac{1}{\rho} \nabla p \cdot d\mathbf{n} \neq 0$ can apply. A particle that moves on a closed path, for example a circular path, can be accelerated or decelerated by the pressure gradient, which changes the vorticity.

So apart from the solenoid term, vorticity is only generated by momentum advection. This can be broken down as follows:

$$\frac{\partial \zeta}{\partial t}_{\text{adv}} = \underbrace{-\mathbf{v} \cdot \nabla \eta}_{\text{Vorticityadvektion}} \underbrace{-\eta \nabla \cdot \mathbf{v}_h}_{\text{Divergenzterm}} + \underbrace{\boldsymbol{\eta}_h \cdot \nabla_h w}_{\text{Drehterm}} \tag{15.57}$$

The *Rotation term* describes the generation of vertical vorticity by horizontal vorticity and a horizontal gradient of the vertical velocity. It applies

$$\boldsymbol{\eta}_h \cdot \nabla_h w = \zeta_x \frac{\partial w}{\partial x} + \zeta_y \frac{\partial w}{\partial y}. \tag{15.58}$$

O.B.d. A. the y-axis of the KS is aligned with $\boldsymbol{\xi}_h$, resulting in

$$\boldsymbol{\eta}_h \cdot \nabla_h w = \zeta_y \frac{\partial w}{\partial y} \tag{15.59}$$

leads. Now assume a convective tube with amplitude W and variance σ^2 , i.e

$$w = w(x, y) = W \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right). \tag{15.60}$$

The KS was again placed in the center of the tube. From this it follows

$$\frac{\partial w}{\partial y} = -\frac{Wy}{\sigma^2} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right). \tag{15.61}$$

For the y-component of the relative vorticity applies

$$\zeta_y = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}. \tag{15.62}$$

From this it follows

$$\boldsymbol{\eta}_h \cdot \nabla_h w = \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}\right) \frac{\partial w}{\partial y} = -\frac{Wy}{\sigma^2} \left[\frac{\partial u}{\partial z} + \frac{Wx}{\sigma^2} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right)\right] \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right). \tag{15.63}$$

If you insert $x = 0$, $y = \pm\sigma$ and approximate all exponential terms by 1/2, it follows

$$\boldsymbol{\eta}_h \cdot \nabla_h w = \mp \frac{W}{2\sigma} \frac{\partial u}{\partial z}. \tag{15.64}$$

Most of the time $\frac{\partial u}{\partial z} > 0$. Thus, the rotation term produces cyclonic vorticity south of the convective tube and anticyclonic vorticity north of the tube. The scale analysis obtained for the case of very strong convection is $\sigma \sim 50 \text{ m}$, $W \sim 10 \text{ m/s}$ and $\frac{\partial u}{\partial z} \sim \frac{20 \text{ m/s}}{2 \text{ km}} = 1 \cdot 10^{-2} \text{ 1/s}$

$$\boldsymbol{\eta}_h \cdot \nabla_h w \sim \frac{10}{100} 10^{-2} 1/\text{s}^2 = 10^{-3} 1/\text{s}^2. \quad (15.65)$$

This is seven orders of magnitude stronger than the synoptic-scale vorticity tendency. This mechanism is important for the formation of tornadoes. The rotation term is all the more effective,

- the stronger the vertical shear of the horizontal wind is, and
- the stronger the convection.

15.1.3.3 Barotropic vorticity equation

In the barotropic case, the solenoid term is omitted and the vertical shear of the horizontal wind is ignored (see section 13.8).

$$\frac{\partial \zeta}{\partial t} = -\mathbf{v}_h \cdot \nabla \eta - \eta \nabla \cdot \mathbf{v} + \boldsymbol{\eta} \cdot \nabla w. \quad (15.66)$$

This is the so-called *barotropic vorticity equation*. In the case of incompressibility, especially in the case of SWEs, $\nabla \cdot \mathbf{v} = 0$, from which it follows

$$\frac{\partial \zeta}{\partial t} = -\mathbf{v}_h \cdot \nabla \eta + \boldsymbol{\eta} \cdot \nabla w \Rightarrow \frac{d\eta}{dt} = \boldsymbol{\eta} \cdot \nabla w. \quad (15.67)$$

Neglecting the horizontal gradients of w , it follows

$$\frac{D\eta}{Dt} = \eta \frac{\partial w}{\partial z}. \quad (15.68)$$

You bet

$$\nabla \cdot \mathbf{v} = \nabla \cdot \mathbf{v}_h + \frac{\partial w}{\partial z} = 0 \quad (15.69)$$

one, where a width-independent curvature term $\propto \frac{w}{r}$ was neglected, follows

$$\frac{D\eta}{Dt} = -\eta \nabla \cdot \mathbf{v}_h. \quad (15.70)$$

In the incompressible, horizontally divergence-free, barotropic case (in addition, the vertical shear of the horizontal wind was ignored), the absolute vorticity is a conserved quantity.

15.1.3.4 Vorticity equation in the p-system

Now the same thing should be done in the p-system. The momentum equations (13.132) - (13.133) in the p-system are vectorial

$$\frac{\partial \mathbf{v}_h}{\partial t} = -\nabla \varphi - \frac{1}{2} \nabla (\mathbf{v}_h \cdot \mathbf{v}_h) + \mathbf{v}_h \times \boldsymbol{\eta}' - \omega \frac{\partial \mathbf{v}_h}{\partial p} + \nabla \times \mathbf{f}_R^{(H)}. \quad (15.71)$$

The modified absolute vorticity $\boldsymbol{\eta}'$ was given by

$$\boldsymbol{\eta}' := f\mathbf{k} + \nabla \times \mathbf{v}_h \quad (15.72)$$

defined. Now you apply the operator $\nabla \times$ to the individual terms:

$$\nabla \times \frac{\partial \mathbf{v}_h}{\partial t} \stackrel{\text{Glg. (B.50)}}{=} \frac{\partial}{\partial t} \nabla \times \mathbf{v}_h \quad (15.73)$$

$$\nabla \times \nabla \varphi \stackrel{\text{Glg. (B.47)}}{=} \mathbf{o} \quad (15.74)$$

$$\nabla \times \mathbf{g} \stackrel{\text{Glg. (B.47)}}{=} \mathbf{o} \quad (15.75)$$

$$\nabla \times \nabla (\mathbf{v}_h \cdot \mathbf{v}_h) \stackrel{\text{Glg. (B.47)}}{=} \mathbf{o} \quad (15.76)$$

$$\nabla \times (\mathbf{v}_h \times \boldsymbol{\eta}') \stackrel{\text{Glg. (B.53)}}{=} -(\mathbf{v}_h \cdot \nabla) \boldsymbol{\eta}' - \boldsymbol{\eta}' \nabla \cdot \mathbf{v}_h + (\boldsymbol{\eta}' \cdot \nabla) \mathbf{v}_h \quad (15.77)$$

$$\nabla \times \left(\omega \frac{\partial \mathbf{v}_h}{\partial p} \right) \stackrel{\text{Glg. (B.51)}}{=} \omega \nabla \times \frac{\partial \mathbf{v}_h}{\partial p} - \frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega \quad (15.78)$$

Therefore applies

$$\frac{\partial}{\partial t} \nabla \times \mathbf{v}_h = -(\mathbf{v}_h \cdot \nabla) \boldsymbol{\eta}' - \boldsymbol{\eta}' \nabla \cdot \mathbf{v}_h + (\boldsymbol{\eta}' \cdot \nabla) \mathbf{v}_h + \omega \nabla \times \frac{\partial \mathbf{v}_h}{\partial p} - \frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega + \nabla \times \mathbf{f}_R^{(H)}. \quad (15.79)$$

15.1.3.5 Formulation in geographical coordinates

By projecting onto the local perpendicular $\mathbf{k}$ one obtains

$$\begin{aligned} \frac{\partial \zeta}{\partial t} &= -\mathbf{k} \cdot [(\mathbf{v}_h \cdot \nabla) \boldsymbol{\eta}'] - (f + \zeta) \nabla \cdot \mathbf{v}_h + \mathbf{k} \cdot [(\boldsymbol{\eta}' \cdot \nabla) \mathbf{v}_h] \\ &\quad - \omega \frac{\partial \zeta}{\partial p} + \mathbf{k} \cdot \left[\frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega \right] + \mathbf{k} \cdot \nabla \times \mathbf{f}_R^{(H)}. \end{aligned} \quad (15.80)$$

One first calculates with Eq. (B.58)

$$\begin{aligned} \mathbf{o} &= (\boldsymbol{\eta}' \cdot \nabla) (\mathbf{v}_h \cdot \mathbf{k}) = \mathbf{k} \cdot [(\boldsymbol{\eta}' \cdot \nabla) \mathbf{v}_h] + \mathbf{v}_h \cdot [(\boldsymbol{\eta}' \cdot \nabla) \mathbf{k}] \\ &\Rightarrow \mathbf{k} \cdot [(\boldsymbol{\eta}' \cdot \nabla) \mathbf{v}_h] = -\mathbf{v}_h \cdot [(\boldsymbol{\eta}' \cdot \nabla) \mathbf{k}], \end{aligned} \quad (15.81)$$

$$\begin{aligned} \mathbf{v}_h \cdot \nabla \boldsymbol{\eta}' &= (\mathbf{v}_h \cdot \nabla) (\boldsymbol{\eta}' \cdot \mathbf{k}) = \boldsymbol{\eta}' \cdot [(\mathbf{v}_h \cdot \nabla) \mathbf{k}] + \mathbf{k} \cdot [(\mathbf{v}_h \cdot \nabla) \boldsymbol{\eta}'] \\ &\Rightarrow \mathbf{k} \cdot [(\mathbf{v}_h \cdot \nabla) \boldsymbol{\eta}'] = \mathbf{v}_h \cdot \nabla \boldsymbol{\eta}' - \boldsymbol{\eta}' \cdot [(\mathbf{v}_h \cdot \nabla) \mathbf{k}]. \end{aligned} \quad (15.82)$$

The findings in Section B.2.1 apply

$$\frac{\partial \mathbf{k}}{\partial x} = \frac{\mathbf{i}}{r}, \quad \frac{\partial \mathbf{k}}{\partial y} = \frac{\mathbf{j}}{r}, \quad \frac{\partial \mathbf{k}}{\partial z} = \mathbf{o}. \quad (15.83)$$

Thus follows

$$\mathbf{v}_h \cdot [(\boldsymbol{\eta}' \cdot \nabla) \mathbf{k}] = \boldsymbol{\eta}' \cdot [(\mathbf{v}_h \cdot \nabla) \mathbf{k}]. \quad (15.84)$$

The vorticity equation in the p-system is:

$$\frac{\partial \zeta}{\partial t} = -v\beta - (f + \zeta) \nabla \cdot \mathbf{v}_h - \mathbf{v}_h \cdot \nabla \zeta - \omega \frac{\partial \zeta}{\partial p} + \mathbf{k} \cdot \left[\frac{\partial \mathbf{v}_h}{\partial p} \times \nabla \omega \right] + \mathbf{k} \cdot \nabla \times \mathbf{f}_R^{(H)}. \quad (15.85)$$

If you calculate the vorticity of the geostrophic wind field you get

$$\zeta_g = \frac{1}{f} \frac{\partial^2 \varphi}{\partial x^2} + \frac{1}{f} \frac{\partial^2 \varphi}{\partial y^2} - \frac{\beta}{f^2} \frac{\partial \varphi}{\partial y} + \frac{\tan(\varphi) u}{r} = \frac{1}{f} \Delta_h \varphi + \frac{\beta}{f} u + \frac{\tan(\varphi) u}{r}. \quad (15.86)$$

For the first term applies

$$\mathcal{O}\left(\frac{1}{f}\Delta\varphi\right) = \mathcal{O}\left(\frac{1}{f}\frac{\Delta p}{\rho L^2}\right) = 10^{-5} \frac{1}{s}. \quad (15.87)$$

The term of the β effect has a magnitude of 10^{-6} 1/s in mid-latitudes. Therefore, a common approximation in the extratropics is to approximate the vorticity by the geostrophic vorticity and to neglect the term of the beta effect.

15.1.3.6 Barotropic vorticity equation in the p-system

If you delete from Eq. (15.85) the friction and all terms containing vertical gradients are obtained

$$\frac{\partial \zeta}{\partial t} = -v\beta - (f + \zeta) \nabla \cdot \mathbf{v}_h - \mathbf{v}_h \cdot \nabla \zeta. \quad (15.88)$$

In the barotropic medium, $\partial w / \partial z \sim \partial \omega / \partial p$ is now constant in height. Under kinematic boundary conditions

$$\omega(p = 0) = \omega(p_{\text{surface}}) = 0 \quad (15.89)$$

thus follows

$$\frac{\partial \omega}{\partial p} = \frac{\omega(p_{\text{surface}}) - \omega(p = 0)}{p_{\text{surface}}} = 0. \quad (15.90)$$

Due to Eq. (13.129) now also applies

$$\nabla \cdot \mathbf{v}_h = -\frac{\partial \omega}{\partial p} = 0. \quad (15.91)$$

From this you get the *barotropic vorticity equation in the p-system*

$$\frac{\partial \zeta}{\partial t} = -v\beta - \mathbf{v}_h \cdot \nabla \zeta. \quad (15.92)$$

Other forms of this equation are:

$$\frac{\partial \eta}{\partial t} = -v\beta - \mathbf{v}_h \cdot \nabla \zeta, \quad (15.93)$$

$$\frac{D_h \zeta}{Dt} = -v\beta, \quad (15.94)$$

$$\frac{D_h \eta}{Dt} = 0. \quad (15.95)$$

Due to Eq. (15.91) $\mathbf{v}_h$ can be represented by a stream function $\psi = \psi(\varphi, \lambda)$, i.e

$$\begin{aligned} \mathbf{v}_h \stackrel{\text{Glg. (15.13)}}{=} \mathbf{k} \times \nabla \psi &= -\frac{\partial \psi}{\partial y} \mathbf{i} + \frac{\partial \psi}{\partial x} \mathbf{j} = -\frac{\partial \psi}{a \partial \varphi} \mathbf{i} + \frac{\partial \psi}{a \cos(\varphi) \partial \lambda} \mathbf{j} \\ \Rightarrow u &= -\frac{\partial \psi}{a \partial \varphi}, \end{aligned} \quad (15.96)$$

$$v = \frac{\partial \psi}{a \cos(\varphi) \partial \lambda}. \quad (15.97)$$

From this it follows

$$\zeta = \Delta \psi. \quad (15.98)$$

Putting this into Eq. (15.92), you get

$$\begin{aligned}
\frac{\partial \zeta}{\partial t} &= -v\beta - u \frac{\partial \zeta}{a \cos(\varphi) \partial \lambda} - v \frac{\partial \zeta}{a \partial \varphi} \\
\Leftrightarrow \Delta \frac{\partial \psi}{\partial t} &= -\frac{\partial \psi}{a \cos(\varphi) \partial \lambda} \beta + \frac{\partial \psi}{a \partial \varphi} \frac{\partial \zeta}{a \cos(\varphi) \partial \lambda} - \frac{\partial \psi}{a \cos(\varphi) \partial \lambda} \frac{\partial \zeta}{a \partial \varphi} \\
\Leftrightarrow \Delta \frac{\partial \psi}{\partial t} &= -\frac{\partial \psi}{a \cos(\varphi) \partial \lambda} \beta + \frac{\mathbf{I}}{a^2 \cos(\varphi)} \left(\frac{\partial \psi}{\partial \varphi} \frac{\partial \zeta}{\partial \lambda} - \frac{\partial \psi}{\partial \lambda} \frac{\partial \zeta}{\partial \varphi} \right) \\
\Leftrightarrow \Delta \frac{\partial \psi}{\partial t} &= -\frac{\partial \psi}{a \cos(\varphi) \partial \lambda} \beta + \frac{\mathbf{I}}{a^2 \cos(\varphi)} \left(\frac{\partial \psi}{\partial \varphi} \Delta \frac{\partial \psi}{\partial \lambda} - \frac{\partial \psi}{\partial \lambda} \Delta \frac{\partial \psi}{\partial \varphi} \right). \tag{15.99}
\end{aligned}$$

The operator

$$J(\zeta, \psi) := \frac{\partial \zeta}{\partial \lambda} \frac{\partial \psi}{\partial \varphi} - \frac{\partial \zeta}{\partial \varphi} \frac{\partial \psi}{\partial \lambda} \tag{15.100}$$

is called *Jacobi operator*. This allows the barotropic vorticity equation to be in the form

$$\Delta \frac{\partial \psi}{\partial t} = -\frac{\partial \psi}{a \cos(\varphi) \partial \lambda} \beta + \frac{\mathbf{I}}{a^2 \cos(\varphi)} J(\Delta \psi, \psi) \tag{15.101}$$

note down. This can be simplified further by using it as an equation for the absolute vorticity

$$\eta = \zeta + f = \Delta \psi + f \tag{15.102}$$

formulated. Then you get

$$\frac{\partial \eta}{\partial t} = \frac{\mathbf{I}}{a^2 \cos(\varphi)} J(\eta, \psi). \tag{15.103}$$

15.1.4 Helicity

One defines the *helicity* Z by

$$Z := \mathbf{v} \cdot \boldsymbol{\xi}. \tag{15.104}$$

The momentum equation Eq. (8.101) is

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{\mathbf{I}}{\rho} \nabla p + \mathbf{v} \times \mathbf{f} + \mathbf{v} \times \boldsymbol{\xi} - \nabla k + \mathbf{g} + \mathbf{f}_R. \tag{15.105}$$

Projecting this onto $\boldsymbol{\xi}$ gives

$$\boldsymbol{\xi} \cdot \frac{\partial \mathbf{v}}{\partial t} = -\frac{\boldsymbol{\xi}}{\rho} \cdot \nabla p + \boldsymbol{\xi} \cdot (\mathbf{v} \times \mathbf{f}) - \boldsymbol{\xi} \cdot \nabla k + \boldsymbol{\xi} \cdot \mathbf{g} + \boldsymbol{\xi} \cdot \mathbf{f}_R. \tag{15.106}$$

The three-dimensional vorticity equation Eq. (15.46) is

$$\frac{\partial \boldsymbol{\xi}}{\partial t} = \frac{\mathbf{I}}{\rho^2} \nabla \rho \times \nabla p - (\mathbf{v} \cdot \nabla) \boldsymbol{\xi} - \mathbf{f} \nabla \cdot \mathbf{v} - \boldsymbol{\xi} \nabla \cdot \mathbf{v} + (\mathbf{f} \cdot \nabla) \mathbf{v} + (\boldsymbol{\xi} \cdot \nabla) \mathbf{v} + \nabla \times \mathbf{f}_R. \tag{15.107}$$

Projecting this onto $\mathbf{v}$ gives

$$\begin{aligned}
\mathbf{v} \cdot \frac{\partial \boldsymbol{\xi}}{\partial t} &= \frac{\mathbf{v}}{\rho^2} \cdot (\nabla_{\mathcal{L}} \times \nabla p) - \mathbf{v} \cdot [(\mathbf{v} \cdot \nabla) \boldsymbol{\xi}] - \mathbf{v} \cdot \mathbf{f} \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \boldsymbol{\xi} \nabla \cdot \mathbf{v} + \mathbf{f} \cdot \nabla k + \boldsymbol{\xi} \cdot \nabla k + \mathbf{v} \cdot (\nabla \times \mathbf{f}_R) \\
\Leftrightarrow \mathbf{v} \cdot \frac{\partial \boldsymbol{\xi}}{\partial t} &= \frac{\mathbf{v}}{\rho^2} \cdot (\nabla_{\mathcal{L}} \times \nabla p) - (\mathbf{v} \cdot \nabla) (\mathbf{v} \cdot \boldsymbol{\xi}) + \boldsymbol{\xi} \cdot [(\mathbf{v} \cdot \nabla) \mathbf{v}] - \mathbf{v} \cdot \mathbf{f} \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \boldsymbol{\xi} \nabla \cdot \mathbf{v} + \mathbf{f} \cdot \nabla k + \boldsymbol{\xi} \cdot \nabla k + \mathbf{v} \cdot (\nabla \times \mathbf{f}_R) \\
\Leftrightarrow \mathbf{v} \cdot \frac{\partial \boldsymbol{\xi}}{\partial t} &= \frac{\mathbf{v}}{\rho^2} \cdot (\nabla_{\mathcal{L}} \times \nabla p) - (\mathbf{v} \cdot \nabla) (\mathbf{v} \cdot \boldsymbol{\xi}) + \boldsymbol{\xi} \cdot \nabla k - \mathbf{v} \cdot \mathbf{f} \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \boldsymbol{\xi} \nabla \cdot \mathbf{v} + \mathbf{f} \cdot \nabla k + \boldsymbol{\xi} \cdot \nabla k + \mathbf{v} \cdot (\nabla \times \mathbf{f}_R) \\
\Leftrightarrow \mathbf{v} \cdot \frac{\partial \boldsymbol{\xi}}{\partial t} &= \frac{\mathbf{v}}{\rho^2} \cdot (\nabla_{\mathcal{L}} \times \nabla p) - (\mathbf{v} \cdot \nabla) Z + \mathbf{z} \boldsymbol{\xi} \cdot \nabla k - \mathbf{v} \cdot \mathbf{f} \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \boldsymbol{\xi} \nabla \cdot \mathbf{v} + \mathbf{f} \cdot \nabla k + \mathbf{v} \cdot (\nabla \times \mathbf{f}_R). \tag{15.108}
\end{aligned}$$

Thus you get

$$\begin{aligned}
\frac{\partial Z}{\partial t} &= \frac{\partial \mathbf{v}}{\partial t} \cdot \boldsymbol{\xi} + \mathbf{v} \cdot \frac{\partial \boldsymbol{\xi}}{\partial t} \\
&= -\frac{\boldsymbol{\xi}}{\rho} \cdot \nabla p + \boldsymbol{\xi} \cdot (\mathbf{v} \times \mathbf{f}) - \boldsymbol{\xi} \cdot \nabla k + \boldsymbol{\xi} \cdot \mathbf{g} + \boldsymbol{\xi} \cdot \mathbf{f}_R \\
&\quad + \frac{\mathbf{v}}{\rho^2} \cdot (\nabla_{\mathcal{L}} \times \nabla p) - (\mathbf{v} \cdot \nabla) Z + \mathbf{z} \boldsymbol{\xi} \cdot \nabla k - \mathbf{v} \cdot \mathbf{f} \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \boldsymbol{\xi} \nabla \cdot \mathbf{v} + \mathbf{f} \cdot \nabla k + \mathbf{v} \cdot (\nabla \times \mathbf{f}_R). \tag{15.109}
\end{aligned}$$

The *helicity equation* is therefore:

$$\begin{aligned}
\frac{\partial Z}{\partial t} &= -(\mathbf{v} \cdot \nabla) Z - \frac{\boldsymbol{\xi}}{\rho} \cdot \nabla p + \boldsymbol{\xi} \cdot (\mathbf{v} \times \mathbf{f}) + (\mathbf{f} + \boldsymbol{\xi}) \cdot \nabla k + \boldsymbol{\xi} \cdot \mathbf{g} + \boldsymbol{\xi} \cdot \mathbf{f}_R \\
&\quad + \frac{\mathbf{v}}{\rho^2} \cdot (\nabla_{\mathcal{L}} \times \nabla p) - \mathbf{v} \cdot (\mathbf{f} + \boldsymbol{\xi}) \nabla \cdot \mathbf{v} + \mathbf{v} \cdot (\nabla \times \mathbf{f}_R). \tag{15.110}
\end{aligned}$$

15.1.5 enstrophy

The square $\boldsymbol{\xi}^2$ of the relative vorticity $\boldsymbol{\xi}$ is called *local enstrophy*. It applies

$$\frac{\partial \boldsymbol{\xi}^2}{\partial t} = \mathbf{z} \boldsymbol{\xi} \cdot \frac{\partial \boldsymbol{\xi}}{\partial t} \tag{15.111}$$

At this point we limit ourselves to two-dimensional, incompressible flows. In this case applies

$$\frac{\partial \eta}{\partial t} + \mathbf{v}_h \cdot \nabla \eta \stackrel{\text{Glg. (15.70)}}{=} \mathbf{o} \Rightarrow \frac{\partial \eta}{\partial t} + \mathbf{v}_h \cdot \nabla \eta + \eta \nabla \cdot \mathbf{v}_h = \frac{\partial \eta}{\partial t} + \nabla \cdot (\eta \mathbf{v}_h) = \mathbf{o}. \tag{15.112}$$

This then applies under kinematic or periodic boundary conditions

$$\bar{\eta} = \bar{\zeta} + \bar{f} = \text{const.} \Rightarrow \bar{\zeta} = \text{const.} \tag{15.113}$$

If you multiply Eq. (15.112) with $\mathbf{z} \eta$, one obtains

$$\begin{aligned}
\frac{\partial \eta^2}{\partial t} + \mathbf{v}_h \cdot \nabla \eta^2 + \mathbf{z} \eta^2 \nabla \cdot \mathbf{v}_h &= \frac{\partial \eta^2}{\partial t} + \mathbf{v}_h \cdot \nabla \eta^2 + \eta^2 \nabla \cdot \mathbf{v}_h = \mathbf{o} \\
\Leftrightarrow \frac{\partial \eta^2}{\partial t} &= -\nabla \cdot (\eta^2 \mathbf{v}_h). \tag{15.114}
\end{aligned}$$

If you integrate this under kinematic or periodic boundary conditions, you get on the f-plane

$$\overline{\eta^2} = \overline{\zeta^2} + \overline{f_o^2} + \mathbf{z} \overline{f_o \zeta} = \overline{\zeta^2} + \overline{f_o^2} + \mathbf{z} \overline{f_o \zeta} = \text{const.} \tag{15.115}$$

With Eq. (15.113) still implies this

$$\overline{\zeta^2} = \text{const.} \quad (15.116)$$

The size $\overline{\zeta^2}$ is called *enstrophy*.

15.2 divergence

The divergence of the horizontal wind is called

$$\delta := \nabla \cdot \mathbf{v}_h. \quad (15.117)$$

According to Eq. (B.112) applies

$$\delta = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} - v \frac{\tan(\varphi)}{a + z}. \quad (15.118)$$

The divergence of the overall wind field is

$$D := \nabla \cdot \mathbf{v} \quad (15.119)$$

designated. With Eq. (B.112) can be done

$$D = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} - v \frac{\tan(\varphi)}{a + z} + \frac{2w}{a + z} \quad (15.120)$$

note down. In the case of eddy-free, non-viscous, incompressible flows, Eq. (8.101) for a current function χ in IS

$$\nabla \left(\frac{\partial \chi}{\partial t} + k + \varphi + \frac{p}{\rho} \right) = \mathbf{o}, \quad (15.121)$$

$$\Leftrightarrow \frac{\partial \chi}{\partial t} + \frac{1}{2} \mathbf{v}^2 + gz + \frac{p}{\rho} = \text{homogen}, \quad (15.122)$$

which is called *time-dependent Bernoulli equation*.

15.2.1 Speed and direction divergence

Analogous to vorticity, horizontal divergence can also be divided into two clear parts. The KS from section 15.1.1 is used again. This time we derive the first component of the equation. (15.27) to s and the second to n from:

$$\begin{aligned} \delta &= \frac{\partial}{\partial s} (V \cos(\beta)) + \frac{\partial}{\partial n} (V \sin(\beta)) \\ &= \cos(\beta) \frac{\partial V}{\partial s} - V \sin(\beta) \frac{\partial \beta}{\partial s} + \sin(\beta) \frac{\partial V}{\partial n} + V \cos(\beta) \frac{\partial \beta}{\partial n} \end{aligned} \quad (15.123)$$

If you look at the coordinate origin, it follows that $\beta = \mathbf{o}$

$$\delta = \frac{\partial V}{\partial s} + V \frac{\partial \beta}{\partial n}. \quad (15.124)$$

The first term describes a divergence due to differences in speed in the direction of flow, this is called speed divergence. The second term denotes a directional fanning out perpendicular to the direction of flow, this is directional divergence.

15.2.2 Divergence equation

There is also a prognostic equation for divergence, called the *divergence equation*. The momentum equation Eq. (8.101) is

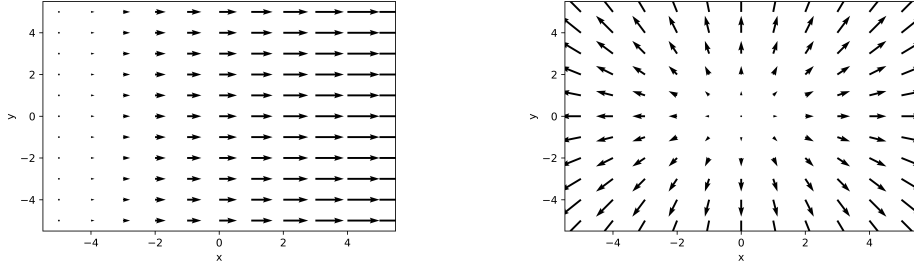


Figure 15.3: Speed divergence (left) and direction divergence (right).

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{\mathbf{I}}{\rho} \nabla p + \mathbf{v} \times \mathbf{f} - (\mathbf{v} \cdot \nabla) \mathbf{v} + \mathbf{g} + \mathbf{f}_R. \quad (15.125)$$

Now you apply the operator $\nabla \cdot$ to the individual terms:

$$\nabla \cdot \frac{\partial \mathbf{v}}{\partial t} \stackrel{\text{Glg. (B.50)}}{=} \frac{\partial D}{\partial t} \quad (15.126)$$

$$\nabla \cdot \left(-\frac{\mathbf{I}}{\rho} \nabla p \right) \stackrel{\text{Glg. (B.49)}}{=} \frac{\mathbf{I}}{\rho^2} \nabla \rho \cdot \nabla p - \frac{\mathbf{I}}{\rho} \Delta p \quad (15.127)$$

$$\nabla \cdot (\mathbf{v} \times \mathbf{f}) \stackrel{\text{Glg. (B.55)}}{=} \mathbf{f} \cdot \boldsymbol{\xi} \quad (15.128)$$

Due to the Poisson equation, the divergence of $\mathbf{g}$ consists only of the centrifugal component. However, since in meteorology a radially symmetric gravity field is usually assumed for analytical derivations, this part is also neglected. So it applies

$$\frac{\partial D}{\partial t} = \frac{\mathbf{I}}{\rho^2} \nabla \rho \cdot \nabla p - \frac{\mathbf{I}}{\rho} \Delta p + \mathbf{f} \cdot \boldsymbol{\xi} - \nabla \cdot [(\mathbf{v} \cdot \nabla) \mathbf{v}] + \nabla \cdot \mathbf{f}_R. \quad (15.129)$$

This is the divergence equation. Using the Lamb transformation one obtains

$$\begin{aligned} \nabla \cdot [(\mathbf{v} \cdot \nabla) \mathbf{v}] &= \Delta k - \nabla \cdot [\mathbf{v} \times (\nabla \times \mathbf{v})] \stackrel{\text{Glg. (B.55)}}{=} \Delta k - \boldsymbol{\xi}^2 + \mathbf{v} \cdot (\nabla \times \boldsymbol{\xi}) \\ &\stackrel{\text{Glg. (B.54)}}{=} \Delta k - \boldsymbol{\xi}^2 - \mathbf{v} \cdot (\Delta \mathbf{v}) + \mathbf{v} \cdot \nabla D. \end{aligned} \quad (15.130)$$

This leads to another form of the divergence equation:

$$\begin{aligned} \frac{\partial D}{\partial t} &= \frac{\mathbf{I}}{\rho^2} \nabla \rho \cdot \nabla p - \frac{\mathbf{I}}{\rho} \Delta p + \mathbf{f} \cdot \boldsymbol{\xi} - \Delta k + \boldsymbol{\xi}^2 \\ &\quad + \mathbf{v} \cdot (\Delta \mathbf{v}) - \mathbf{v} \cdot \nabla D + \nabla \cdot \mathbf{f}_R \end{aligned} \quad (15.131)$$

15.2.2.1 Divergence equation in the p-system

The momentum equations (13.132) - (13.133) in the p-system are vectorial

$$\frac{\partial \mathbf{v}_h}{\partial t} = -\nabla \Phi - \mathbf{f} \mathbf{k} \times \mathbf{v}_h - (\mathbf{v}_h \cdot \nabla) \mathbf{v}_h - \omega \frac{\partial \mathbf{v}_h}{\partial p} + \nabla \cdot \mathbf{f}_R^{(H)}. \quad (15.132)$$

For the preparation, it makes sense to add a $\mathbf{g}$ here and interpret $-\nabla \Phi$ as a three-dimensional vector with $-g$ in the z-component. Thus, applying $\nabla \cdot$ to $-\nabla \Phi + \mathbf{g} = -\Delta_h \Phi$, for which we simply note $\Delta \Phi$ in the further derivation. By applying the operator $\nabla \cdot$ to the individual terms one obtains

$$\begin{aligned}
& \nabla \cdot \frac{\partial \mathbf{v}_h}{\partial t} \stackrel{\text{Glg. (B.50)}}{=} \frac{\partial \delta}{\partial t}, \\
& -\nabla \cdot \nabla \Phi = -\Delta \Phi, \\
& -\nabla \cdot (f \mathbf{k} \times \mathbf{v}_h) \stackrel{\text{Glg. (B.55)}}{=} -\mathbf{v}_h \cdot [\nabla \times (f \mathbf{k})] + f \mathbf{k} \cdot (\nabla \times \mathbf{v}_h) \stackrel{\text{Glg. (B.51)}}{=} -\mathbf{v}_h \cdot [-\mathbf{k} \times \nabla f + f \nabla \times \mathbf{k}] + f \zeta \\
& \quad = \mathbf{v}_h \cdot (\mathbf{k} \times \beta \mathbf{j}) + f \zeta = -u \beta + f \zeta, \\
& \nabla \cdot \left(-\omega \frac{\partial \mathbf{v}_h}{\partial p} \right) \stackrel{\text{Glg. (B.49)}}{=} -\omega \frac{\partial \delta}{\partial p} - \frac{\partial \mathbf{v}_h}{\partial p} \cdot \nabla \omega.
\end{aligned} \tag{15.133}$$

Thus follows

$$\frac{\partial \delta}{\partial t} = -\Delta \Phi - u \beta + f \zeta - \nabla \cdot [(\mathbf{v}_h \cdot \nabla) \mathbf{v}_h] - \omega \frac{\partial \delta}{\partial p} - \frac{\partial \mathbf{v}_h}{\partial p} \cdot \nabla \omega + \nabla \cdot \mathbf{f}_R^{(H)}. \tag{15.134}$$

This is the divergence equation in the p-system. Using the Lamb transformation one obtains

$$\begin{aligned}
\nabla \cdot [(\mathbf{v}_h \cdot \nabla) \mathbf{v}_h] &= \Delta k - \nabla \cdot [\mathbf{v}_h \times (\nabla \times \mathbf{v}_h)] \stackrel{\text{Glg. (B.55)}}{=} \Delta k - (\nabla \times \mathbf{v}_h)^2 + \mathbf{v}_h \cdot (\nabla \times (\nabla \times \mathbf{v}_h)) \\
&\stackrel{\text{Glg. (B.54)}}{=} \Delta k - (\nabla \times \mathbf{v}_h)^2 - \mathbf{v}_h \cdot (\Delta \mathbf{v}_h) + \mathbf{v}_h \cdot \nabla \delta.
\end{aligned} \tag{15.135}$$

This leads to another form of the divergence equation:

$$\begin{aligned}
\frac{\partial \delta}{\partial t} &= -\Delta \Phi - u \beta + f \zeta - \Delta k + (\nabla \times \mathbf{v}_h)^2 + \mathbf{v}_h \cdot (\Delta \mathbf{v}_h) - \mathbf{v}_h \cdot \nabla \delta \\
&\quad - \omega \frac{\partial \delta}{\partial p} - \frac{\partial \mathbf{v}_h}{\partial p} \cdot \nabla \omega + \nabla \cdot \mathbf{f}_R^{(H)}
\end{aligned} \tag{15.136}$$

15.2.2.2 Balance equation

If you insert $\delta = \omega = \circ$ here, the *balance equation* follows

$$\Delta \Phi = -u \beta + f \zeta - \Delta k + (\nabla \times \mathbf{v}_h)^2 + \mathbf{v}_h \cdot (\Delta \mathbf{v}_h). \tag{15.137}$$

If you neglect the non-linear terms, you get the *linear balance equation*

$$\Delta \Phi = -u \beta + f \zeta. \tag{15.138}$$

Using a current function ψ , it follows

$$\Delta \Phi = \beta \frac{\partial \psi}{\partial y} + f \Delta \psi. \tag{15.139}$$

15.3 Potential vorticity

15.3.1 Ertel's vortex theorem

One defines a preliminary form of the potential vorticity P_ψ by

$$P_\psi := a \boldsymbol{\eta} \cdot \nabla \psi, \tag{15.140}$$

where a is the specific volume and ψ is an arbitrary function of space and time. If you differentiate this partially according to time, you get:

$$\frac{\partial P_\psi}{\partial t} = \frac{\partial a}{\partial t} \boldsymbol{\eta} \cdot \nabla \psi + a \frac{\partial (\nabla \times \mathbf{v})}{\partial t} \cdot \nabla \psi + a \boldsymbol{\eta} \cdot \nabla \frac{\partial \psi}{\partial t}. \quad (15.141)$$

First, Eq. (15.46) notated in terms of a

$$\frac{\partial}{\partial t} \text{rot}(\mathbf{v}) = \nabla p \times \nabla a - (\mathbf{v} \cdot \nabla) \boldsymbol{\eta} - \boldsymbol{\eta} \nabla \cdot \mathbf{v} + (\boldsymbol{\eta} \cdot \nabla) \mathbf{v} + \nabla \times \mathbf{f}_R \quad (15.142)$$

In section 15.1, an equation for $\frac{\partial \mathbf{v}}{\partial t}$ was derived by projecting this equation onto the local perpendicular $\mathbf{k}$; the same procedure is used here with a projection onto $\nabla \psi$. One first calculates with Eq. (B.58)

$$\begin{aligned} (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \nabla \psi) &= \nabla \psi \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{v}] + \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \nabla \psi] \\ \Rightarrow \nabla \psi \cdot [(\boldsymbol{\eta} \cdot \nabla) \mathbf{v}] &= (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \nabla \psi) - \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \nabla \psi], \end{aligned} \quad (15.143)$$

$$\begin{aligned} (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \nabla \psi) &= \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi] + \nabla \psi \cdot [(\mathbf{v} \cdot \nabla) \boldsymbol{\eta}] \\ \Rightarrow \nabla \psi \cdot [(\mathbf{v} \cdot \nabla) \boldsymbol{\eta}] &= (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \nabla \psi) - \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi]. \end{aligned} \quad (15.144)$$

So you get

$$\begin{aligned} a \frac{\partial (\nabla \times \mathbf{v})}{\partial t} \cdot \nabla \psi &= a (\nabla p \times \nabla a) \cdot \nabla \psi - a (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \nabla \psi) + a \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi] \\ &\quad - a (\nabla \psi \cdot \boldsymbol{\eta}) \nabla \cdot \mathbf{v} + a (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \nabla \psi) - a \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \nabla \psi] + a \mathbf{f}_R \cdot \nabla \psi. \end{aligned} \quad (15.145)$$

It follows

$$\begin{aligned} \frac{\partial P_\psi}{\partial t} &= a \boldsymbol{\eta} \cdot \nabla \left(\frac{\partial \psi}{\partial t} \right) + a (\nabla p \times \nabla a) \cdot \nabla \psi - a (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \nabla \psi) + a \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi] \\ &\quad - a (\nabla \psi \cdot \boldsymbol{\eta}) \nabla \cdot \mathbf{v} + a (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \nabla \psi) - a \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \nabla \psi] \\ &\quad + \frac{\partial a}{\partial t} \boldsymbol{\eta} \cdot \nabla \psi + a \mathbf{f}_R \cdot \nabla \psi \\ &= a \boldsymbol{\eta} \cdot \nabla \left(\frac{\partial \psi}{\partial t} \right) + a (\nabla p \times \nabla a) \cdot \nabla \psi - a (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \nabla \psi) + a \boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi] \\ &\quad + a (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \nabla \psi) - a \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \nabla \psi] - (\mathbf{v} \cdot \nabla a) (\boldsymbol{\eta} \cdot \nabla \psi) + a \mathbf{f}_R \cdot \nabla \psi. \end{aligned} \quad (15.146)$$

With Eq. (B.56) follows

$$\boldsymbol{\eta} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi] - \mathbf{v} \cdot [(\boldsymbol{\eta} \cdot \nabla) \nabla \psi] = 0. \quad (15.147)$$

The *Ertel's vortex theorem* is therefore:

$$\begin{aligned} \frac{\partial P_\psi}{\partial t} &= a \boldsymbol{\eta} \cdot \nabla \left(\frac{\partial \psi}{\partial t} \right) + a (\nabla p \times \nabla a) \cdot \nabla \psi - a (\mathbf{v} \cdot \nabla) (\boldsymbol{\eta} \cdot \nabla \psi) \\ &\quad + a (\boldsymbol{\eta} \cdot \nabla) (\mathbf{v} \cdot \nabla \psi) - (\mathbf{v} \cdot \nabla a) (\boldsymbol{\eta} \cdot \nabla \psi) + a \mathbf{f}_R \cdot \nabla \psi. \end{aligned} \quad (15.148)$$

This can be done with the material derivation

$$\frac{DP_\psi}{Dt} = a \boldsymbol{\eta} \cdot \nabla \left(\frac{D\psi}{Dt} \right) + a (\nabla p \times \nabla a) \cdot \nabla \psi + a \mathbf{f}_R \cdot \nabla \psi \quad (15.149)$$

rephrase.

15.3.2 Definition and properties of PV

The *potential vorticity* P is defined by

$$P := a\boldsymbol{\eta} \cdot \nabla\theta, \quad (15.150)$$

It is therefore created by entering into Eq. (15.140) for ψ the potential temperature θ sets in. This is a function of pressure and specific volume, so it varies in Eq. (15.148) the term with the vector product. This applies to adiabatic processes:

$$\frac{\partial P}{\partial t} = -a(\mathbf{v} \cdot \nabla)(\boldsymbol{\eta} \cdot \nabla\psi) - (\boldsymbol{\eta} \cdot \nabla\psi)(\mathbf{v} \cdot \nabla a) + a\mathbf{f}_R \cdot \nabla\theta \quad (15.151)$$

$$\Leftrightarrow \frac{\partial P}{\partial t} = -(\mathbf{v} \cdot \nabla)(a\boldsymbol{\eta} \cdot \nabla\psi) + a\mathbf{f}_R \cdot \nabla\theta, \quad (15.152)$$

In this case, the potential vorticity is a conserved quantity except for the friction:

$$\frac{DP}{Dt} = a\mathbf{f}_R \cdot \nabla\theta \quad (15.153)$$

For the potential vorticity, Eq. (B.115)

$$P = a\boldsymbol{\eta} \cdot \nabla\theta = a\mathbf{f} \cdot \nabla\theta + a \left[\left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} - \frac{v}{r} \right) \frac{\partial \theta}{\partial x} + \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} + \frac{u}{r} \right) \frac{\partial \theta}{\partial y} + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} - \frac{u \tan(\varphi)}{r} \right) \frac{\partial \theta}{\partial z} \right]. \quad (15.154)$$

Here we now make the following approximations:

- shallow atmosphere (see section 13.3)
- Neglecting the vertical speed when calculating the rotation of the wind field

The quantity obtained in this way is denoted by P_i . Then you get

$$P_i = a\eta \frac{\partial \theta}{\partial z} + a \left[-\frac{\partial v}{\partial z} \frac{\partial \theta}{\partial x} + \frac{\partial u}{\partial z} \frac{\partial \theta}{\partial y} \right]. \quad (15.155)$$

In a hydrostatic atmosphere one can use Eq. (15.155) transform the vertical derivatives into the p-system:

$$P_i = -gf \frac{\partial \theta}{\partial p} - g \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} - \frac{u \tan(\varphi)}{a} \right) \frac{\partial \theta}{\partial p} + g \left[\frac{\partial v}{\partial p} \frac{\partial \theta}{\partial x} - \frac{\partial u}{\partial p} \frac{\partial \theta}{\partial y} \right] \quad (15.156)$$

If you transform the horizontal derivatives with Eq. (12.7) follows a generalized vertical coordinate μ

$$\frac{P_i}{g} = \dots \Big|_{\mu} - \left(\frac{\partial \mu}{\partial x} \right)_z \frac{\partial v}{\partial \mu} \frac{\partial \theta}{\partial p} + \left(\frac{\partial \mu}{\partial y} \right)_z \frac{\partial u}{\partial \mu} \frac{\partial \theta}{\partial p} + \frac{\partial v}{\partial p} \frac{\partial \theta}{\partial \mu} \left(\frac{\partial \mu}{\partial x} \right)_z - \frac{\partial u}{\partial p} \frac{\partial \theta}{\partial \mu} \left(\frac{\partial \mu}{\partial y} \right)_z, \quad (15.157)$$

where the formal values of Eq. (15.156) same terms were abbreviated. The formally new terms disappear in the two cases $\mu = p, \theta$. This means you can record the potential vorticity

$$P_i = -g\eta_p \frac{\partial \theta}{\partial p} + g \left[\frac{\partial v}{\partial p} \left(\frac{\partial \theta}{\partial x} \right)_p - \frac{\partial u}{\partial p} \left(\frac{\partial \theta}{\partial y} \right)_p \right], \quad (15.158)$$

where the index p means that partial derivatives are to be formed in the p -system. In isentropic coordinates only the first term remains,

$$P_i = -g\eta_\theta \left(\frac{\partial p}{\partial \theta} \right)^{-1} \equiv \frac{\eta_\theta}{\sigma_\theta}, \quad (15.159)$$

where the *hydrostatic stability in the θ -system*, defined by

$$\sigma_\theta := -\frac{1}{g} \frac{\partial p}{\partial \theta}, \quad (15.160)$$

was introduced. Due to the simple form of Eq. (15.159) P_i is also called *isentropic potential vorticity*. In the barotropic case, Eq. (15.158) the terms between the square brackets, you get

$$P_{i,b} = -g\eta_p \frac{\partial \theta}{\partial p} \quad (15.161)$$

for the so-called *barotropic potential vorticity* $P_{i,b}$.

15.3.3 Incompressible potential vorticity

In the dynamics of SWEs, the *incompressible potential vorticity* (incompressible PV) q is defined by

$$q := \frac{\eta}{h} = \frac{\zeta + f}{h} = \frac{\mathbf{k} \cdot (\nabla \times \mathbf{v}) + f}{h}, \quad (15.162)$$

where h is the depth. According to Eq. (B.57) applies

$$(\mathbf{v} \cdot \nabla) \mathbf{v} = \nabla k - \mathbf{v} \times (\nabla \times \mathbf{v}) \quad (15.163)$$

with the specific kinetic energy $k = \frac{1}{2} \mathbf{v}^2$. For the second term, Eq. (13.17)

$$\mathbf{v} \times (\nabla \times \mathbf{v}) = \mathbf{v} \times \left[\frac{u \tan(\varphi)}{r} \mathbf{k} + \mathbf{k} \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) + j \frac{\partial u}{\partial z} - i \frac{\partial v}{\partial z} \right]. \quad (15.164)$$

Due to the disappearance of vertical shear in the barotropic case

$$\mathbf{v} \times (\nabla \times \mathbf{v}) = \mathbf{v} \times \left[\frac{u \tan(\varphi)}{r} \mathbf{k} + \mathbf{k} \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \right] = \mathbf{v} \times \mathbf{k} \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} + \frac{u \tan(\varphi)}{r} \right) = \mathbf{v} \times \mathbf{k} \zeta = -\mathbf{k} \times \zeta \mathbf{v}. \quad (15.165)$$

The vertical component is of no further interest here. Now one can use Eq. for the momentum equation of the shallow water equations. Write (13.171) neglecting friction

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \mathbf{k} \times \zeta \mathbf{v} &= -g \nabla (h + b) - \nabla k - f \mathbf{k} \times \mathbf{v} \\ \Leftrightarrow \frac{\partial \mathbf{v}}{\partial t} + q h \mathbf{k} \times \mathbf{v} &= -g \nabla (h + b) - \nabla k. \end{aligned} \quad (15.166)$$

It applies

$$\frac{Dq}{Dt} = \frac{1}{h} \frac{D\eta}{Dt} - \frac{\eta}{h^2} \frac{Dh}{Dt} \stackrel{\text{Glg. (13.172)}}{=} -\frac{\eta}{h} \nabla \cdot \mathbf{v} - \frac{\eta}{h^2} (-h \nabla \cdot \mathbf{v}) = 0. \quad (15.167)$$

The incompressible PV is therefore a conserved quantity. In the middle latitudes, the planetary vorticity is an order of magnitude larger than the relative one, thus it follows from the fact that the incompressible potential vorticity is preserved

$$h \text{ nimmt ab} \Rightarrow (\zeta + f) \text{ nimmt ab} \Rightarrow \zeta \text{ nimmt ab,} \quad (15.168)$$

where a positive sign of f and therefore also of η was assumed. If f is negative, then ζ must grow. If a westerly flow encounters an orographic obstacle, anticyclonic relative vorticity arises. This is called *orographic β -effect*. An important example is the formation of planetary waves in the Rocky Mountains.

Eq. (15.167) can be in the form

$$\frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q = 0 \quad (15.169)$$

note down. Combining this with Eq. (13.172), one obtains

$$h \frac{\partial q}{\partial t} + h \mathbf{v} \cdot \nabla q + q \frac{\partial h}{\partial t} + q h \nabla \cdot \mathbf{v} + q \mathbf{v} \cdot \nabla h = 0$$

$$\Leftrightarrow \frac{\partial (hq)}{\partial t} + \nabla \cdot (hq\mathbf{v}) = 0. \quad (15.170)$$

The equations of motion have wave solutions. This is obtained by inserting a complex harmonic approach $\psi_0 e^{-i\omega t}$ into the respective system of equations and looking for non-trivial solutions, here ψ_0 is a complex amplitude vector. Occasionally a zonal background current is recorded due to climatological relevance. A solution is instability if $\Im(\omega) > 0$, i.e. the amplitude increases exponentially.

16.1 kinematics

Waves are periodic changes in space and time. The maximum magnitude deflection from the rest position is the amplitude. The time $T > 0$ until the movement pattern is repeated at a fixed location is called the period duration; its inverse is the frequency f . The angular frequency ω is defined as

$$\omega := 2\pi f = \frac{2\pi}{T}. \quad (16.1)$$

Analogously, the wavelength $\lambda > 0$ is the length after which the movement pattern repeats itself. Wavenumber κ and circular wavenumber k are analogous to frequency and circular frequency defined by

$$\kappa := \frac{1}{\lambda}, \quad k := \frac{2\pi}{\lambda}. \quad (16.2)$$

A wave of size a is described by an equation of the form

$$a(x, t) = Af(kx - \omega t + \varphi). \quad (16.3)$$

Here f is a real or complex-valued, 2π -periodic function, i.e. $f(\xi + 2\pi) = f(\xi)$ for each $\xi \in \mathbb{R}$. This can, but does not have to be, a trigonometric function. f is often chosen to be complex-valued, e.g. $f(x) = \exp(ix)$ if this shortens the mathematical description or makes it more clear. However, before you calculate quantities that you want to compare with measured quantities, you have to project everything onto the real axis. The argument $kx - \omega t + \varphi$ is also called the *phase* of the wave, in the complex plane this is the angle that the number includes with the real axis. φ is the phase shift that allows the phase of the wave at $x, t = 0$ not to be equal to zero. You can often do without φ in derivations by shifting the time or location coordinates accordingly. k and ω can also have imaginary parts, e.g. B. with waves that propagate exponentially into a medium (so-called *evanescent waves*), or with instabilities in which the amplitude increases exponentially over a certain period of time. Likewise, the prefactor A can also be complex and thus contain a phase shift.

In general, a wave can also propagate in a three-dimensional space, in which case we first write in general terms

$$a(\mathbf{r}, t) = Af(\varphi(\mathbf{r}, t)) \quad (16.4)$$

with $\varphi = \varphi(\mathbf{r}, t)$ as the phase function. The phase function can, for example, have the shape

$$\varphi(\mathbf{r}, t) = \mathbf{k} \cdot \mathbf{r} - \omega t \quad (16.5)$$

have, here $\mathbf{k} = (k_x, k_y, k_z)^T$ is called the wave vector. Its magnitude is equal to the circular wave number and points in the direction of propagation of the wave. If one introduces Eq. (16.5) after the time, follows

$$\frac{d\varphi(\mathbf{r}, t)}{dt} = \mathbf{k} \cdot \frac{d\mathbf{r}}{dt} - \omega \quad (16.6)$$

If you set the left side equal to zero, i.e. move with a point of constant phase, and choose a trajectory parallel to $\mathbf{k}$, you get the phase velocity

$$c = \frac{\omega}{k} = \frac{\lambda}{T} = \lambda f. \quad (16.7)$$

The dependency

$$\omega = \omega(k) \quad (16.8)$$

is called *dispersion relation*. Now consider the equation $f(x, t) = f_1(x, t) + f_2(x, t)$ of two waves:

$$f_1(x, t) = -\cos(k_1 x - \omega_1 t) \quad (16.9)$$

$$f_2(x, t) = \cos(k_2 x - \omega_2 t) \quad (16.10)$$

$$f(x, t) = -\cos(k_1 x - \omega_1 t) + \cos(k_2 x - \omega_2 t) \quad (16.11)$$

With Eq. (A.61) follows

$$\begin{aligned} -\cos(a) + \cos(\beta) &= 1 - \cos(a) - 1 + \cos(\beta) = 2\sin^2\left(\frac{a}{2}\right) - 2\sin^2\left(\frac{\beta}{2}\right) \\ &= 2\sin^2\left(\frac{a}{2}\right) - 2\sin^2\left(\frac{a}{2}\right)\sin^2\left(\frac{\beta}{2}\right) - 2\sin^2\left(\frac{\beta}{2}\right) + 2\sin^2\left(\frac{a}{2}\right)\sin^2\left(\frac{\beta}{2}\right) \\ &= 2\left[\sin^2\left(\frac{a}{2}\right)\cos^2\left(\frac{\beta}{2}\right) - \cos^2\left(\frac{a}{2}\right)\sin^2\left(\frac{\beta}{2}\right)\right] \\ &= 2\left[\sin\left(\frac{a}{2}\right)\cos\left(\frac{\beta}{2}\right) - \cos\left(\frac{a}{2}\right)\sin\left(\frac{\beta}{2}\right)\right]\left[\sin\left(\frac{a}{2}\right)\cos\left(\frac{\beta}{2}\right) + \cos\left(\frac{a}{2}\right)\sin\left(\frac{\beta}{2}\right)\right] \\ &= 2\sin\left(\frac{a-\beta}{2}\right)\sin\left(\frac{a+\beta}{2}\right). \end{aligned} \quad (16.12)$$

So it applies

$$f(x, t) = 2\sin\left(\frac{\Delta k x - \Delta \omega t}{2}\right)\sin(\bar{k}x - \bar{\omega}t) \quad (16.13)$$

with

$$\Delta k := k_2 - k_1, \quad \Delta \omega := \omega_2 - \omega_1, \quad (16.14)$$

$$\bar{k} := \frac{k_1 + k_2}{2}, \quad \bar{\omega} := \frac{\omega_1 + \omega_2}{2}. \quad (16.15)$$

So the envelope $\sin\left(\frac{\Delta k x - \Delta \omega t}{2}\right)$ moves with the speed

$$v_e = \frac{\Delta \omega}{\Delta k}. \quad (16.16)$$

One therefore defines the *group velocity* c_{gr} by

$$c_{\text{gr}} := \frac{\partial \omega}{\partial k}. \quad (16.17)$$

It can therefore be derived from the dispersion relation. It is the speed at which wave packets move, i.e. at which energy is transported. Is

$$c_{\text{gr}} = c \quad (16.18)$$

regardless of k , the wave is called *dispersion-free*. You can vector the group speed

$$c_{\text{gr}} = \nabla_k \omega. \quad (16.19)$$

generalize. You can write with $\omega = ck$

$$c_{\text{gr}} = \frac{d\omega}{dk} = c + k \frac{dc}{dk} = c + k \frac{d\lambda}{dk} \frac{dc}{d\lambda} = c - \frac{2\pi}{k} \frac{dc}{dy} = c - \lambda \frac{dc}{d\lambda}. \quad (16.20)$$

In the case $dc/d\lambda < 0$ one speaks of *abnormal dispersion*. In this case the energy propagates faster than the phase velocity. In the case

$$\frac{dc}{d\lambda} \lambda > c \Leftrightarrow \frac{dc}{d\lambda} > \frac{c}{\lambda} = f \quad (16.21)$$

or

$$\frac{d\omega}{dk} < 0 \quad (16.22)$$

propagates the energy in a direction opposite to the wave vector.

If the character of a wave allows this, it is categorized either as a *longitudinal wave*, in which the oscillators oscillate parallel to the wave vector, or as a *transverse wave*, in which they oscillate perpendicular to it. For mechanical transverse waves, the *wave height* H as double amplitude and the *steepness* S of a wave that passes through are introduced as further kinematic variables

$$S := \frac{H}{\lambda} \quad (16.23)$$

is defined and is therefore dimensionless.

16.2 Categorization of waves in geofluids

Barotropic waves (see section 16.5) require boundary surfaces and have their amplitude maximum at these. Therefore they are also referred to as *external waves* or surface waves. The shallow water equations are usually sufficient to describe such waves.

Barocline waves (see section 16.6), however, exist inside a medium; they are therefore also referred to as *internal waves*.

A limiting case here are waves at a sharp interface ($N \gg 0$) inside a medium, such as. B. at an inversion or at a density jump (see, for example, the illustration at the end of section 16.5.2). They can often be described mathematically using the formulas for surface waves, but are usually classified as internal waves. Capillary waves (see section 16.4) are surface waves, but barotropy plays no role and the shallow water equations are not sufficient to describe them. Therefore they represent a special category.

16.3 Justification for linearization

If A, B are two phenomena and $f(A + B)$ is, for example, a prediction, then in general it holds

$$f(A + B) \neq f(A) + f(B), \quad (16.24)$$

The total effect of $A + B$ is therefore not the sum of the individual effects A, B , since f is not a linear map.

However, when searching for analytical solutions to a nonlinear system of equations, especially when searching for wave solutions, one is very interested in linearization. This is sometimes more sometimes less justified. It is assumed that for a quantity $A = A_0 + A'$ with A_0 as the background state and A' as the disturbance

$$\mathcal{O}(A_0) = \mathcal{O}(A') + \mathbf{1}, \quad (16.25)$$

therefore applies

$$\mathcal{O}(A'^2) = \mathcal{O}(A_0) - \mathbf{2}. \quad (16.26)$$

One therefore ignores all terms in which products of the perturbations occur. This leads to a linearization of the system of equations. For the derivatives, we assume a plane wave in the x-direction with angular frequency ω and angular wave number k , which only affects the disturbances

$$\mathcal{O}\left(\frac{\partial A'}{\partial t}\right) = \mathcal{O}(\omega A'), \quad (16.27)$$

$$\mathcal{O}\left(\frac{\partial A'}{\partial x}\right) = \mathcal{O}(k A') \quad (16.28)$$

$$\mathcal{O}\left(\frac{\frac{\partial A'}{\partial t}}{A \frac{\partial A'}{\partial x}}\right) = \mathcal{O}\left(\frac{\omega}{Ak}\right) = \mathcal{O}\left(\frac{c}{A}\right). \quad (16.29)$$

From Eq. (16.29) it follows that one can neglect the advective terms if the phase velocity $c = \frac{\omega}{k}$ is much larger than the fluid particle velocity.

If it is possible to eliminate all nonlinear terms of a system of equations, then we know that two independent solutions to this system of equations do not affect each other. Examples are sound waves and electromagnetic waves. The linearity of these systems makes it possible to independently superimpose different sounds or signals.

16.3.1 Example: sound waves

Sound waves are compression waves, but due to adiabatic pressures and densities can be clearly mapped to one another. A wave propagating in the x direction is considered. The perturbation approach for velocity and density is

$$u = U + u', \quad \rho = \rho_o + \rho'. \quad (16.30)$$

The system of equations is with the abbreviated replacements

$$\rho' \rightarrow \rho, \quad (16.31)$$

$$u' \rightarrow u \quad (16.32)$$

and the approximations derived in the previous section

$$\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} = -\frac{1}{\rho_o} \frac{\partial p}{\partial x} \quad (16.33)$$

$$\frac{\partial \rho}{\partial t} + U \frac{\partial \rho}{\partial x} = -\rho_o \frac{\partial u}{\partial x} \quad (16.34)$$

$$\rho(p) = \rho_o \left(\frac{p}{p_o} \right)^{c_v/c_p} \quad (16.35)$$

The first equation is the momentum equation, the second is the continuity equation, and the third is the potential density equation Eq. (9.44). In order to be in Eq. (16.34) to express the change in density through pressure, one uses the chain rule:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial p} \frac{\partial p}{\partial t} = \frac{\rho_o c_v}{p_o c_p} \left(\frac{p}{p_o} \right)^{c_v/c_p - 1} \frac{\partial p}{\partial t} = \frac{\rho_o c_v}{p_o c_p} \frac{\partial p}{\partial t}, \quad (16.36)$$

analogously for $\frac{\partial}{\partial x}$. The derivation of the density according to the pressure was evaluated at the point $p = p_o$ because the pressure fluctuations are very small. Now you make an approach

$$u = u_o \exp[i(kx - \omega t)], \quad p = P \exp[i(kx - \omega t)] \quad (16.37)$$

with possibly complex amplitudes u_o, P . If you insert this into the system of equations, it follows

$$-i\omega u_o + Uiku_o = -\frac{1}{\rho_o} ikP, \quad (16.38)$$

$$\begin{aligned} -\frac{\rho_o c_v}{p_o c_p} i\omega P + Uik \frac{\rho_o c_v}{p_o c_p} P &= -\rho_o iku_o \\ \Leftrightarrow -i\omega P + UikP &= -\frac{p_o c_p}{c_v} iku_o. \end{aligned} \quad (16.39)$$

As a matrix equation this becomes

$$\begin{pmatrix} -i\omega + Uik & \frac{1}{\rho_\theta} ik \\ ik \frac{p_o c_p}{c_v} & -i\omega + Uik \end{pmatrix} \begin{pmatrix} u_p \\ P \end{pmatrix} = \mathbf{0}. \quad (16.40)$$

Non-trivial solutions exist for

$$(\omega - Uk)^2 - k^2 \frac{p_o c_p}{\rho_\theta c_v} = 0 \Leftrightarrow \omega = Uk \pm k \sqrt{\frac{p_o c_p}{\rho_\theta c_v}}. \quad (16.41)$$

So for the phase velocity c it follows

$$c = U \pm \sqrt{R_d T \kappa}. \quad (16.42)$$

The equation of state was used here, T is the equilibrium temperature and $\kappa = c_p/c_v > 1$ is the adiabatic exponent. However, the value of c also depends on the humidity. You could therefore determine the humidity by measuring the speed of sound in combination with a temperature measurement. It should be noted that sound waves are dispersion-free, but the phase velocity is space and time dependent as it depends on the temperature and humidity.

16.3.1.1 Entropy form of the pressure gradient

If you use the equation with Eq. (10.87) obtained formulation

$$-\frac{1}{\rho} \nabla p = -c^{(p)} T + T \nabla s = -c^{(p)} T + c^{(p)} \frac{T}{\theta} \nabla \theta \quad (16.43)$$

for the pressure gradient acceleration, further insights into sound waves are obtained. Since sound waves are adiabatic, the portion of the pressure gradient that is related to the gradient of entropy is not expected to contribute to sound waves. It is different with the temperature gradient. In order to obtain a closed system of equations, a prognostic equation for the temperature must therefore be found. The adiabatic form of Eq. (9.14) is

$$\frac{\partial T}{\partial t} = -\nabla \cdot (T \mathbf{v}) - \left(\frac{R_d}{c^{(V)}} - 1 \right) T \nabla \cdot \mathbf{v}. \quad (16.44)$$

It is therefore recorded as a one-dimensional system of equations, neglecting advection

$$\frac{\partial w}{\partial t} = -c^{(p)} \frac{\partial T}{\partial z}, \quad (16.45)$$

$$\frac{\partial T}{\partial t} = -\frac{R_d}{c^{(V)}} T \frac{\partial w}{\partial z}. \quad (16.46)$$

In order to verify that this actually describes sound waves, one makes the approach

$$w = w_1 \exp(ikz - i\omega t), \quad T = T_o + T_1 \exp(ikz - i\omega t). \quad (16.47)$$

The density is assumed to be homogeneous. If you insert this into the equations (16.45) - (16.46), it follows

$$-i\omega w_1 = -c^{(p)} ik \frac{T_1}{\rho}, \quad -i\omega T_1 = -\frac{R_d}{c^{(V)}} T_o ik w_1. \quad (16.48)$$

In matrix notation you get

$$\begin{pmatrix} -i\omega & c^{(p)} ik \frac{1}{\rho} \\ \frac{R_d}{c^{(V)}} T_o ik & -i\omega \end{pmatrix} \begin{pmatrix} w_1 \\ T_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (16.49)$$

By setting the determinant to zero you get

$$\omega^2 = \kappa R_d T k^2. \quad (16.50)$$

This results in the same dispersion relation as Eq. (16.42). This verifies that the terms listed in the equations (16.45) - (16.46) do indeed describe sound waves.

16.4 Capillary waves

In the case $\eta = \hat{\eta} \exp(ikx - i\omega t)$ follows

$$-\frac{\mathbf{1}}{\rho} \frac{\partial p_k}{\partial x} = -\frac{k^2 \sigma}{\rho} \frac{\partial \eta}{\partial x}. \quad (16.51)$$

Adding this to the right-hand side of Eq. (16.66), is obtained

$$-g \frac{\partial \eta}{\partial x} \rightarrow -g \frac{\partial \eta}{\partial x} - \frac{\sigma k^2}{\rho} \frac{\partial \eta}{\partial x} = -g \left(\mathbf{1} + \frac{k^2 \sigma}{\rho g} \right) \frac{\partial \eta}{\partial x}, \quad (16.52)$$

So you have to

$$g \rightarrow g \left(\mathbf{1} + \frac{k^2 \sigma}{\rho g} \right) \quad (16.53)$$

replace, the rest of the derivation carries over. So you get the dispersion relation of the capillary waves

$$\omega^2 = kg \left(\mathbf{1} + \frac{k^2 \sigma}{\rho g} \right) \tanh(kD). \quad (16.54)$$

In the case of very short waves, the limiting case is obtained

$$\omega^2 = \frac{k^3 \sigma}{\rho} \Rightarrow c = \sqrt{\frac{2\pi\sigma}{\rho\lambda}}. \quad (16.55)$$

In this limiting case, capillary waves are abnormally dispersed.

In order to derive a boundary wall length λ_K , above which capillary effects become important, one calculates

$$\frac{k_K^2 \sigma}{\rho g} \stackrel{!}{\geq} \frac{\mathbf{1}}{\mathbf{10}} \Leftrightarrow \lambda_K \leq \sqrt{\frac{40\pi^2 \sigma}{\rho g}}. \quad (16.56)$$

The surface tension of water is approximately $\sigma \sim 75$ mN/m, from which it follows

$$\lambda_K \sim 5, 5 \text{ cm}. \quad (16.57)$$

16.5 Barotropic waves

16.5.1 Inertial waves

In the case of inertial waves, a vanishing horizontal pressure gradient is assumed, so that only the Coriolis force remains. The momentum equations of the SWEs Eq. (13.171) becomes, neglecting the advective terms

$$\frac{du}{dt} = f_\circ v, \quad \frac{dv}{dt} = -f_\circ u. \quad (16.58)$$

A location-independent value f_o is used for the Coriolis parameter in order to avoid the β effect. You make an approach

$$u = U \exp(-i\omega t), \quad v = V \exp(-i\omega t) \quad (16.59)$$

with possibly complex amplitudes U, V . If you plug this into the system of equations, you get

$$-i\omega U = f_o V, \quad -i\omega V = -f_o U. \quad (16.60)$$

As a matrix equation this becomes

$$\begin{pmatrix} -i\omega & -f_o \\ f_o & -i\omega \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \mathbf{0}. \quad (16.61)$$

Non-trivial solutions exist for

$$-\omega^2 + f_o^2 = 0, \quad (16.62)$$

so for

$$\omega = \pm f. \quad (16.63)$$

The particles move in a circular path with a radius

$$R_I = \frac{V}{f_o}. \quad (16.64)$$

If you use a speed of $1 \frac{\text{m}}{\text{s}}$, for example $R_I = 10 \text{ km}$ with $f_o = 10^{-4} \text{ s}^{-1}$. Applies to the period

$$T = \frac{2\pi}{f_o} \approx \frac{1 \text{ d}}{2 \sin(\varphi)}, \quad (16.65)$$

$d = 24 \text{ h}$ is the duration of a day. Typical inertial periods are on the order of one day.

Since the total derivatives $\frac{D}{Dt}$ were used, a trajectory was implicitly calculated. This trajectory is a circular path, but only assuming a location-independent Coriolis parameter. In general, however, the particle trajectories are not closed circular paths due to the beta effect. Likewise, no wind field $\mathbf{v}_h(\mathbf{r}, t)$ was determined.

16.5.2 Water surface waves

At this point one assumes the absence of a zonal base current $U = 0$. A. you also align the x-direction with the wave vector, so that the linearized system of equations here

$$\frac{\partial u}{\partial t} = -g \frac{\partial \eta}{\partial x}, \quad (16.66)$$

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0 \quad (16.67)$$

is. One assumes a homogeneous depth $D > 0$ and requires this as a boundary condition

$$w(z = -D) \stackrel{!}{=} 0. \quad (16.68)$$

Now there are the approaches

$$u = U(z) \exp(ikx - i\omega t), \quad w = W(z) \exp(ikx - i\omega t). \quad (16.69)$$

The surface deflection η and the vertical velocity w hang over

$$\frac{\partial \eta}{\partial t}(z = \mathfrak{o}) \stackrel{!}{=} w(z = \mathfrak{o}), \quad (16.70)$$

$$\Rightarrow -i\omega \hat{\eta} = W(\mathfrak{o}) \quad (16.71)$$

together, where $\hat{\eta}$ is the amplitude of the surface deflection. Eq. (16.66) therefore results in $z = \mathfrak{o}$

$$-i\omega U(\mathfrak{o}) = g \frac{k}{\omega} W(\mathfrak{o}) \Rightarrow \omega^2 = igk \frac{W(\mathfrak{o})}{U(\mathfrak{o})}. \quad (16.72)$$

From Eq. (16.67) follows

$$ikU(z) + W' = \mathfrak{o} \Rightarrow W' = -ikU. \quad (16.73)$$

This and the equations (16.68) and (16.71) are through

$$U(z) = \frac{\hat{\eta}\omega}{\sinh(kD)} \cosh[k(D+z)], \quad (16.74)$$

$$W(z) = -\frac{i\hat{\eta}\omega}{\sinh(kD)} \sinh[k(D+z)]. \quad (16.75)$$

fulfilled. It follows from Eq. (16.72) is the dispersion relation

$$\omega^2 = gk \tanh(kD). \quad (16.76)$$

In the case $\lambda \gg D$ it follows

$$\omega^2 = k^2 gD \quad (16.77)$$

as the dispersion relation of the so-called *shallow water waves*. In the opposite case $\lambda \ll D$ the dispersion relation follows the *deep water waves*

$$\omega^2 = gk. \quad (16.78)$$

In the case of a density discontinuity $\varrho_1 < \varrho_2$ with a lighter fluid above a heavier fluid, the pressure gradient term is below the wave

$$\begin{aligned} -\frac{1}{\varrho_2} \frac{\partial p}{\partial x} &= -\frac{1}{\varrho_2} \frac{\partial (g\varrho_2 \eta - g\varrho_1 \eta)}{\partial x} = -\frac{g}{\varrho_2} \frac{\partial (\varrho_2 \eta - \varrho_1 \eta)}{\partial x} = -\frac{g}{\varrho_2} \frac{\partial [\eta (\varrho_2 - \varrho_1)]}{\partial x} \\ &= -\frac{g(\varrho_2 - \varrho_1)}{\varrho_2} \frac{\partial \eta}{\partial x} = -g \frac{\Delta \varrho}{\varrho_2} \frac{\partial \eta}{\partial x} \end{aligned} \quad (16.79)$$

with $\Delta \varrho := \varrho_2 - \varrho_1$, where η is to be understood as the deflection of the density discontinuity. The rest of the derivation carries over, whereby the substitution $g \rightarrow g' := g \frac{\Delta \varrho}{\varrho_2}$ has to be made. For the dispersion relation one obtains

$$\omega^2 = g' k \tanh(k(z_w - z_o)), \quad (16.80)$$

where z_w denotes the position of the density discontinuity and z_o denotes the depth coordinate of the bottom.

16.5.2.1 Stokes drift

Define

$$\gamma := \frac{\hat{\eta}\omega}{\sinh(kD)}, \quad (16.81)$$

then Eq. (16.74) as

$$U(z) = \gamma \cosh[k(D+z)] \quad (16.82)$$

note down. If you integrate this from $z = -D$ to $z = \eta$, it follows

$$\int_{-D}^{\eta} \gamma \cosh[k(D+z)] dz = \frac{\gamma}{k} \sinh(k(D+\eta)) \stackrel{\text{Glg. (A.56)}}{=} \frac{\gamma}{k} [\sinh(kD) \cosh(k\eta) + \cosh(kD) \sinh(k\eta)]. \quad (16.83)$$

Developing this to first order in $k\eta$ (slope $\ll 1$), it follows

$$\int_{-D}^{\eta} \gamma \cosh[k(D+z)] dz \approx \frac{\gamma}{k} [\sinh(kD) + \cosh(kD) k\eta]. \quad (16.84)$$

Multiplying this by the real part of $\exp(ikx - i\omega t)$ gives the expression

$$\frac{d\dot{v}_h}{dy} = \frac{\gamma}{k} [\sinh(kD) + \cosh(kD) k\eta] \cos(kx - \omega t) \quad (16.85)$$

for the vertically integrated volume flow density. If you insert the real part of the surface deflection $\eta = \hat{\eta}e^{ikx - i\omega t}$, you get

$$\frac{d\dot{v}_h}{dy} = \frac{\gamma}{k} [\sinh(kD) + \cosh(kD) k\hat{\eta}\cos(kx - \omega t)] \cos(kx - \omega t). \quad (16.86)$$

If you integrate this over a period it follows

$$\frac{d\dot{v}_h}{dy} = \frac{\gamma}{k} \cosh(kD) k\hat{\eta} \frac{1}{2} = \frac{\hat{\eta}^2 \omega}{2 \tanh(kD)} = \frac{\hat{\eta}^2}{2} \sqrt{\frac{gk}{\tanh(kD)}}. \quad (16.87)$$

This volume flow in the direction of the wave vector is called *Stokes drift*. Because of

$$\bar{u}(z) = 0 \quad (16.88)$$

for $z < -\hat{\eta}$ this volume flow arises exclusively in the area of the surface wave itself due to the increase in the amplitude of the horizontal velocity with height.

16.5.3 Poincare waves

Poincaré waves are the waves of the linearized shallow water equations on the f-plane, so the equations (13.173) - (13.174) form the underlying system of equations. These equations are in components in plane geometry

$$\frac{\partial u}{\partial t} = fv - g \frac{\partial \eta}{\partial x}, \quad (16.89)$$

$$\frac{\partial v}{\partial t} = -fu - g \frac{\partial \eta}{\partial y}, \quad (16.90)$$

$$\frac{\partial \eta}{\partial t} = -H \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right). \quad (16.91)$$

Here η is the surface deflection and H is the average depth. You make an approach

$$u = u_o \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)], \quad v = v_o \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)], \quad \eta = \hat{\eta} \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]. \quad (16.92)$$

with a horizontal wave vector $\mathbf{k} = (k_x, k_y)^T$ and possibly complex amplitudes u_o, v_o, η_o . If you put this in, you get

$$-i\omega u_o = f v_o - g i k_x \hat{\eta}, \quad (16.93)$$

$$-i\omega v_o = -f u_o - g i k_y \hat{\eta}, \quad (16.94)$$

$$-i\omega \hat{\eta} = -H i k_x u_o - H i k_y v_o \quad (16.95)$$

$$\Leftrightarrow -i\omega u_o - f v_o + g i k_x \hat{\eta} = 0, \quad (16.96)$$

$$-i\omega v_o + f u_o + g i k_y \hat{\eta} = 0, \quad (16.97)$$

$$-i\omega \hat{\eta} + H i k_x u_o + H i k_y v_o = 0. \quad (16.98)$$

In matrix notation this is:

$$\begin{pmatrix} -i\omega & -f & g i k_x \\ f & -i\omega & g i k_y \\ H i k_x & H i k_y & -i\omega \end{pmatrix} \begin{pmatrix} u_o \\ v_o \\ \hat{\eta} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \quad (16.99)$$

Non-trivial solutions exist here if and only if

$$\begin{aligned} &\Leftrightarrow (-i\omega) \left[(-i\omega)^2 - f^2 H g k_y^2 \right] - f \left[-f(-i\omega) - f^2 H g k_x k_y \right] + H i k_x \left[-f g i k_y - (-i\omega) g i k_x \right] = 0 \\ &\Leftrightarrow (-i\omega) \left[(-i\omega)^2 + H g k_y^2 \right] - f \left[-f(-i\omega) + H g k_x k_y \right] + H i k_x \left[-f g i k_y - (-i\omega) g i k_x \right] = 0 \\ &\Leftrightarrow i\omega \left[-(-i\omega)^2 - H g k_y^2 \right] + f \left[f(-i\omega) - H g k_x k_y \right] + H i k_x \left(-f g i k_y + i\omega g i k_x \right) = 0 \\ &\Leftrightarrow i\omega \left[-(i\omega)^2 - H g k_y^2 \right] + f \left(-f i\omega - H g k_x k_y \right) + H i k_x \left(-f g i k_y - \omega g k_x \right) = 0 \\ &\Leftrightarrow i\omega \left(\omega^2 - H g k_y^2 \right) + f \left(-f i\omega - H g k_x k_y \right) + H i k_x \left(-f g i k_y - \omega g k_x \right) = 0 \\ &\Leftrightarrow \omega \left(\omega^2 - H g k_y^2 \right) + f \left(-f\omega + i H g k_x k_y \right) + H k_x \left(-f g i k_y - \omega g k_x \right) = 0 \\ &\Leftrightarrow \omega \left(\omega^2 - H g k_y^2 \right) - f^2 \omega + f i H g k_x k_y - H k_x f g i k_y - H k_x \omega g k_x = 0 \\ &\Leftrightarrow \omega \left(\omega^2 - H g k_y^2 \right) - f^2 \omega - H k_x \omega g k_x = 0 \\ &\Leftrightarrow \omega \left(\omega^2 - H g k_y^2 - f^2 - H g k_x^2 \right) = 0 \\ &\Leftrightarrow \omega \left[\omega^2 - f^2 - H g \left(k_x^2 + k_y^2 \right) \right] = 0 \end{aligned} \quad (16.100)$$

applies. So the dispersion relation of Poincaré waves is:

$$\omega \left(\omega^2 - f^2 - H g k^2 \right) = 0. \quad (16.101)$$

This equation has the three solutions

$$\omega = 0, \quad (16.102)$$

$$\omega = \sqrt{f^2 + H g k^2}, \quad (16.103)$$

$$\omega = -\sqrt{f^2 + H g k^2}. \quad (16.104)$$

Eq. (16.102) is the geostrophic mode, the other two equations describe Poincaré waves in the true sense. Eq. (16.104) describes a wave propagating in the direction $-\mathbf{k}$ and is therefore not a physically new wave mode. For these propagating solutions $\omega^2 \geq f^2$ applies, so the magnitude of the Coriolis parameter is a lower bound of the angular frequency. applies to the phase speed

$$c^2 = \frac{\omega^2}{k^2} = gH + \frac{f^2}{k^2} = gH + f^2 L^2 \frac{1}{4\pi^2} \quad (16.105)$$

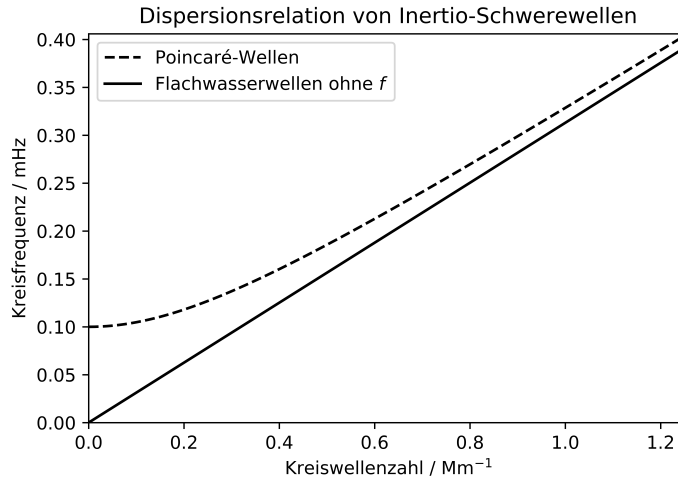


Figure 16.1: The dispersion relation of Poincaré waves compared to the dispersion of shallow water waves without Coriolis acceleration. $f = 10^{-4} \text{ 1/s}$ and $H = 10 \text{ km}$ were calculated.

with L as the wavelength. The Poincaré waves therefore have a higher phase speed than gravity waves without the rotation of the earth. The shorter the waves become, the smaller the influence of the Coriolis force becomes, but for long waves ω goes towards f . The expression for c^2 of the Poincaré waves is higher than that of gravity waves without Coriolis force by the expression $f^2 L^2 \frac{1}{4\pi^2}$. To determine a cutoff wavelength R_o from which the effect of the Coriolis force becomes clear, one sets

$$f_o^2 R_o^2 \frac{1}{4\pi^2} = \frac{gH}{4\pi^2} \approx 0,025gH. \quad (16.106)$$

This gives the barotropic Rossby radius

$$R_o = \frac{\sqrt{gH}}{|f|}. \quad (16.107)$$

If you use typical values, $R_o \approx 2000 \text{ km}$ follows.

Poincaré waves are also known in English as *inertia-gravity waves*. This is because the restoring forces in this wave mode are gravity and the Coriolis force. The German translation „Inertial gravity wave“ is rather unusual. Another name is *Sverdrup wave*.

16.5.4 Kelvin waves

One starts again from the system of equations (16.89) - (16.91), but this time one imagines the half-plane $x < 0$ as a coast, so that only the remaining half-plane $x \geq 0$ can be flowed by the fluid. So the boundary condition is:

$$u(x=0) = 0. \quad (16.108)$$

We are now looking for solutions that fulfill this globally. To do this, we start again from the f -plane. The system of equations reduces to

$$0 = -g \frac{\partial \eta}{\partial x} + fv, \quad (16.109)$$

$$\frac{\partial v}{\partial t} = -g \frac{\partial \eta}{\partial y}, \quad (16.110)$$

$$\frac{\partial \eta}{\partial t} + H \frac{\partial v}{\partial y} = 0. \quad (16.111)$$

From Eq. (16.109) it follows that v is geostrophically balanced, so one can eliminate v from the remaining two equations:

$$\frac{\partial^2 \eta}{\partial t \partial x} = -f \frac{\partial \eta}{\partial y}, \quad (16.112)$$

$$\frac{\partial \eta}{\partial t} + H \frac{g}{f} \frac{\partial^2 \eta}{\partial x \partial y} = 0. \quad (16.113)$$

Here you do the harmonic wave approach

$$\eta = \eta_0 \exp [i (k_x x + k_y y - \omega t)], \quad (16.114)$$

from which follows

$$-i \omega k_x = -f i k_y \Rightarrow \omega k_x = -f k_y, \quad (16.115)$$

$$-i \omega + H \frac{g}{f} i k_x i k_y = 0 \Rightarrow i \omega = -H \frac{g}{f} k_x k_y. \quad (16.116)$$

From Eq. (16.115) follows

$$k_x = -\frac{i}{\omega} f k_y, \quad (16.117)$$

what in Eq. (16.116) is used

$$i \omega = -H \frac{g}{f} k_y \left(-\frac{i}{\omega} f k_y \right) = i H \frac{g}{\omega} k_y^2 \quad (16.118)$$

results. Define κ by

$$\kappa := \frac{\omega}{\sqrt{gH}} > 0 \quad (16.119)$$

with an angular frequency $\omega > 0$ assumed to be positive, follows

$$k_y = \pm \kappa. \quad (16.120)$$

This results in transformed

$$\omega = \pm \kappa \sqrt{gH}. \quad (16.121)$$

With Eq. (16.115) follows

$$k_x = \mp i f \frac{1}{\sqrt{gH}}. \quad (16.122)$$

η must not increase exponentially as a function of the distance from the coast, therefore when $f > 0$ the negative sign in Eq. (16.120), at $f < 0$ the positive. In the northern hemisphere the Kelvin wave has the coast to the right of the direction of propagation, in the southern hemisphere to the left.

The penetration lengths l of the Kelvin waves are:

$$l = l(f, H) = \frac{2\pi \sqrt{gH}}{|f|} = 2\pi R_o \quad (16.123)$$

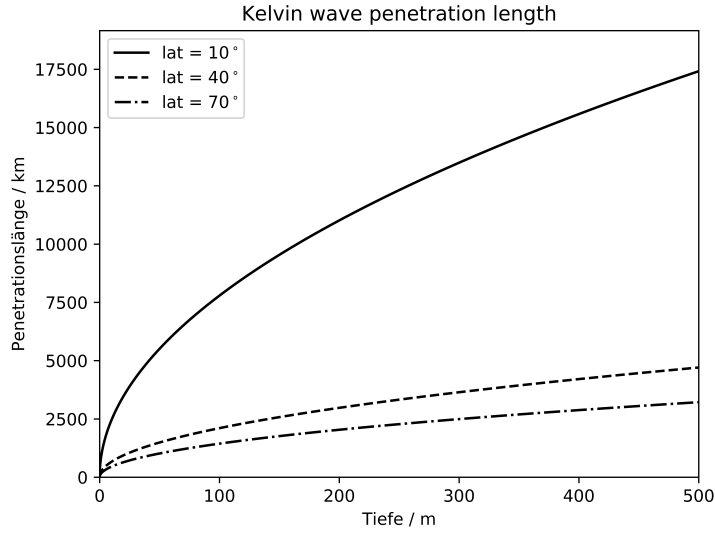


Figure 16.2: Penetration lengths of Kelvin waves.

with that in Eq. (16.107) defined Rossby radius R_o .

Fig. 16.2 shows the typical penetration lengths of Kelvin waves, which are quickly in the range of 1000 - 10000 km, i.e. in the range of ten to several hundred percent of a quarter of the earth's circumference. This extension far exceeds the validity of the f-plane.

16.5.4.1 Equatorial Kelvin waves

At the equator you cannot set $f = f_o$, you set the β plane instead

$$f = \beta y \quad (16.124)$$

with

$$\beta := \left. \frac{\partial f}{\partial y} \right|_{\varphi=0} \quad (16.125)$$

to. The equations are therefore (16.89) - (16.91)

$$\frac{\partial u}{\partial t} = -g \frac{\partial \eta}{\partial x} + \beta y v, \quad (16.126)$$

$$\frac{\partial v}{\partial t} = -g \frac{\partial \eta}{\partial y} - \beta y u, \quad (16.127)$$

$$\frac{\partial \eta}{\partial t} + H \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = 0. \quad (16.128)$$

Now you look for solutions with $v = 0$. In this case applies

$$\frac{\partial u}{\partial t} = -g \frac{\partial \eta}{\partial x}, \quad (16.129)$$

$$0 = -g \frac{\partial \eta}{\partial y} - \beta y u, \quad (16.130)$$

$$\frac{\partial \eta}{\partial t} + H \frac{\partial u}{\partial x} = 0. \quad (16.131)$$

Over

$$u = -\frac{g}{\beta y} \frac{\partial \eta}{\partial y} \quad (16.132)$$

u can be eliminated:

$$-\frac{g}{\beta y} \frac{\partial^2 \eta}{\partial t \partial y} = -g \frac{\partial \eta}{\partial x} \quad (16.133)$$

$$\frac{\partial \eta}{\partial t} - \frac{gH}{\beta y} \frac{\partial^2 \eta}{\partial x \partial y} = 0 \quad (16.134)$$

The approach

$$\eta = \hat{\eta} \exp [i (k_x x + k_y y - \omega t)] \quad (16.135)$$

performs

$$-\frac{g}{\beta y} k_y \omega = -g i k_x \Rightarrow k_y = \frac{i}{\omega} \beta y i k_x, \quad (16.136)$$

$$-i\omega + \frac{gH}{\beta y} k_x k_y = 0 \Rightarrow \omega^2 = gH k_x^2. \quad (16.137)$$

So it applies

$$k_x = \pm \frac{\omega}{\sqrt{gH}}. \quad (16.138)$$

For k_y follows

$$k_y = \frac{i}{\omega} \beta y i k_x = \pm i \frac{\beta y}{\sqrt{gH}}. \quad (16.139)$$

Only the plus sign comes into question. So the solution is

$$\eta = \hat{\eta} \exp \left[i \left(k_x x + i \frac{\beta y^2}{\sqrt{gH}} - \sqrt{gH} k_x t \right) \right]. \quad (16.140)$$

To estimate the meridional extent y_o of these waves, one sets

$$1 = \frac{2\omega y_o^2}{\sqrt{gH}} \quad (16.141)$$

to. From this it follows

$$y_o = \sqrt{R \frac{\sqrt{gH}}{2\omega}} = 2071 \text{ km} \quad (16.142)$$

with R as the equatorial radius and $H = 1 \text{ km}$.

16.5.5 Rossby-Haurwitz fashions

Rossby-Haurwitz modes are the eigenmodes of the barotropic vorticity equation Eq. (15.92) on the sphere. Therefore, the notation from section 15.1.3.6 is adopted in this section. Spherical surface functions $Y_{l,m}(\varphi, \lambda)$ with $l \geq 0$

and $-l \leq m \leq l$ satisfy

$$\Delta Y_{l,m} \stackrel{\text{Glg. (C.166)}}{=} -\frac{l(l+1)}{a^2} Y_{l,m}. \quad (16.143)$$

Do the approach for the current function $\psi = \psi(\varphi, \lambda, t)$

$$\psi = Y_{l,m} e^{-i\omega t}, \quad (16.144)$$

follows from this

$$J(\zeta, \psi) = J(\Delta\psi, \psi) \propto \frac{\partial\psi}{\partial\lambda} \frac{\partial\psi}{\partial\varphi} - \frac{\partial\psi}{\partial\varphi} \frac{\partial\psi}{\partial\lambda} = 0. \quad (16.145)$$

If you put Eq. (16.144) into the barotropic vorticity equation in the form Eq. (15.101), you get

$$\begin{aligned} \Delta \frac{\partial\psi}{\partial t} &= -\frac{\partial\psi}{a \cos(\varphi)} \frac{\partial}{\partial\lambda} \beta + \frac{1}{a^2 \cos(\varphi)} J(\Delta\psi, \psi) = -\frac{\partial\psi}{a \cos(\varphi)} \frac{\partial}{\partial\lambda} \beta \\ \Delta \frac{\partial\psi}{\partial t} &= -\frac{\partial\psi}{a^2 \cos(\varphi)} \frac{\partial}{\partial\lambda} 2\omega \cos(\varphi) = -\frac{\partial\psi}{a^2 \partial\lambda} 2\Omega \\ \Rightarrow -i\omega l \frac{l(l+1)}{a^2} &= -\frac{2\Omega}{a^2} im \\ \Rightarrow \omega \frac{l(l+1)}{a^2} &= \frac{2\Omega}{a^2} m \end{aligned} \quad (16.146)$$

From this follows the dispersion relation of the Rossby-Haurwitz modes:

$$\omega(l, m) = \frac{m}{l(l+1)} 2\Omega \quad (16.147)$$

In the case $l = 0$, $m = 0$ and Eq. (16.146) is satisfied for every ω . From Eq. (16.147) follows

$$-\frac{1}{(l+1)} 2\Omega \leq \omega(l, m) \leq \frac{1}{(l+1)} 2\Omega. \quad (16.148)$$

For the phase velocity (expressed as zonal angular velocity) one obtains

$$\frac{\omega}{\frac{2\pi}{\Delta\lambda}} = \frac{\omega \Delta\lambda}{2\pi} = \frac{\omega 2\pi}{2\pi m} = \frac{\omega}{m} = \frac{1}{l(l+1)} 2\Omega > 0. \quad (16.149)$$

Rossby-Haurwitz fashions always propagate to the East. Using Eq. (15.139), which is

$$\Delta\Phi = \beta \frac{\partial\psi}{\partial y} + f\Delta\psi, \quad (16.150)$$

The geopotential Φ can be determined from ψ . First you set a Rossby-Haurwitz fashion

$$\psi = \psi_0 Y_{l,m} e^{-i\omega t} \quad (16.151)$$

one, this implies

$$\begin{aligned} \Delta\Phi &= \frac{2\Omega \cos(\varphi)}{a^2 \cos(\varphi)} \frac{\partial\psi}{\partial\varphi} - \frac{2\Omega \sin(\varphi)}{a^2} l(l+1) \psi_0 Y_{l,m} e^{-i\omega t} \\ \Rightarrow \Delta\Phi &= \frac{2\Omega}{a^2} \frac{\partial\psi}{\partial\varphi} - \frac{2\Omega \sin(\varphi)}{a^2} l(l+1) \psi_0 Y_{l,m} e^{-i\omega t}. \end{aligned} \quad (16.152)$$

The approach is now made for the geopotential Φ

$$\Phi = \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \Phi_{l',m'} Y_{l',m'}. \quad (16.153)$$

If you put this in, you get

$$\begin{aligned} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} -\frac{l'(l'+1)}{a^2} \Phi_{l',m'} Y_{l',m'} &= \frac{2\Omega}{a^2} \frac{\partial \psi}{\partial \varphi} - \frac{2\Omega \sin(\varphi)}{a^2} l(l+1) \psi_0 Y_{l,m} e^{-i\omega t} \\ \Rightarrow \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} -l'(l'+1) \Phi_{l',m'} Y_{l',m'} &= 2\Omega \frac{\partial \psi}{\partial \varphi} - 2\Omega \sin(\varphi) l(l+1) \psi_0 Y_{l,m} e^{-i\omega t}. \end{aligned} \quad (16.154)$$

Eq. (C.180) is

$$\sin(\varphi) Y_{l,m} = \sqrt{\frac{l^2 - m^2}{4l^2 - 1}} Y_{l-1,m} + \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} Y_{l+1,m}. \quad (16.155)$$

This implies

$$\sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} -l'(l'+1) \Phi_{l',m'} Y_{l',m'} = 2\Omega \frac{\partial \psi}{\partial \varphi} - 2\Omega l(l+1) \psi_0 \left[\sqrt{\frac{l^2 - m^2}{4l^2 - 1}} Y_{l-1,m} + \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} Y_{l+1,m} \right] e^{-i\omega t}. \quad (16.156)$$

16.5.6 Barotropic Rossby waves

In section 16.5.3 $\beta = 0$ was assumed. In this case, the Poincaré waves derived there are the most general wave solutions. A new type of waves arises when the width dependence of f is taken into account.

One assumes a homogeneous zonal base current U . One assumes $u_0 = 0$, and one also assumes $k_y = 0$, the disturbances should only be x -dependent. You already know:

- Since U is homogeneous and $u_0 = 0$, $v = v(x, t)$, the solutions are divergence-free.

Therefore one can use the barotropic vorticity equation. You do the approach

$$v = v_0 \exp[i(kx - \omega t)] \quad (16.157)$$

then apply

$$\zeta = ikv, \quad \frac{\partial \zeta}{\partial t} = k\omega v, \quad \frac{\partial \zeta}{\partial x} = -k^2 v. \quad (16.158)$$

Plugging this into the barotropic vorticity equation you get

$$k\omega v_0 = Uk^2 v_0 - v_0 \beta \Leftrightarrow \omega = Uk - \frac{\beta}{k}. \quad (16.159)$$

Eq. (16.159) is the dispersion relation of barotropic Rossby waves. If they span a complete circle of latitude, they are also referred to as *planetary waves*.

The following applies to the phase velocity of barotropic Rossby waves

$$c = U - \frac{\beta}{k^2}. \quad (16.160)$$

In the hypothetical case $U \rightarrow 0$, $L = 2\pi a$ and $\varphi = 0$ holds

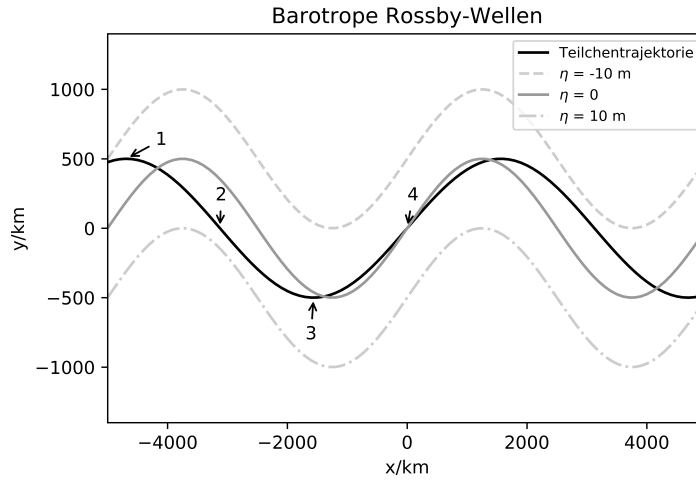


Figure 16.3: Illustration of the principle of conservation of absolute vorticity. 1: f maximum, ζ minimum, 2: $f = f_0$, $\zeta = 0$, 3: f minimum, ζ maximum, 4: $f = f_0$, $\zeta = 0$. Note also that the wavelength of the particle trajectory is larger than that of the wave.

$$|c| = 2\omega \frac{1}{a} \frac{4\pi^2 a^2}{4\pi^2} = 2\omega a = 930 \frac{\text{m}}{\text{s}}. \quad (16.161)$$

This is an amount limit of c . No wave can propagate faster than the speed $2\omega a$, and the system of governing equations cannot transmit information faster.

16.5.6.1 Clear understanding

The y component of the momentum equation in the shallow water model is

$$\frac{Dv}{Dt} = -fu - g \frac{\partial \eta}{\partial y}. \quad (16.162)$$

Do a linear Taylor expansion for f

$$f = f_0 + \beta y. \quad (16.163)$$

A homogeneous zonal base current U can be geostrophically balanced by surface deflection

$$0 = -f_0 U - g \frac{\partial \eta}{\partial y}. \quad (16.164)$$

In this case, Eq. (16.162) to

$$\frac{D^2 y}{Dt^2} = -\beta U y. \quad (16.165)$$

This corresponds to a harmonic oscillator with the natural frequency

$$\omega_{\text{ind}} = \sqrt{\beta U}. \quad (16.166)$$

Therefore $U > 0$ must be western. The natural frequency was marked with an index ind because it is the individual oscillation frequency of the particles and not the frequency ω of the wave.

Another clear explanation comes from the barotropic vorticity equation, which is:

$$f + \zeta = \text{const.} \quad (16.167)$$

If a particle is deflected northward from its resting position in the northern hemisphere when there is a western background current, then f increases. Therefore ζ must decrease and the particle acquires anticyclonic relative vorticity. It then oscillates southward beyond its rest position, with f decreasing. Therefore, the particle acquires cyclonic relative vorticity and veers northward again. The mechanism of barotropic Rossby waves is the conservation of absolute vorticity, see also Fig. 16.3.

Barotropic Rossby waves are relevant in the atmosphere and ocean despite the extensive simplifications (barotropy and freedom from divergence). In the atmosphere, due to their freedom from divergence, they are most applicable to the middle troposphere and provide a simple view of the meandering polar jet. The term wave number is often used here; a wave of wave number n has a zonal spatial period of $\frac{2\pi}{n}$ as an angle. Rossby waves always propagate westward in the ocean due to the small easterly (east-facing) base current (it is $\beta \geq 0$ over the entire Earth).

16.5.7 Oceanic tide

The oceanic tide is a global phenomenon, so advection ($\propto \mathbf{1}/\lambda$) can be neglected. Barotropy can also be assumed. Therefore, the linear shallow water equations Equations (13.173) - (13.174) are used as an equation system. These are in components

$$\frac{\partial u}{\partial t} = -\frac{\partial (gd + U)}{a \cos(\varphi) \partial \lambda} + 2\Omega \sin(\varphi) v, \quad (16.168)$$

$$\frac{\partial v}{\partial t} = -\frac{\partial (gd + U)}{a \partial \varphi} - 2\Omega \sin(\varphi) u, \quad (16.169)$$

$$\frac{\partial d}{\partial t} = -D \left(\frac{\partial u}{a \cos(\varphi) \partial \lambda} + \frac{\partial v}{a \partial \varphi} - v \frac{\tan(\varphi)}{a} \right). \quad (16.170)$$

Here $U = U(\varphi, \lambda, t)$ is the *tidal potential*. Ω is the angular velocity of the Earth's rotation. These equations are also known as Laplace's tidal equations (*Laplace's tidal equations (LTEs)*). The approach is taken here

$$u = \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{u}_{l,m} Y_{l,m}(\varphi, \lambda) e^{-i\omega t}, \quad v = \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{v}_{l,m} Y_{l,m}(\varphi, \lambda) e^{-i\omega t}, \quad (16.171)$$

$$d = \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{d}_{l,m} Y_{l,m}(\varphi, \lambda) e^{-i\omega t}, \quad U = \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{U}_{l,m} Y_{l,m}(\varphi, \lambda) e^{-i\omega t}, \quad (16.172)$$

Here $Y_{l,m}(\varphi, \lambda)$ are spherical surface functions, see section C.5. They apply

$$\frac{\partial Y_{l,m}}{\partial \varphi} \stackrel{\text{Glg. (C.167)}}{=} -m \tan(\varphi) Y_{l,m} - \sqrt{l^2 - m^2 + l - m} Y_{l,m+1} \exp(-i\lambda), \quad (16.173)$$

$$\frac{\partial Y_{l,m}}{\partial \lambda} \stackrel{\text{Glg. (C.168)}}{=} i m Y_{l,m}, \quad (16.174)$$

$$\sin(\varphi) Y_{l,m} \stackrel{\text{Glg. (C.171)}}{=} \sqrt{\frac{l^2 - m^2}{4l^2 - 1}} Y_{l-1,m} + \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} Y_{l+1,m}. \quad (16.175)$$

With the abbreviations

$$f_{l,m} = \sqrt{l^2 - m^2 + l - m}, \quad g_{l,m} = \sqrt{\frac{l^2 - m^2}{4l^2 - 1}}, \quad h_{l,m} = \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} \quad (16.176)$$

you can do this in the form

$$\frac{\partial Y_{l,m}}{\partial \varphi} \stackrel{\text{Glg. (C.178)}}{=} -m \tan(\varphi) Y_{l,m} - f_{l,m} Y_{l,m+1} \exp(-i\ell), \quad (16.177)$$

$$\frac{\partial Y_{l,m}}{\partial \lambda} \stackrel{\text{Glg. (C.179)}}{=} im Y_{l,m}, \quad (16.178)$$

$$\sin(\varphi) Y_{l,m} \stackrel{\text{Glg. (C.180)}}{=} g_{l,m} Y_{l-1,m} + h_{l,m} Y_{l+1,m} \quad (16.179)$$

note down. Put all of this into the LTEs and you get

$$\begin{aligned} & -i\omega \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{u}_{l,m} Y_{l,m} \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^l -im \frac{g\tilde{d}_{l,m} + \tilde{U}_{l,m}}{a \cos(\varphi)} Y_{l,m} + \mathbf{z} \Omega \tilde{v}_{l,m} (g_{l,m} Y_{l-1,m} + h_{l,m} Y_{l+1,m}), \end{aligned} \quad (16.180)$$

$$\begin{aligned} & -i\omega \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{v}_{l,m} Y_{l,m} \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{g\tilde{d}_{l,m} + \tilde{U}_{l,m}}{a} (m \tan(\varphi) Y_{l,m} + f_{l,m} Y_{l,m+1} \exp(-i\ell)) - \mathbf{z} \Omega \tilde{u}_{l,m} (g_{l,m} Y_{l-1,m} + h_{l,m} Y_{l+1,m}), \end{aligned} \quad (16.181)$$

$$\begin{aligned} & -i\omega \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{d}_{l,m} Y_{l,m} \\ &= -\frac{D}{a} \sum_{l=0}^{\infty} \sum_{m=-l}^l im \frac{\tilde{u}_{l,m}}{\cos(\varphi)} Y_{l,m} - \tilde{v}_{l,m} (m \tan(\varphi) Y_{l,m} + f_{l,m} Y_{l,m+1} \exp(-i\ell)) - \tilde{v}_{l,m} \tan(\varphi) Y_{l,m} \\ &= -\frac{D}{a} \sum_{l=0}^{\infty} \sum_{m=-l}^l im \frac{\tilde{u}_{l,m}}{\cos(\varphi)} Y_{l,m} - \tilde{v}_{l,m} [(m + \mathbf{1}) \tan(\varphi) Y_{l,m} + f_{l,m} Y_{l,m+1} \exp(-i\ell)]. \end{aligned} \quad (16.182)$$

Coastlines, bathymetry and ground friction modify this significantly.

16.5.7.1 Clear understanding

In contrast to many clear illustrations, it is less the vertical but predominantly the horizontal component of $-\nabla U$ that is relevant for the oceanic tide. However, what is somewhat counterintuitive is the fact that in most places it is not the period ~ 25 hours that predominates, but rather the first harmonic of the lunar tide with a period of ~ 12.5 hours. To understand this clearly, place a KS at the center of the earth and align the negative x-axis with the moon. Lunar quantities (relative to the moon) are denoted by the index l and terrestrial quantities by the index t . For the x-coordinate x_S of the center of gravity one obtains

$$x_S = \frac{m_l x_l + m_t x_t}{m_l + m_t} = \frac{m_l x_l}{m_l + m_t} = \frac{\mathbf{1}}{\mathbf{1} + \frac{m_t}{m_l}} x_l = -\mathbf{o}, 73a. \quad (16.183)$$

The center of gravity of the moon and earth is therefore within the earth. At point $x = -a$, the tidal force $\mathbf{f}_T$ is directed towards the moon. At $x = a$ applies

$$f_{T,x} = \omega_l^2 (a - x_S) - \frac{Gm_l}{(a - x_l)^2} = \mathbf{1}, 73\omega_l^2 a - \frac{Gm_l}{(a - x_l)^2}. \quad (16.184)$$

ω_l is the angular velocity of the moon's rotation around the earth. It is easy to verify that

$$f_{T,x} > \mathbf{o} \quad (16.185)$$

applies. At the two points considered so far, the tidal force has no horizontal component. If you move away from these points, the horizontal tidal force is directed towards these points. This implies that there must be another point on every semicircle between $x = -a$ and $x = a$ where $\mathbf{f}_T = -\nabla U$ has no horizontal component. This suggests that the period ~ 12.5 hours is more dominant than the lunar fundamental period.

16.6 Baroclinic waves

16.6.1 Vertical modes

Here we assume a flat subsurface at a depth of $z = -D < 0$ and demand the boundary conditions

$$w(z = 0) = 0, \quad (16.186)$$

$$w(z = -D) = 0. \quad (16.187)$$

The following system of equations is used, whereby one of A. starts from a wave propagating in the x direction:

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p'}{\partial x}, \quad (16.188)$$

$$\frac{\partial w}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p'}{\partial z}, \quad (16.189)$$

$$\frac{\partial \rho'}{\partial t} = -\rho_0 \frac{\partial u}{\partial x} - \rho_0 \frac{\partial w}{\partial z}. \quad (16.190)$$

Here is

$$\rho = \rho_0 + \rho' \quad (16.191)$$

with a homogeneous background density ρ_0 and a fluctuation ρ' . Analogously, one decomposes the pressure p , where should apply

$$\frac{\partial p_0}{\partial z} = -g\rho_0. \quad (16.192)$$

You now make the approaches

$$u = U(z) \exp(ikx - i\omega t), \quad v = V(z) \exp(ikx - i\omega t), \quad (16.193)$$

$$p' = P(z) \exp(ikx - i\omega t), \quad \rho' = \tilde{\rho}(z) \exp(ikx - i\omega t). \quad (16.194)$$

If you insert this into the applicable system of equations, it follows

$$-i\omega U = -\frac{ikP}{\rho_0} \Rightarrow \omega U = \frac{kP}{\rho_0}, \quad (16.195)$$

$$-i\omega W = -\frac{P'}{\rho_0} \Rightarrow \omega W = -i\frac{P'}{\rho_0}, \quad (16.196)$$

$$-i\omega \tilde{\rho} = -\rho_0 ikU - \rho_0 W' \Rightarrow \omega \tilde{\rho} = \rho_0 kU - i\rho_0 W'. \quad (16.197)$$

The third equation is always satisfiable, $\tilde{\rho}(z)$ can be chosen accordingly. For W you do the approach

$$W(z) = \hat{w} \sin\left(n\pi \frac{z}{D}\right) \quad (16.198)$$

with $n \geq 1$. From Eq. (16.196) follows

$$P' = \rho_0 i\omega \hat{w} \sin\left(n\pi \frac{z}{D}\right). \quad (16.199)$$

Therefore you bet for P

$$P(z) = -\frac{D\rho_0 i\omega \hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) \quad (16.200)$$

to. Putting this into Eq. (16.196) follows

$$U(z) = \frac{kP}{\omega \rho_o} = -\frac{ki\hat{w}D}{n\pi} \cos\left(n\pi \frac{z}{D}\right). \quad (16.201)$$

So it applies

$$\begin{aligned} u(x, z, t) &= \frac{Dk\hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) \exp\left[i\left(kx - \omega t - \frac{\pi}{2}\right)\right] \\ \Rightarrow u(x, z, t) &= -i \frac{Dk\hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) \exp[i(kx - \omega t)] \\ \Rightarrow u(x, z, t) &= -i \frac{Dk\hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) [\cos(kx - \omega t) + i\sin(kx - \omega t)] \\ \Rightarrow u(x, z, t) &= \frac{Dk\hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) [-i\cos(kx - \omega t) + \sin(kx - \omega t)] \\ \Rightarrow \Re(u(x, z, t)) &= \frac{Dk\hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) \sin(kx - \omega t). \end{aligned} \quad (16.202)$$

The horizontal divergence δ at the surface results in

$$\delta(z = 0) = \frac{\partial \Re(u(x, z, t))}{\partial x} = \frac{Dk^2 \hat{w}}{n\pi} \cos\left(n\pi \frac{z}{D}\right) \cos(kx - \omega t). \quad (16.203)$$

Vertical modes therefore lead to alternating stripes of divergence and convergence at the surface. In the area of convergence, the surface waves are compressed horizontally, which destabilizes the wave field. Conversely, the wave field is stabilized in the area of divergence, which also contributes to the fact that in this area the water comes from the depths to the surface and this water has not yet been exposed to the effects of wind.

The mode $n = 0$ is also called external mode because it has no internal vertical structure.

16.6.2 Gravity waves

Baroclinic gravity waves are the baroclinic analogue of Poincaré waves. First you make a perturbation of the shape

$$u = U + u', \quad v = v', \quad w = w', \quad (16.204)$$

$$p = p_o(z) + p', \quad \theta = \theta_o(z) + \theta', \quad f = f_o. \quad (16.205)$$

Because of Eq. (16.205) is Eq. (16.204) no restriction of the background current to the x-direction; by rotating the coordinate system around the vertical axis, the background wind can assume any direction. In particular, all curvature terms are neglected and one can use Cartesian coordinates (x, y, z) . The background state is supposed to be hydrostatic, so

$$\frac{\partial p_o}{\partial z} = -g\rho_o(z) \quad (16.206)$$

fulfill. A dry adiabatic system is assumed; in such a system the first law of thermodynamics becomes true

$$\frac{D\theta}{Dt} = 0 \quad \Leftrightarrow \quad \frac{D\theta}{Dt} + \frac{D\theta'}{Dt} = 0 \quad \Leftrightarrow \quad \frac{D\theta'}{Dt} + w' \frac{d\theta_o}{dz} = 0. \quad (16.207)$$

One now introduces an approximate material derivation $\tilde{\frac{D}{Dt}}$ in which disturbing products are neglected. Equal signs are noted below for this purpose. This gives you

$$\frac{\tilde{D}\theta'}{Dt} + w' \frac{d\theta_o}{dz} = 0. \quad (16.208)$$

If you multiply this equation by $\frac{g}{\theta_o}$, it follows

$$\frac{\tilde{D}b'}{Dt} + w' \frac{g}{\theta_o} \frac{d\theta_o}{dz} = 0, \quad (16.209)$$

where the definition of the so-called *buoyancy*

$$b' := g \frac{\theta'}{\theta_o} \quad (16.210)$$

was used. From Eq. (16.253) can be seen

$$\frac{g}{\theta_o} \frac{d\theta_o}{dz} = N^2, \quad (16.211)$$

what on

$$\frac{\tilde{D}b'}{Dt} + w' N^2 = 0 \quad (16.212)$$

leads. With Eq. (9.69) is obtained

$$\begin{aligned} \frac{Dp}{Dt} + \frac{c^{(p)}}{c^{(V)}} p \nabla \cdot \mathbf{v} &= 0 \\ \Leftrightarrow \frac{1}{\kappa p} \frac{Dp}{Dt} + \nabla \cdot \mathbf{v} &= 0 \\ \Leftrightarrow \frac{1}{\kappa \rho R_d T} \frac{Dp}{Dt} + \nabla \cdot \mathbf{v} &= 0. \end{aligned} \quad (16.213)$$

With Eq. (16.42) this can be expressed in terms of the speed of sound:

$$\frac{1}{c_s^2 \rho} \frac{Dp}{Dt} + \nabla \cdot \mathbf{v} = 0 \quad (16.214)$$

If you linearize this equation, you get

$$\begin{aligned} \frac{1}{c_s^2 \rho} \frac{\tilde{D}p}{Dt} + \nabla \cdot \mathbf{v}' &= 0 \\ \Leftrightarrow \frac{1}{c_s^2 \rho_o} \frac{\tilde{D}p'}{Dt} + \frac{1}{c_s^2 \rho_o} w' \frac{dp_o}{dz} + \nabla \cdot \mathbf{v}' &= 0 \\ \Leftrightarrow \frac{1}{c_s^2 \rho_o} \frac{\tilde{D}p'}{Dt} - \frac{g}{c_s^2} w' + \nabla \cdot \mathbf{v}' &= 0. \end{aligned} \quad (16.215)$$

For the vertical equation of motion one obtains using Eq. (13.151)

$$\frac{\tilde{D}w'}{Dt} = -g - \frac{1}{\rho} \frac{\partial p}{\partial z} = -\frac{1}{\rho} \frac{\partial p'}{\partial z} - \left(\frac{1}{\rho} \right)' \frac{\partial p_o}{\partial z} \approx -\frac{1}{\rho_o} \frac{\partial p'}{\partial z} + \frac{\rho'}{\rho_o^2} \frac{\partial p_o}{\partial z} = -\frac{1}{\rho_o} \frac{\partial p'}{\partial z} - \frac{g \rho'}{\rho_o}. \quad (16.216)$$

To express the perturbation in the density through perturbations in the potential temperature and pressure, write down Eq. (9.65) in the form

$$\rho = \frac{p_{\text{ref}}^{R_d/c^{(p)}}}{R_d} \frac{p^{1/\kappa}}{\theta}. \quad (16.217)$$

In the first order, this applies

$$\varrho' = \frac{1}{z} \frac{\varrho_o}{p_o} p' - \frac{\varrho_o}{\theta} \theta' \approx \frac{p'}{c_s^2} - \frac{\varrho_o}{\theta_o} \theta' \quad (16.218)$$

From this it follows

$$\frac{\tilde{D}w'}{Dt} = -\frac{1}{\varrho_o} \frac{\partial p'}{\partial z} - \frac{gp'}{\varrho_o c_s^2} + \frac{g}{\theta_o} \theta' = -\frac{1}{\varrho_o} \frac{\partial p'}{\partial z} - \frac{gp'}{\varrho_o c_s^2} + b'. \quad (16.219)$$

In summary, the linearized system of equations is:

$$\frac{\tilde{D}u'}{Dt} = fv' - \frac{1}{\varrho_o} \frac{\partial p'}{\partial x}, \quad (16.220)$$

$$\frac{\tilde{D}v'}{Dt} = -fu' - \frac{1}{\varrho_o} \frac{\partial p'}{\partial y}, \quad (16.221)$$

$$\frac{\tilde{D}w'}{Dt} = b' - \frac{1}{\varrho_o} \frac{\partial p'}{\partial z} - \frac{g}{c_s^2} \frac{p'}{\varrho_o}, \quad (16.222)$$

$$\frac{\tilde{D}b'}{Dt} = -w' N^2, \quad (16.223)$$

$$\frac{1}{c_s^2 \varrho_o} \frac{\tilde{D}p'}{Dt} = \frac{g}{c_s^2} w' - \nabla \cdot \mathbf{v}'. \quad (16.224)$$

Terms that would disappear with the hydrostatic approximation were marked **blue**, and all terms that would disappear if sound waves were ignored were marked **red**. The vertical dependency on ϱ_o is disturbing. Therefore one defines

$$u'' := \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} u', \quad v'' := \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} v', \quad w'' := \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} w', \quad (16.225)$$

$$b'' := \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} b', \quad p'' := \sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} p'. \quad (16.226)$$

which is called *Bretherton transformation*. The index SFC denotes the values on the earth's surface. The transformation is essentially done by multiplying the system of equations by $\sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}}$. The vertical leads require special attention:

$$\frac{dw'}{dz} = \sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} \frac{dw''}{dz} - \frac{1}{2} \sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} w'' \frac{1}{\varrho_o} \frac{d\varrho_o}{dz} = \sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} \frac{dw''}{dz} + \frac{H}{2} w' \quad (16.227)$$

$$\frac{dp'}{dz} = \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} \frac{dp''}{dz} + \frac{1}{2} \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} p'' \frac{1}{\varrho_o} \frac{d\varrho_o}{dz} = \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} \frac{dp''}{dz} + \frac{1}{2} p' \frac{1}{\varrho_o} \frac{d\varrho_o}{dz} = \sqrt{\frac{\varrho_o}{\varrho_{\text{SFC}}}} \frac{dp''}{dz} - \frac{H}{2} p' \quad (16.228)$$

This was done

$$\frac{1}{\varrho_o} \frac{d\varrho_o}{dz} = -\frac{1}{H} \quad (16.229)$$

with the scale height H used. From this it follows

$$-\frac{\mathbf{I}}{\varrho_o} \frac{\partial p'}{\partial z} = -\sqrt{\frac{\mathbf{I}}{\varrho_o \varrho_{\text{SFC}}}} \frac{dp''}{dz} + \frac{H}{2\varrho_o} p' = -\sqrt{\frac{\mathbf{I}}{\varrho_o \varrho_{\text{SFC}}}} \frac{dp''}{dz} + \frac{H}{2\sqrt{\varrho_o \varrho_{\text{SFC}}}} p'', \quad (16.230)$$

$$-\frac{\partial w'}{\partial z} = -\sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} \frac{dw''}{dz} - \frac{H}{2} w' = -\sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} \frac{dw''}{dz} - \frac{H}{2} \sqrt{\frac{\varrho_{\text{SFC}}}{\varrho_o}} w''. \quad (16.231)$$

In summary, this leads to the following system of equations:

$$\frac{\tilde{D}u''}{Dt} = fv'' - \frac{\mathbf{I}}{\varrho_{\text{SFC}}} \frac{\partial p''}{\partial x} \quad (16.232)$$

$$\frac{\tilde{D}v''}{Dt} = -fu'' - \frac{\mathbf{I}}{\varrho_{\text{SFC}}} \frac{\partial p''}{\partial y} \quad (16.233)$$

$$\frac{\tilde{D}w''}{Dt} = bw'' - \frac{\mathbf{I}}{\varrho_{\text{SFC}}} \frac{\partial p''}{\partial z} + \left(\frac{\mathbf{I}}{2H} - \frac{g}{c_s^2} \right) \frac{p''}{\varrho_{\text{SFC}}}, \quad (16.234)$$

$$\frac{\tilde{D}b''}{Dt} = -w'' N^2 \quad (16.235)$$

$$\frac{\mathbf{I}}{c_s^2 \varrho_{\text{SFC}}} \frac{\tilde{D}p''}{Dt} = \left(\frac{g}{c_s^2} - \frac{\mathbf{I}}{2H} \right) w'' - \nabla_h \cdot \mathbf{v}_h'' - \frac{\partial w''}{\partial z} \quad (16.236)$$

An approach is now made for each of the five occurring variables

$$\psi'' = A_\psi \exp[i(kx + ly + mz - \omega t)], \quad (16.237)$$

where A_ψ can be complex. It applies

$$\frac{\tilde{D}A_\psi}{Dt} = i(Uk - \omega)A_\psi = -i\omega_I A_\psi, \quad (16.238)$$

where the definition of the so-called *intrinsic frequency*

$$\omega_I := \omega - kU \quad (16.239)$$

was used. This is the frequency that would be measured in the coordinate system moving at speed U . If you write down the derived system of equations as a matrix A and neglect the sound wave terms (red terms), you get

$$A \cdot \begin{pmatrix} A_u \\ A_v \\ A_w \\ A_b \\ A_{p/\varrho_{\text{SFC}}} \end{pmatrix} = \begin{pmatrix} -i\omega_I & -f & 0 & 0 & ik \\ f & -i\omega_I & 0 & 0 & il \\ 0 & 0 & -i\omega_I & -\mathbf{I} & im - \frac{1}{2H} \\ 0 & 0 & N^2 & -i\omega_I & 0 \\ ik & il & im + \frac{1}{2H} & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} A_u \\ A_v \\ A_w \\ A_b \\ A_{p/\varrho_{\text{SFC}}} \end{pmatrix} = 0. \quad (16.240)$$

Nontrivial solutions exist if the determinant A of A vanishes:

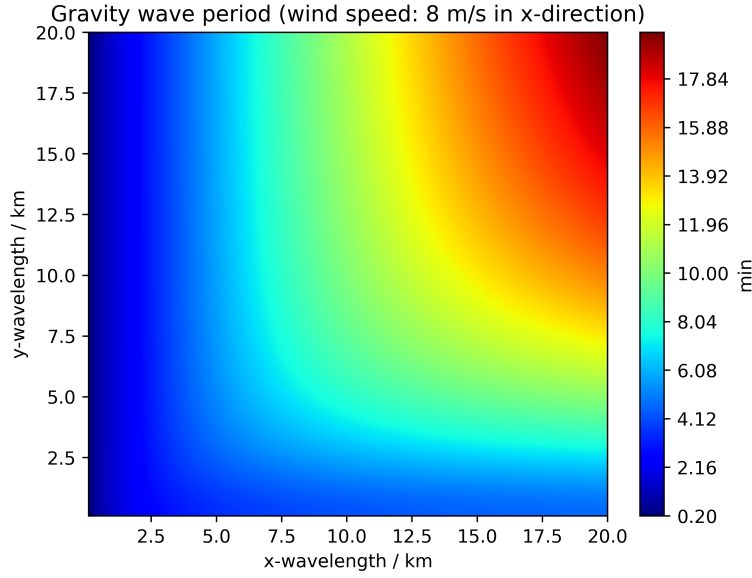


Figure 16.4: Dispersion relation of gravity waves. A vertical wavelength of 2 km was assumed.

$$\begin{aligned}
 A &\stackrel{!}{=} 0 \\
 \Leftrightarrow 0 &= -i\omega_I \left\{ -i\omega_I \left[i\omega_I \left(-m^2 - \frac{1}{4H^2} \right) \right] - il [-i\omega_I^2 l + N^2 il] \right\} \\
 &\quad + f \left\{ f \left[i\omega_I \left(-m^2 - \frac{1}{4H^2} \right) \right] - il [-\omega_I^2 ik + ikN^2] \right\} \\
 &\quad + ik [f(-\omega_I^2 il + ilN^2) - ik(i\omega_I^3 - N^2 i\omega_I)] \\
 \Leftrightarrow 0 &= (f^2 - \omega_I^2) i\omega_I \left(-m^2 - \frac{1}{4H^2} \right) - \omega_I l [-i\omega_I^2 l + N^2 il] + k^2 (i\omega_I^3 - N^2 i\omega_I)
 \end{aligned} \tag{16.241}$$

The magenta colored terms cancel each other out. The geostrophic mode $\omega_I = 0$ is of no further interest here, which is why division by $i\omega_I$ can be done:

$$\begin{aligned}
 0 &= (f^2 - \omega_I^2) \left(-m^2 - \frac{1}{4H^2} \right) + \omega_I^2 l^2 - N^2 l^2 + k^2 (\omega_I^2 - N^2) \\
 \Leftrightarrow \omega_I^2 \left(k^2 + l^2 + m^2 + \frac{1}{4H^2} \right) &= f^2 \left(m^2 + \frac{1}{4H^2} \right) + N^2 (l^2 + k^2)
 \end{aligned}$$

$$\Leftrightarrow \omega_I^2 = \frac{f^2 \left(m^2 + \frac{1}{4H^2} \right) + N^2 (k^2 + l^2)}{m^2 + \frac{1}{4H^2} + k^2 + l^2} \tag{16.242}$$

This is the *Dispersion relation of gravity waves*, this is also visualized in Fig. 16.4. ω_I^2 is a weighted average of the shares f^2 and N^2 with the weighting factors $m^2 + \frac{1}{4H^2}$ and $k^2 + l^2$. So ω_I^2 is always between f^2 and N^2 .

Often one wants to know the period of the expected oscillation as a function of the atmospheric background state (U, N) . The period assuming that the wave vector is parallel to the background wind is shown in Fig. 16.5.

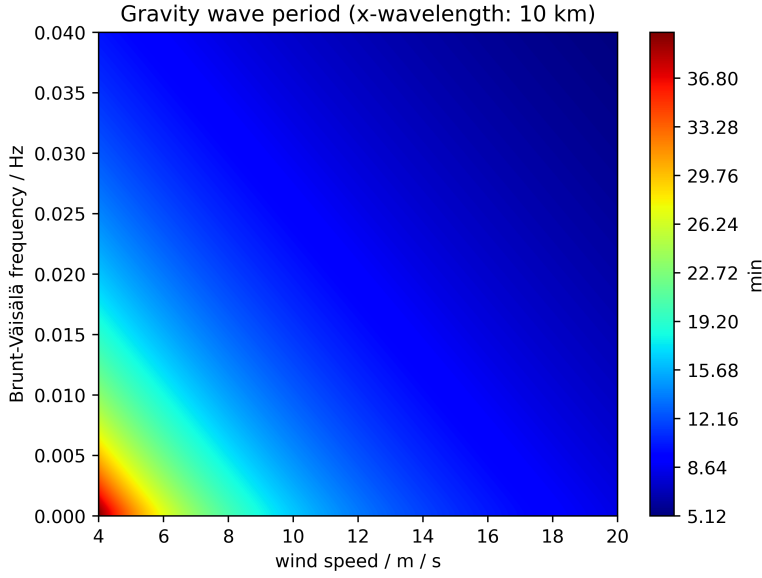


Figure 16.5: Period lengths of gravity waves depending on the atmospheric background state. A vertical wavelength of 2 km and $k_y = 0$ was assumed.

16.6.2.1 Borderline cases

For $k^2 + l^2 \rightarrow 0$ (waves that do not propagate horizontally relative to the base current) one obtains from Eq. (16.242) Inertial waves:

$$\lim_{k^2 + l^2 \rightarrow 0} \omega^2 = f^2 \quad (16.243)$$

For $m^2 + \frac{1}{4H^2} \rightarrow \infty$ one gets from Eq. (16.242) oscillations with frequency N :

$$\lim_{m^2 + \frac{1}{4H^2} \rightarrow \infty} \omega^2 = N^2 \quad (16.244)$$

$H \rightarrow \infty$ can be interpreted as neglecting vertical density fluctuations. $m \rightarrow 0$ means that the wave vector is oriented purely horizontally. These waves arise in a continuous, thermally stable medium when a particle is deflected vertically. A particle of density $\rho_o = \rho(z_o)$ has its rest position at the height z_o , which is shown here above. A. is set to $z_o = 0$. If you deflect the particle vertically, the equation of motion is:

$$\frac{d^2 z}{dt^2} = -\frac{1}{\rho_o} \frac{\partial p}{\partial z} - g = g \frac{\rho}{\rho_o} - g = \frac{g}{\rho_o} (\rho - \rho_o), \quad (16.245)$$

Let $z(t)$ be the deflection. It was assumed that the particle does not change its density during the deflection. If one approximates the deviation $\rho(z) - \rho_o$ using a Taylor expansion

$$\rho(t) - \rho_o = \frac{\partial \rho}{\partial z}(z=0)z, \quad (16.246)$$

this follows for the oscillation equation

$$\frac{d^2 z}{dt^2}(t) = \frac{g}{\rho_o} \frac{\partial \rho}{\partial z} z(t). \quad (16.247)$$

If you set $z = Z_1 \exp(iNt) + Z_2 \exp(-iNt)$, this follows for the angular frequency

$$N^2 = -\frac{g}{\rho} \frac{\partial \rho}{\partial z}, \quad (16.248)$$

N is the *Brunt-Väisälä frequency*, it is a measure of stability. If you insert N into (16.247), you get

$$\frac{d^2 z}{dt^2} = -N^2 z. \quad (16.249)$$

This shows that in the case $N^2 > 0$ a sine wave follows as the solution, while in the case $N^2 < 0$ a real exponential function is the solution because the particle is accelerated away from its origin. In the case $N^2 > 0$ the stratification is *stable*, while in the case $N^2 < 0$ it is *unstable*. Stable stratification is also referred to as strong stratification. In the case $N^2 = 0$ the stratification is *neutral*.

The above derivation is not yet completely complete because incompressibility was assumed. Strictly speaking, it is not the density that is retained during the deflection, but rather the potential density relative to the reference level. If $\tilde{\rho}(z)$ denotes the density of the particle at a deflection z , then equation (16.245) becomes

$$\frac{d^2 z}{dt^2} = \frac{1}{\tilde{\rho}(z)} g \rho(z) - g = \frac{g}{\tilde{\rho}(z)} (\rho(z) - \tilde{\rho}(z)). \quad (16.250)$$

The expression $\rho(z) - \tilde{\rho}(z)$ is the density difference between the surrounding fluid and the particle under consideration. If you bring both systems adiabatic to $z = 0$, then according to Eq. (9.44) for their density difference

$$\Delta \rho = (\rho(z) - \tilde{\rho}(z)) \left(\frac{p_0}{p} \right)^{1/\gamma}. \quad (16.251)$$

Here $p := p(z)$ and $p_0 := p(0)$. In the first order $p = p_0$, $\Delta \rho$ is then the difference of the potential densities with respect to the reference level $z = 0$. Therefore you can also use the potential densities ρ_θ (related to $z = 0$). One obtains in the first order

$$\frac{d^2 z}{dt^2} = \frac{g}{\tilde{\rho}(z)} (\rho_\theta(z) - \rho_\theta(0)) = \frac{g}{\tilde{\rho}(z)} \frac{\partial \rho_\theta}{\partial z} z. \quad (16.252)$$

For the Brunt-Väisälä frequency follows

$$N^2 = -\frac{g}{\rho_\theta} \frac{\partial \rho_\theta}{\partial z}. \quad (16.253)$$

This is the general expression for the Brunt-Väisälä frequency in a compressible medium. N^2 is a field that can depend on all three coordinates and time. The potential density must always be related to the level at which you are. In a dry atmosphere N^2 can also be expressed in terms of the potential temperature θ :

$$\rho_\theta = \frac{p_0}{R_d \theta} \quad (16.254)$$

Thus follows

$$\frac{\partial \rho_\theta}{\partial z} = -\frac{p_0}{R_d \theta^2} \frac{\partial \theta}{\partial z}. \quad (16.255)$$

For the Brunt-Väisälä frequency this means

$$N^2 = \frac{g}{\theta} \frac{\partial \theta}{\partial z}. \quad (16.256)$$

Such waves, which are also referred to in English as *buoyancy oscillations* (the German translation „stratification wave“ is rather unusual) arise, for example, as lee waves behind orography, in this case sinusoidal trajectories

$(ut, z_o \sin(Nt))^T$ result. When saturation is reached, clouds form in the wave crests.

16.6.2.2 Hydrostatic gravity waves

Neglecting the blue terms in Eq. (16.242) provides the *dispersion relation of hydrostatic gravity waves*:

$$\omega_I^2 = f^2 + N^2 \frac{k^2 + l^2}{m^2 + \frac{1}{4H^2}} \quad (16.257)$$

16.6.2.3 Group speed

From this equation it follows

$$\nabla_{\mathbf{k}} \omega_I^2 = \begin{pmatrix} \frac{2N^2 k}{m^2 + \frac{1}{4H^2}} \\ \frac{2N^2 l}{m^2 + \frac{1}{4H^2}} \\ -2m \frac{N^2(k^2 + l^2)}{(m^2 + \frac{1}{4H^2})^2} \end{pmatrix}. \quad (16.258)$$

With $\omega' = \text{sign}(\omega) \sqrt{\omega^2}' = \frac{1}{2\omega} (\omega^2)'$ one obtains for the group velocity of hydrostatic baroclinic gravity waves

$$\mathbf{c}_{\text{gr}} = \frac{1}{\omega_I} \begin{pmatrix} \frac{N^2 k}{m^2 + \frac{1}{4H^2}} \\ \frac{N^2 l}{m^2 + \frac{1}{4H^2}} \\ -m \frac{N^2(k^2 + l^2)}{(m^2 + \frac{1}{4H^2})^2} \end{pmatrix} = \frac{1}{\omega_I} \frac{N^2}{m^2 + \frac{1}{4H^2}} \begin{pmatrix} k \\ l \\ -m \frac{k^2 + l^2}{m^2 + \frac{1}{4H^2}} \end{pmatrix}. \quad (16.259)$$

Horizontally, the group velocity points in the same direction as the phase velocity. Vertically, the two velocities have opposite signs. For the vertical wavelength l_z applies

$$m^2 = \frac{4\pi^2}{l_z^2} \Rightarrow \frac{m^2}{\frac{1}{4H^2}} = \frac{16\pi^2 H^2}{l_z^2} \approx 158 \frac{H^2}{l_z^2}. \quad (16.260)$$

Often applies

$$\frac{m^2}{\frac{1}{4H^2}} \gg 1. \quad (16.261)$$

Under this condition applies

$$\mathbf{c}_{\text{gr}} = \frac{\text{sign}(\omega_I)}{\sqrt{f^2 + \frac{N^2}{m^2}(k^2 + l^2)}} \frac{N^2}{m^2} \begin{pmatrix} k \\ l \\ -\frac{k^2 + l^2}{m} \end{pmatrix} = \frac{\text{sign}(\omega_I)}{\sqrt{f^2 m^2 + N^2(k^2 + l^2)}} \frac{N^2}{m} \begin{pmatrix} k \\ l \\ -\frac{k^2 + l^2}{m} \end{pmatrix} \quad (16.262)$$

$$\Rightarrow \mathbf{c}_{\text{gr}} \cdot \mathbf{k} \propto k^2 + l^2 - (k^2 + l^2) = 0. \quad (16.263)$$

Phase velocity and group velocity are therefore perpendicular to each other.

16.6.2.4 Amplitude behavior

From the Bretherton transformation equations (16.225) - (16.226) and Eq. (16.229) follows

$$u' := \sqrt{\frac{\rho_{\text{SFC}}}{\rho_o}} u'' = \exp\left(\frac{z}{2H}\right) u'', \quad v' := \sqrt{\frac{\rho_{\text{SFC}}}{\rho_o}} v'' = \exp\left(\frac{z}{2H}\right) v'', \quad (16.264)$$

$$w' := \sqrt{\frac{\rho_{\text{SFC}}}{\rho_o}} w'' = \exp\left(\frac{z}{2H}\right) w'', \quad p' := \sqrt{\frac{\rho_o}{\rho_{\text{SFC}}}} p'' = \exp\left(-\frac{z}{2H}\right) p''. \quad (16.265)$$

The amplitude of the movements increases exponentially with height, and the height of the pressure fluctuations decreases exponentially.

16.6.2.5 Lee waves

Lee waves are stationary, i.e. $\omega = 0$. From this it follows

$$\omega_I = \omega - Uk = -Uk \Rightarrow \omega_I^2 = U^2 k^2. \quad (16.266)$$

If one assumes hydrostatic gravity waves, this can be done using Eq. (16.257), from this it follows

$$\omega_I^2 = U^2 k^2 = f^2 + \frac{N^2 (k^2 + l^2)}{m^2 + \frac{1}{4H^2}}. \quad (16.267)$$

Assuming $m^2 \gg \frac{1}{4H^2}$, $f = 0$ and $l = 0$, it follows

$$\omega_I^2 = U^2 k^2 = \frac{N^2 k^2}{m^2} \Rightarrow U^2 = \frac{N^2}{m^2} \Rightarrow m^2 = \frac{N^2}{U^2}. \quad (16.268)$$

This follows for the intrinsic phase velocity

$$\mathbf{c}_{I,\text{ph}} = \frac{\omega_I}{\sqrt{k^2 + m^2}} \frac{\mathbf{k}}{|\mathbf{k}|} = -\frac{Uk}{k^2 + m^2} \begin{pmatrix} k \\ 0 \\ m \end{pmatrix} \quad (16.269)$$

as well as for the intrinsic group speed

$$\mathbf{c}_{I,\text{gr}} = \nabla_{\mathbf{k}} \omega_I = \begin{pmatrix} -\frac{N}{U} \\ 0 \\ \frac{Nk}{m^2} \end{pmatrix}. \quad (16.270)$$

The intrinsic phase velocity is directed downwards and against the wind direction, the intrinsic group velocity is also negative in the x direction, but directed upwards.

In the case of non-hydrostatic gravity waves, Eq. (16.242), also under the assumptions $f = 0$ and $l = 0$,

$$\begin{aligned} U^2 k^2 &= \frac{N^2 k^2}{m^2 + \frac{1}{4H^2} + k^2} \Leftrightarrow U^2 \left(k^2 + m^2 + \frac{1}{4H^2} \right) = N^2 \\ \Leftrightarrow m^2 &= \frac{N^2}{U^2} - k^2 - \frac{1}{4H^2}. \end{aligned} \quad (16.271)$$

In the case $m^2 < 0$ the waves are vertically evanescent, so they cannot propagate vertically. This is the case for

$$\begin{aligned} \frac{N^2}{U^2} - k^2 - \frac{1}{4H^2} &< 0 & \Leftrightarrow k^2 &> \frac{N^2}{U^2} - \frac{1}{4H^2} \\ \Leftrightarrow \frac{4\pi^2}{l_x^2} &> \frac{N^2}{U^2} - \frac{1}{4H^2} & \Leftrightarrow \frac{l_x^2}{4\pi^2} &< \frac{1}{\frac{N^2}{U^2} - \frac{1}{4H^2}} \\ \Leftrightarrow l_x &< \frac{2\pi}{\sqrt{\frac{N^2}{U^2} - \frac{1}{4H^2}}}. \end{aligned} \quad (16.272)$$

Those spectral components of the orography that fulfill this inequality cannot generate upward propagating waves. Substituting typical values of $N = 0.02$ Hz, $U = 8$ m/s and $H = 8$ km gives $l_x \approx 2.5$ km. With higher wind speed, l_x increases.

16.6.3 Rossby waves

In order to understand so-called *Rossby waves*, one uses the quasi-geostrophic equation system derived in Sect. 13.11, consisting of the trend equation Eq. (13.226) and ω -equation Eq. (13.231), but here in discretized form. The prognostic (state-determining) variables here are two current functions ψ_1, ψ_3 . The resulting five layers are summarized in Tab. 16.1. The boundary conditions $\omega_0 = \omega_4 = 0$ are used for calculation.

This approach is called *quasigeostrophic two-layer model*.

Index	Druck / hPa	definierte Funktion
0	0	$\omega_0 = 0$ (Randbedingung)
1	250	ψ_1
2	500	ω_2
3	750	ψ_3
4	1000	$\omega_4 = 0$ (Randbedingung)

Table 16.1: Overview of the quasi-geostrophic two-layer model. See [17].

For the quasi-geostrophic potential vorticities applies

$$q_1 = f + \Delta\psi_1 + \frac{f_0}{\sigma} \frac{\frac{\partial\psi}{\partial p}\big|_1 - \frac{\partial\psi}{\partial p}\big|_0}{\Delta p} = f + \Delta\psi_1 + \frac{f_0}{\sigma\Delta p^2} (\psi_3 - \psi_1) - \frac{f_0}{\sigma\Delta p} \frac{\partial\psi}{\partial p}\bigg|_0, \quad (16.273)$$

$$q_3 = f + \Delta\psi_3 + \frac{f_0}{\sigma} \frac{\frac{\partial\psi}{\partial p}\big|_4 - \frac{\partial\psi}{\partial p}\big|_3}{\Delta p} = f + \Delta\psi_3 - \frac{f_0}{\sigma\Delta p^2} (\psi_3 - \psi_1) + \frac{f_0}{\sigma\Delta p} \frac{\partial\psi}{\partial p}\bigg|_4. \quad (16.274)$$

$\Delta p := 500$ hPa is defined. No statement can be made about the last terms within the framework of this model, so they are assumed to be constant and are therefore ignored. One further defines a barotropic and a baroclinic component of the current function:

$$\psi_M := \frac{\psi_1 + \psi_3}{2}, \quad \psi_T := \frac{\psi_1 - \psi_3}{2}. \quad (16.275)$$

In addition, a baroclinic potential vorticity is defined:

$$q_T := \frac{q_1 - q_3}{2} = \frac{\zeta_1 - \zeta_3}{2} - \frac{f_0}{\sigma\Delta p^2} (\psi_1 - \psi_3) \quad (16.276)$$

Furthermore, the *stability wave number* K is given by

$$K^2 := \frac{2f_0}{\sigma\Delta p^2} \quad (16.277)$$

defined. This allows you to take notes

$$q_1 = f + \zeta_1 - K^2\psi_T, \quad q_3 = f + \zeta_3 + K^2\psi_T, \quad q_T = \zeta_T - K^2\psi_T. \quad (16.278)$$

Now you make a disruption approach

$$\psi = \bar{\psi} + \psi' = -\bar{u}y + \psi' \quad (16.279)$$

with a mean homogeneous zonal flow vector $\bar{u}$. Now we assume a special case: we assume that the background wind is at level 1

$$\bar{u}_1 = \bar{u}_T \quad (16.280)$$

blowing and around level 3 the background wind

$$\bar{u}_3 = -\bar{u}_T. \quad (16.281)$$

Then apply

$$\bar{\psi}_1 = -\bar{u}_T y, \quad \bar{\psi}_3 = \bar{u}_T y. \quad (16.282)$$

From this it follows

$$\bar{\psi}_T = -\bar{u}_T y. \quad (16.283)$$

For the ground state $\bar{\mathbf{v}}_h$ one can therefore note

$$\bar{\mathbf{v}}_{h_1} = \begin{pmatrix} \bar{u}_T \\ 0 \end{pmatrix}, \quad (16.284)$$

$$\bar{\mathbf{v}}_{h_3} = \begin{pmatrix} -\bar{u}_T \\ 0 \end{pmatrix}. \quad (16.285)$$

Let the field $\bar{u}_T$ be independent of y , then the following applies

$$\bar{\zeta}_1 = \bar{\zeta}_3 = 0. \quad (16.286)$$

For the potential vorticities applies

$$\bar{q}_1 = f_0 + \beta y - K^2 \bar{\psi}_T = f_0 + (\beta + K^2 \bar{u}_T) y, \quad (16.287)$$

$$\bar{q}_3 = f_0 + \beta y + K^2 \bar{\psi}_T = f_0 + (\beta - K^2 \bar{u}_T) y. \quad (16.288)$$

This field is stationary:

$$\left(\frac{\partial}{\partial t} + \bar{\mathbf{v}}_{h_1} \cdot \nabla \right) \bar{q}_1 = 0 \quad (16.289)$$

$$\left(\frac{\partial}{\partial t} + \bar{\mathbf{v}}_{h_3} \cdot \nabla \right) \bar{q}_3 = 0 \quad (16.290)$$

If one also applies the perturbation approach to the form of material derivation used here and to the potential vorticity, it follows

$$\frac{D_h^{(g)}}{Dt} = \frac{\partial}{\partial t} + \bar{\mathbf{v}}_h \cdot \nabla + \mathbf{v}'_h \cdot \nabla, \quad (16.291)$$

$$q = \bar{q} + q'. \quad (16.292)$$

Now one assumes again that the disturbances only have meridional components, i.e

$$\mathbf{v}'_{h,g,1} = \begin{pmatrix} 0 \\ v'_1 \end{pmatrix}, \quad (16.293)$$

$$\mathbf{v}'_{h,g,3} = \begin{pmatrix} 0 \\ v'_3 \end{pmatrix}. \quad (16.294)$$

Apply to the power functions

$$v'_1 = \frac{\partial \psi'_1}{\partial x}, \quad v'_3 = \frac{\partial \psi'_3}{\partial x}. \quad (16.295)$$

This follows for the potential vorticities

$$q'_1 = \frac{\partial^2 \psi'_1}{\partial x^2} - K^2 \psi'_T, \quad q'_3 = \frac{\partial^2 \psi'_3}{\partial x^2} + K^2 \psi'_T. \quad (16.296)$$

To examine the tendency equations, write down

$$\frac{\partial \bar{q}}{\partial t} + \bar{\mathbf{v}}_h \cdot \nabla \bar{q} + \frac{\partial q'}{\partial t} + \bar{\mathbf{v}}_h \cdot \nabla q' + \mathbf{v}'_h \cdot \nabla \bar{q} + \mathbf{v}'_h \cdot \nabla q' = 0. \quad (16.297)$$

The first two terms result in zero, as already noted. The final dot product also disappears due to the orthogonality of the vectors involved. Therefore apply

$$\left(\frac{\partial}{\partial t} + \bar{u}_T \frac{\partial}{\partial x} \right) q'_1 + (\beta + K^2 \bar{u}_T) \frac{\partial \psi'_1}{\partial x} = 0, \quad (16.298)$$

$$\left(\frac{\partial}{\partial t} - \bar{u}_T \frac{\partial}{\partial x} \right) q'_3 + (\beta - K^2 \bar{u}_T) \frac{\partial \psi'_3}{\partial x} = 0. \quad (16.299)$$

Since the equations (16.298) - (16.299) are linear, one can understand the solutions as superpositions of plane waves and therefore makes an approach

$$\psi'_1 = A_1 \exp[i(kx - \omega t)] =: A_1 f(x, t), \quad (16.300)$$

$$\psi'_3 = A_3 \exp[i(kx - \omega t)] =: A_3 f(x, t). \quad (16.301)$$

This gives you

$$q'_1 = -k^2 A_1 f - K^2 \frac{A_1 - A_3}{2} f, \quad (16.302)$$

$$q'_3 = -k^2 A_3 f + K^2 \frac{A_1 - A_3}{2} f. \quad (16.303)$$

So the system of equations to be solved is

$$(\omega - k\bar{u}_T) \left(k^2 A_1 + K^2 \frac{A_1 - A_3}{2} \right) + (\beta + K^2 \bar{u}_T) k A_1 = 0, \quad (16.304)$$

$$(\omega + k\bar{u}_T) \left(k^2 A_3 - K^2 \frac{A_1 - A_3}{2} \right) + (\beta - K^2 \bar{u}_T) k A_3 = 0. \quad (16.305)$$

In matrix notation this is:

$$\begin{pmatrix} M_{1,1} & M_{1,2} \\ M_{2,1} & M_{2,2} \end{pmatrix} \begin{pmatrix} A_1 \\ A_3 \end{pmatrix} = 0 \quad (16.306)$$

with the matrix coefficients

$$M_{1,1} = (\omega - k\bar{u}_T) \left(k^2 + \frac{K^2}{2} \right) + (\beta + K^2 \bar{u}_T) k, \quad (16.307)$$

$$M_{1,2} = -\frac{K^2}{2} (\omega - k\bar{u}_T), \quad (16.308)$$

$$M_{2,1} = -\frac{K^2}{2} (\omega + k\bar{u}_T), \quad (16.309)$$

$$M_{2,2} = (\omega + k\bar{u}_T) \left(k^2 + \frac{K^2}{2} \right) + (\beta - K^2 \bar{u}_T) k. \quad (16.310)$$

Setting the determinant to zero results in

$$\begin{aligned}
M_{1,1}M_{2,2} - M_{2,1}M_{1,2} &\stackrel{!}{=} 0 \\
\Rightarrow (\omega^2 - k^2\bar{u}_T^2) \left(k^2 + \frac{K^2}{2}\right)^2 + 2k \left(k^2 + \frac{K^2}{2}\right) (\omega\beta + kK^2\bar{u}_T^2) + (\beta^2 - K^4\bar{u}_T^2) k^2 - \frac{K^4}{4} (\omega^2 - k^2\bar{u}_T^2) &= 0 \\
\Rightarrow (\omega^2 - k^2\bar{u}_T^2) (k^4 + k^2K^2) + 2k \left(k^2 + \frac{K^2}{2}\right) (\omega\beta + kK^2\bar{u}_T^2) + (\beta^2 - K^4\bar{u}_T^2) k^2 &= 0 \\
\Rightarrow (\omega^2 - k^2\bar{u}_T^2) (k^2 + K^2) + \left(2k + \frac{K^2}{k}\right) (\omega\beta + kK^2\bar{u}_T^2) + \beta^2 - K^4\bar{u}_T^2 &= 0 \\
\Rightarrow (\omega^2 - k^2\bar{u}_T^2) (k^2 + K^2) + 2k (\omega\beta + kK^2\bar{u}_T^2) + \frac{K^2\omega\beta}{k} + \beta^2 &= 0 \\
\Rightarrow \omega^2 k^2 + \omega^2 K^2 - k^4\bar{u}_T^2 + k^2 K^2\bar{u}_T^2 + 2k\omega\beta + \frac{K^2\omega\beta}{k} + \beta^2 &= 0 \\
\Rightarrow \omega^2 [k^2 + K^2] + \omega \left[2k\beta + \frac{K^2\beta}{k}\right] - k^4\bar{u}_T^2 + k^2 K^2\bar{u}_T^2 + \beta^2 &= 0 \\
\Rightarrow \omega^2 + \omega \frac{\beta}{k} \frac{2k^2 + K^2}{k^2 + K^2} + \frac{k^2 K^2\bar{u}_T^2 - k^4\bar{u}_T^2 + \beta^2}{k^2 + K^2} &= 0 \\
\Rightarrow \omega_{1,2} = -\frac{\beta}{2k} \frac{2k^2 + K^2}{k^2 + K^2} \pm \sqrt{\frac{\beta^2}{4k^2} \frac{(2k^2 + K^2)^2}{(k^2 + K^2)^2} - \frac{k^2 K^2\bar{u}_T^2 - k^4\bar{u}_T^2 + \beta^2}{k^2 + K^2}} \\
\Rightarrow \omega_{1,2} = -\frac{\beta}{2k} \frac{2k^2 + K^2}{k^2 + K^2} \pm \frac{1}{k^2 + K^2} \sqrt{\frac{\beta^2}{4k^2} (4k^4 + K^4 + 4k^2 K^2) - (k^2 + K^2) (k^2 K^2\bar{u}_T^2 - k^4\bar{u}_T^2 + \beta^2)} \\
\Rightarrow \omega_{1,2} = -\frac{\beta}{2k} \frac{2k^2 + K^2}{k^2 + K^2} \\
\pm \frac{1}{k^2 + K^2} \sqrt{\beta^2 k^2 + \frac{\beta^2 K^4}{4k^2} + \beta^2 K^2 - k^4 K^2\bar{u}_T^2 - k^2 \beta^2 - K^4 k^2\bar{u}_T^2 - K^2 \beta^2 + k^6\bar{u}_T^2 + K^2 k^4\bar{u}_T^2} \\
\Rightarrow \omega_{1,2} = -\frac{\beta}{k} \frac{k^2 + K^2/2}{k^2 + K^2} \pm \frac{1}{k^2 + K^2} \sqrt{\frac{\beta^2 K^4}{4k^2} + \bar{u}_T^2 k^2 (k^4 - K^4)}. \tag{16.311}
\end{aligned}$$

Assuming $k < K$, one maximizes the expression at the root by setting $\bar{u}_T = 0$, from which it follows

$$c = \frac{\omega}{k} \leq -\frac{\beta}{k^2 + K^2}, \tag{16.312}$$

Baroclinic Rossby waves always propagate westward. Baroclinic Rossby waves are also called planetary waves when they span a complete circle of latitude.

16.6.4 Natural oscillations of a hydrostatic atmosphere

Write down the equations summarized in Section 13.7 in their adiabatic form:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \omega \frac{\partial u}{\partial p} = -\frac{\partial \Phi}{\partial x} + fv, \tag{16.313}$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \omega \frac{\partial v}{\partial p} = -\frac{\partial \Phi}{\partial y} - fu, \tag{16.314}$$

$$\frac{\partial^2 \Phi}{\partial p \partial t} + \left(u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y}\right) \frac{\partial \Phi}{\partial p} + \frac{a^2}{g^2} N^2 \omega = 0, \tag{16.315}$$

$$\frac{\partial \omega}{\partial p} = -\nabla \cdot \mathbf{v}_h. \tag{16.316}$$

If you neglect advection, you get

$$\frac{\partial u}{\partial t} = -\frac{\partial \Phi}{\partial x} + fv, \quad (16.317)$$

$$\frac{\partial v}{\partial t} = -\frac{\partial \Phi}{\partial y} - fu, \quad (16.318)$$

$$\frac{\partial^2 \Phi}{\partial p \partial t} + \sigma \omega = 0, \quad (16.319)$$

$$\frac{\partial \omega}{\partial p} = -\nabla \cdot \mathbf{v}_h. \quad (16.320)$$

with the static stability parameter $\sigma = \frac{a^2}{g^2} N^2$. This is the underlying system of equations for this section. If you write down the derivatives and differential operators in geographical coordinates, you get.

$$\frac{\partial u}{\partial t} = -\frac{1}{a \cos(\varphi)} \frac{\partial \Phi}{\partial \lambda} + fv, \quad (16.321)$$

$$\frac{\partial v}{\partial t} = -\frac{1}{a} \frac{\partial \Phi}{\partial \varphi} - fu, \quad (16.322)$$

$$\frac{\partial^2 \Phi}{\partial p \partial t} + \sigma \omega = 0, \quad (16.323)$$

$$\frac{\partial \omega}{\partial p} = -\frac{1}{a \cos(\varphi)} \frac{\partial u}{\partial \lambda} - \frac{1}{a} \frac{\partial v}{\partial \varphi} - \frac{v}{a} \tan(\varphi). \quad (16.324)$$

Now we divide it into a background state $\bar{\psi}$ and deviations ψ' , where σ is a property of the background state. One assumes $\bar{u} = \bar{v} = \bar{\omega} = 0$. As approaches for fields ψ are used

$$\psi' = \psi_0 \left(\frac{p}{p_0} \right)^{\chi} h(\varphi) \exp(im\lambda - i\gamma t) \quad (16.325)$$

with a complex amplitude ψ_0 , a zonal wavenumber $m \in \mathbb{N}$ and a continuously differentiable function $h(\varphi)$. p_0 is a reference pressure and $\chi > 0$ is a parameter. If you insert this and the definition of f into the equations (16.321) - (16.324), you get

$$-i\gamma u_0 = -\frac{im\Phi_0}{a \cos(\varphi)} + 2\Omega \sin(\varphi) v_0, \quad (16.326)$$

$$-i\gamma h v_0 = -\frac{\Phi_0 h'}{a} - 2\Omega \sin(\varphi) u_0 h, \quad (16.327)$$

$$-i\gamma \frac{\chi}{p} \Phi_0 = -\sigma \omega_0, \quad (16.328)$$

$$\frac{\chi}{p} h \omega_0 = -\frac{imh}{a \cos(\varphi)} u_0 - \frac{v_0 h'}{a} - \frac{v_0}{a} h \tan(\varphi). \quad (16.329)$$

The fractions are multiplied away:

$$-i\gamma a \cos(\varphi) u_0 = -im\Phi_0 + 2\Omega a \cos(\varphi) \sin(\varphi) v_0 = -im\Phi_0 + \Omega a \sin(2\varphi) v_0, \quad (16.330)$$

$$-i\gamma a h v_0 = -h' \Phi_0 - 2\Omega a \sin(\varphi) h u_0, \quad (16.331)$$

$$-i\gamma \chi \Phi_0 = -\sigma p \omega_0, \quad (16.332)$$

$$\chi h a \cos(\varphi) \omega_0 = -imh p u_0 - ph' \cos(\varphi) v_0 - ph \sin(\varphi) v_0. \quad (16.333)$$

If you bring everything to the left side, you get

$$-i\gamma a \cos(\varphi) u_o + im\Phi_o - \Omega a \sin(2\varphi) v_o = o, \quad (16.334)$$

$$-i\gamma a h v_o + h'\Phi_o + 2\Omega a \sin(\varphi) h u_o = o, \quad (16.335)$$

$$-i\gamma \chi \Phi_o + \sigma p \omega_o = o, \quad (16.336)$$

$$\chi h a \cos(\varphi) \omega_o + imhp u_o + ph' \cos(\varphi) v_o + ph \sin(\varphi) v_o = o. \quad (16.337)$$

The terms are now sorted in the order $u_o, v_o, \Phi_o, \omega_o$:

$$\begin{array}{ccccccc} -i\gamma a \cos(\varphi) u_o & -\Omega a \sin(2\varphi) v_o & +im\Phi_o & +o & = o, \\ 2\Omega a \sin(\varphi) h u_o & -i\gamma a h v_o & +h'\Phi_o & +o & = o, \\ o & +o & -i\gamma \chi \Phi_o & +\sigma p \omega_o & = o, \\ imhp u_o & + [ph' \cos(\varphi) + ph \sin(\varphi)] v_o & +o & +\chi h a \cos(\varphi) \omega_o & = o. \end{array} \quad (16.338)$$

This leads directly to matrix notation

$$M \cdot \mathbf{x} = o \quad (16.339)$$

with

$$M := \begin{pmatrix} -i\gamma a \cos(\varphi) & -\Omega a \sin(2\varphi) & im & o, \\ 2\Omega a \sin(\varphi) h & -i\gamma a h & h' & o, \\ o & o & -i\gamma \chi & \sigma p, \\ imhp & ph' \cos(\varphi) + ph \sin(\varphi) & o & \chi h a \cos(\varphi) \end{pmatrix} \quad (16.340)$$

and

$$\mathbf{v} := \begin{pmatrix} u_o \\ v_o \\ \Phi_o \\ \omega_o \end{pmatrix}. \quad (16.341)$$

16.6.4.1 Atmospheric tide

Important differences between the atmospheric and the oceanic tide (see section 16.5.7) are as follows:

- The oceanic tide can be viewed as barotropic, effects of the ocean's baroclinicity play a minor role.
- In the atmosphere, baroclinity is much more relevant; the barotropic approximation would filter out essential structural elements of the atmospheric tide.
- The oceanic tide is generated primarily by fluctuations in gravity caused by the moon. This leads to a base period of just under 25 hours.
- The atmospheric tide is driven primarily by radiation and by processes triggered by radiation (chemical reactions and convection).
- Due to barotropy, the oceanic tide is virtually independent of height, while the amplitude of the atmospheric tide increases exponentially with height. This means that the tide plays a role in the atmosphere, especially in the mesosphere (50 - 80 km), where it can reach large amplitudes. In the troposphere their amplitude is small.

16.7 Instabilities

If one finds angular frequencies with a positive imaginary part when a plane wave is introduced as a disturbance into a system of equations and subsequent linearization (justified for small amplitudes), then a *instability* is present. The amplitude of the wave grows exponentially in this initial linear time before nonlinear effects become dominant and cause the wave to break with subsequent dissipation of the kinetic energy.

16.7.1 Stratification instability

The atmosphere over a given point on the earth's surface has the stratification $T = T(z)$. Usually is

$$\frac{\partial T}{\partial z} < 0, \quad (16.342)$$

at $\frac{\partial T}{\partial z} > 0$ one speaks of an *inversion*. The dry adiabatic temperature gradient is according to Eq. (9.47)

$$\Gamma_d = \frac{g}{c^{(p)}} \quad (16.343)$$

defined. In the case

$$\frac{\partial T}{\partial z} < -\Gamma_d \quad (16.344)$$

The layering is *unstable*, and even *unconditionally unstable*, since both a saturated and an unsaturated air particle that is deflected from its rest position does not return to it.

However, if the air is saturated, the cooling that occurs as a result of the uplift causes condensation or resublimation to occur, releasing phase transition heat. If you deflect the particle vertically at z , the *lifted condensation level (LCL)* z_{LCL} is the height at which it would be saturated, so it satisfies the equation

$$p_v^{(S)}(T(z) - \Gamma_d(z_{\text{LCL}} - z)) \equiv p_v(z) \left(1 - \frac{\Gamma_d(z_{\text{LCL}} - z)}{T(z)} \right)^{\frac{g}{R_d \Gamma_d}}. \quad (16.345)$$

During the subsequent further uplift, it is initially assumed that all the water remains in the cloud, which is referred to as *reversible wet adiabates*; Occasionally the word pseudoadiabatic is used instead of wet adiabatic, since the question of whether this process is adiabatic or not depends on which system you are looking at: if you look at the air including the condensates as a system, the process is adiabatic because it does not exchange heat with its surroundings; However, if you only look at the gas phase, the process is diabatic. In the case of *irreversible wet adiabates*, which will be discussed in more detail in section 16.7.1.3, it is assumed that all the water rains out. This will now be considered. So assume that the air in a particle with volume V and constant mass m consists of a mixture of moist air and condensation products of a phase, with all components having the same temperature T . With the first law of thermodynamics Eq. (9.10) is obtained

$$\begin{aligned} c^{(V)} \frac{dT}{dz} + p \frac{d}{dz} \frac{1}{\rho} &= \frac{1}{\rho} \frac{dq}{dz} \\ \Rightarrow \frac{dT}{dz} &= \frac{1}{c^{(V)}} \left[\frac{1}{\rho} \frac{dq}{dz} - p \frac{d}{dz} \frac{1}{\rho} \right] = \frac{1}{\rho c^{(V)}} \left[\frac{dq}{dz} + \frac{p}{\rho} \frac{d\rho}{dz} \right] = -\frac{g}{c^{(V)}} \left[\frac{dq}{dp} + \frac{p}{\rho} \frac{d\rho}{dp} \right]. \end{aligned} \quad (16.346)$$

The basic hydrostatic equation was used here. For the heat output per volume due to the phase transition dq applies

$$dq = \frac{c_c}{v_h} dm_c \quad (16.347)$$

with m_c as the condensed or resublimated mass and c_c as the phase transition heat. With the equation of state for water vapor applies

$$\begin{aligned} p_v &= \rho_v R_v T \Rightarrow m_v = \frac{V_v p_v}{R_v T} = \frac{V_h p_v}{R_v T} = \frac{m_h R_h p_v^{(S)}(T)}{p R_v} \\ \Rightarrow dm_c &= -dm_v = \frac{m_h R_h p_v^{(S)}(T)}{p R_v} \left(\frac{dp}{p} - \frac{dp_v^{(S)}}{p_v^{(S)}} + \frac{dm_c}{m_h} \right) \\ \Rightarrow dm_c \left(1 - \frac{R_h p_v^{(S)}(T)}{p R_v} \right) &= \frac{m_h R_h p_v^{(S)}(T)}{p R_v} \left(\frac{dp}{p} - \frac{dp_v^{(S)}}{p_v^{(S)}} \right) \\ \Rightarrow dm_c &= m_h \frac{\frac{dp}{p} - \frac{dp_v^{(S)}}{p_v^{(S)}}}{\frac{p R_v}{R_h p_v^{(S)}} - 1}. \end{aligned} \quad (16.348)$$

Here $p_v^{(S)} = p_v^{(S)}(T)$ is the saturation vapor pressure. It follows

$$\begin{aligned}
 dq &= \frac{c_c}{T} \frac{dp - \frac{p}{p_v^{(S)}} dp_v^{(S)}}{\frac{pR_v}{p_v^{(S)}} - R_h} \\
 \Rightarrow \frac{dq}{dp} &= \frac{c_c}{\frac{pR_v}{p_v^{(S)}} - R_h T} \left(1 - \frac{p}{p_v^{(S)}} \frac{dp_v^{(S)}}{dp} \right) = \frac{c_c}{\frac{pR_v}{p_v^{(S)}} - TR_h} \left(1 + \frac{1}{g\varrho} \frac{dT}{dz} \frac{p}{p_v^{(S)}} \frac{dp_v^{(S)}}{dT} \right) \\
 &= \frac{c_c}{TpR_v - Tp_v^{(S)}R_h} \left(p_v^{(S)} + \frac{p}{g\varrho} \frac{dT}{dz} \frac{dp_v^{(S)}}{dT} \right) \\
 &= \frac{c_c p_v^{(S)}}{TpR_v - Tp_v^{(S)}R_h} + \frac{p}{Tg\varrho} \frac{c_c}{pR_v - p_v^{(S)}R_h} \frac{dp_v^{(S)}}{dT} \frac{dT}{dz}.
 \end{aligned} \tag{16.349}$$

Putting this into Eq. (16.346) and applying the chain rule again, you get

$$\begin{aligned}
 \frac{dT}{dz} &= -\frac{g}{c^{(V)}} \left[\frac{c_c p_v^{(S)}}{TpR_v - Tp_v^{(S)}R_h} \right. \\
 &\quad \left. + \frac{p}{Tg\varrho} \frac{c_c}{pR_v - p_v^{(S)}R_h} \frac{dp_v^{(S)}}{dT} \frac{dT}{dz} + \frac{p}{\varrho} \frac{\partial \varrho}{\partial p} - \frac{p}{g\varrho^2} \frac{\partial \varrho}{\partial T} \frac{dT}{dz} \right].
 \end{aligned} \tag{16.350}$$

Now you need an equation of state. applies to the density

$$\varrho = \varrho_h + \varrho_c = \frac{p}{R_h T} + \varrho_c. \tag{16.351}$$

This is what you get

$$\begin{aligned}
 \frac{dT}{dz} &= \frac{g}{c^{(V)}} \left[-\frac{c_c p_v^{(S)}}{TpR_v - Tp_v^{(S)}R_h} \right. \\
 &\quad \left. - \frac{p}{Tg\varrho} \frac{c_c}{pR_v - p_v^{(S)}R_h} \frac{dp_v^{(S)}}{dT} \frac{dT}{dz} - \frac{p}{\varrho R_h T} - \frac{p^2}{R_h g \varrho^2 T^2} \frac{dT}{dz} \right] \\
 &= \frac{g}{c^{(V)}} \left[-\frac{c_c p_v^{(S)}}{TpR_v - Tp_v^{(S)}R_h} - \frac{p}{Tg\varrho} \frac{c_c}{pR_v - p_v^{(S)}R_h} \frac{dp_v^{(S)}}{dT} \frac{dT}{dz} \right. \\
 &\quad \left. - 1 + \frac{\varrho_c}{\varrho} - \frac{1}{g} \left(1 - \frac{\varrho_c}{\varrho} \right) \frac{p}{\varrho T} \frac{dT}{dz} \right].
 \end{aligned} \tag{16.352}$$

This is now converted to $\frac{dT}{dz}$:

$$\begin{aligned}
 \frac{dT}{dz} &\left(1 + \frac{p}{Tc^{(V)}\varrho} \frac{c_c}{pR_v - p_v^{(S)}R_h} \frac{dp_v^{(S)}}{dT} + \frac{1}{c^{(V)}} \left(1 - \frac{\varrho_c}{\varrho} \right) \frac{p}{\varrho T} \right) \\
 &= \frac{g}{c^{(V)}} \left(\frac{\varrho_c}{\varrho} - 1 \right) - \frac{gc_c p_v^{(S)}(T)}{c^{(V)} T (R_v p - p_v^{(S)} R_h)} \\
 \Rightarrow \frac{dT}{dz} &= -\frac{g}{c^{(p)}} \frac{1 - \frac{\varrho_c}{\varrho} + \frac{c_c p_v^{(S)}}{T(R_v p - p_v^{(S)} R_h)}}{\frac{c^{(V)}}{c^{(p)}} + \frac{p}{T\varrho c^{(p)}} \frac{c_c}{pR_v - p_v^{(S)}R_h} \frac{dp_v^{(S)}}{dT} + \left(1 - \frac{\varrho_c}{\varrho} \right) \frac{p}{c^{(p)} T \varrho}} \\
 &= -\Gamma_d \beta
 \end{aligned} \tag{16.353}$$

Here is

$$\beta = \beta(p, T, \rho_c) := \frac{\mathbf{1} - \frac{\rho_c}{\rho} + \frac{c_v p_v^{(S)}}{T(R_v p - p_v^{(S)} R_h)}}{\frac{c^{(V)}}{c^{(p)}} + \frac{p}{T \rho c^{(p)}} \frac{c_v}{p R_v - p_v^{(S)} R_h} \frac{dp_v^{(S)}}{dT} + \left(\mathbf{1} - \frac{\rho_c}{\rho}\right) \frac{p}{c^{(p)} T \rho}}. \quad (16.354)$$

The Clausius-Clapeyron equation can be used for the derivative $\frac{dp_v^{(S)}}{dT}$. The so-called *moist adiabatic temperature gradient* is now given by

$$\Gamma_h := \Gamma_d \beta \quad (16.355)$$

defined. If you put in Eq. (16.354) $\rho_c = 0$ and $p_v \ll p$, but keeps terms with $\frac{dp_v^{(S)}}{dT}$, follows

$$\frac{dT}{dz} = -\frac{g}{c^{(p)}} \frac{\mathbf{1} + \frac{c_v p_v^{(S)}}{T R_v p}}{\frac{c^{(V)}}{c^{(p)}} + \frac{p}{T \rho c^{(p)}} \frac{c_v}{p R_v} \frac{dp_v^{(S)}}{dT} + \frac{p}{c^{(p)} T \rho}}. \quad (16.356)$$

If you insert the equation of state of ideal gases $p = \rho R_d T$ here, you get the expression that is often found in the literature

$$\begin{aligned} \frac{dT}{dz} &= -\frac{g}{c^{(p)}} \frac{\mathbf{1} + \frac{c_v p_v^{(S)}}{T R_v p}}{\frac{c^{(V)}}{c^{(p)}} + \frac{R_d}{c^{(p)}} \frac{c_v}{p R_v} \frac{dp_v^{(S)}}{dT} + \frac{c^{(p)} - c^{(V)}}{c^{(p)}}} \\ \Leftrightarrow \frac{dT}{dz} &= -\frac{g}{c^{(p)}} \frac{\mathbf{1} + \frac{c_v p_v^{(S)}}{T R_v p}}{\mathbf{1} + \frac{R_d c_v}{R_v c^{(p)} p} \frac{dp_v^{(S)}}{dT}} \equiv -\Gamma_d \beta' \end{aligned} \quad (16.357)$$

with a simplified factor

$$\beta' = \beta'(p, T) := \frac{\mathbf{1} + \frac{c_v p_v^{(S)}}{T R_v p}}{\mathbf{1} + \frac{\frac{M_v}{M_d} c_v}{p c^{(p)}} \frac{dp_v^{(S)}}{dT}} \stackrel{\text{Glg. (5.237)}}{\approx} \frac{\mathbf{1} + \frac{c_v p_v^{(S)}}{T R_v p}}{\mathbf{1} + \frac{\frac{M_v}{M_d} c_v^2 p_v^{(S)}}{R_v c^{(p)} T^2 p}}$$

$$\Leftrightarrow \beta' \stackrel{\text{Glg. (5.172)}}{\approx} \frac{\mathbf{1} + \frac{c_v r^{(S)}}{T R_d}}{\mathbf{1} + \frac{c_v^2 r^{(S)}}{R_v c^{(p)} T^2}}, \quad (16.358)$$

which no longer depends on the density of the water that has already condensed out. In the case $\frac{dp_v^{(S)}}{dT} = p_v^{(S)} = 0$ it follows

$$\Gamma_h = \Gamma_d. \quad (16.359)$$

In the case of saturated air and

$$\frac{\partial T}{\partial z} < -\Gamma_h \quad (16.360)$$

the layering is also *labile*. In the case

$$-\Gamma_d \leq \frac{\partial T}{\partial z} < -\Gamma_h \quad (16.361)$$

the layering is *conditionally unstable*, since only a saturated particle does not return to its rest position when it is deflected, so the instability depends on the humidity. In the case of unsaturated air and

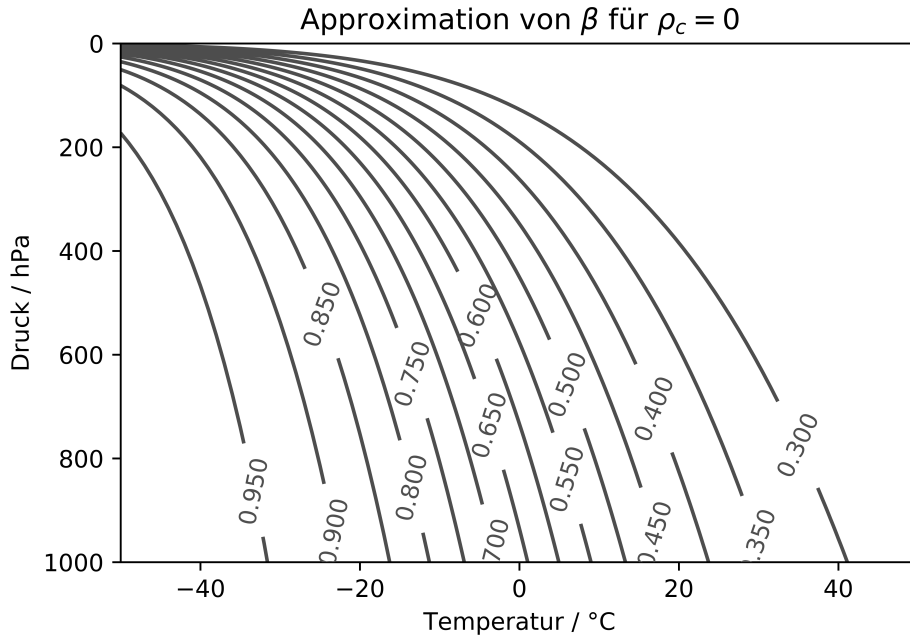


Figure 16.6: Approximation of β according to Eq. (16.358).

$$\frac{\partial T}{\partial z} = -\Gamma_d \quad (16.362)$$

or saturated air and

$$\frac{\partial T}{\partial z} = -\Gamma_h \quad (16.363)$$

one speaks of *neutral stratification*.

16.7.1.1 Equivalent potential temperature

To create the so-called *equivalent potential temperature* θ_e (also: pseudoequivalent potential temperature or, more rarely, pseudopotential temperature) of a particle, two steps are necessary:

1. Raise the particle dry adiabatically to its LCL.
2. Raise the particle irreversibly moist adiabatically to an infinite height. The potential temperature then obtained is θ_e .

This size is not only adjusted for the pressure difference, but also for the existing moisture, which could lead to an increase in temperature in the form of phase transition enthalpy. It is therefore well suited to comparing the temperatures of different air masses.

16.7.1.2 Reversible equivalent potential temperature

The reversible equivalent potential temperature is defined analogously to the equivalent potential temperature, except that a reversible wet adiabatic is pursued in step 2 from section 16.7.1.1.

16.7.1.3 CAPE

The derivations carried out in this section refer to a vertical column of air, where dynamic, i.e. h. Effects caused by the velocity field are not taken into account. One defines a function $f(z, z')$ as the specific force, i.e. the acceleration, that acts on the particle at z if it is brought adiabatically to the level z' and assumes a hydrostatic atmosphere, i.e.

$$f(z, z') := -\frac{\mathbf{I}}{\rho'(z, z')} \frac{\partial p(z')}{\partial z} - g \stackrel{\text{Glg. (13.122)}}{=} \frac{g\rho(z')}{\rho'(z, z')} - g = g \frac{\rho(z') - \rho'(z, z')}{\rho'(z, z')}, \quad (16.364)$$

where $\rho'(z, z')$ is the density of the particle at z after moving it adiabatically to z' . One also defines a function $\tilde{F}(z, z')$ by

$$\tilde{F}(z, z') := g \int_z^{z'} \frac{\rho(z'') - \rho'(z, z'')}{\rho'(z, z'')} dz'' \quad (16.365)$$

as the work done by the layering on a particle that was deflected adiabatically from z to z' . Usually you choose $z = z_{2m} := z_{SFC} + 2 \text{ m}$, you define

$$\begin{aligned} F(z) &:= \tilde{F}(z_{2m}, z) = g \int_{z_{2m}}^z \frac{\rho(z'') - \rho'(z_{2m}, z'')}{\rho'(z_{2m}, z'')} dz'' = g \int_{z_{2m}}^z \frac{\rho(z') - \rho'(z_{2m}, z')}{\rho'(z_{2m}, z')} dz' \\ &= g \int_{z_{2m}}^z \frac{\rho(z') - \rho'(z')}{\rho'(z')} dz' \end{aligned} \quad (16.366)$$

with the misuse of the term

$$\rho'(z') := \rho'(z_{2m}, z'). \quad (16.367)$$

The same applies to the integrand

$$f(z') := g \frac{\rho(z') - \rho'(z')}{\rho'(z')} \quad (16.368)$$

defined. Many of the quantities commonly used in connection with convection can be defined in terms of the functions F and f . The so-called *convectively available potential energy CAPE* is defined by

$$\text{CAPE} := \int_{z_{2m}}^{\infty} \Theta(f(z)) dz, \quad (16.369)$$

where Θ denotes the Θ function. Realistically, of course, you don't integrate to infinity, but only up to a height z_T , where the tropopause is typically located, since there is no longer any instability above that anyway. In the case of dry air one can write for f

$$f(z') = g \frac{\frac{p}{R_d T} - \frac{p}{R_d T'}}{\frac{p}{R_d T'}} = g \frac{\frac{1}{T} - \frac{1}{T'}}{\frac{1}{T'}} = g \frac{T' - T}{T} = g \frac{\theta' \left(\frac{p}{p_o}\right)^{R_d/c_d^{(p)}} - \theta \left(\frac{p}{p_o}\right)^{R_d/c_d^{(p)}}}{\theta \left(\frac{p}{p_o}\right)^{R_d/c_d^{(p)}}} = g \frac{\theta' - \theta}{\theta}. \quad (16.370)$$

In the case of moist air one can replace $T \rightarrow T_v$, here T_v is the value in Eq. (5.164) defined virtual temperature, since at this temperature the dry air would have the same density as the existing moist air. The *level of free convection* z_{LFC} is the height at which the adiabatic rising particle is lighter than the surroundings for the first time

$$z_{LFC} := \inf\{z | f(z) > 0\}. \quad (16.371)$$

When the particle reaches this height, it will continue to rise, which is called *free convection*, i.e. convection that would also take place without dynamic forcing. It is called analogous

$$z_{EL} := \sup\{z | f(z) > 0, z < z_T\} \quad (16.372)$$

as *equilibrium level (equilibrium level)*. To be on the safe side, the deep stratosphere was excluded. This is the height at which a freely rising particle would be heavier than its surroundings. Often in Eq. (16.369) omitted the Θ function and only integrated from z_{LFC} to z_{EL} , which is correct if there is thermal lability in exactly one height interval, which is often the case. The *maximum cloud top* is defined as the height at which such a particle would

have lost its kinetic energy again, i.e

$$z_{\text{MCT}} := \inf\{z \mid \tilde{F}(z_{\text{LFC}}, z) < 0\}. \quad (16.373)$$

The phenomenon $z_{\text{MCT}} > z_{\text{EL}}$ leads to the development of gravity waves at the tropopause (*overshooting tops*) in the case of long-range convection, which is generally the case wherever a stable height interval follows an unstably layered height interval.

If a particle has reached the so-called *release temperature* at a height of two meters, it can rise into the LFC even without dynamic drive, i.e

$$0 \equiv g \int_{z_{2m}}^{z_{\text{LFC}}} \frac{\rho(z') - \tilde{\rho}'(z')}{\tilde{\rho}'(z')}, \quad (16.374)$$

where $\tilde{\rho}'(z')$ is the density of the particle lifted adiabatically from z_{2m} to z' , which would be the trigger temperature at a height of two meters. So the energy CIN that has to be overcome

$$\text{CIN} := -\tilde{F}(z_{2m}, z_{\text{LFC}}). \quad (16.375)$$

is called *convective barrier* or *convective inhibition*. The height at which a particle heated to the trigger temperature would be saturated during adiabatic ascent is called *convective condensation level (CCL)*. This is at least as big as the LCL, so

$$z_{\text{CCL}} \geq z_{\text{LCL}}. \quad (16.376)$$

16.7.2 Kelvin-Helmholtz instability

The *Kelvin-Helmholtz instability* is the instability of a vertically sheared horizontal flow.

16.7.2.1 In discrete layering

The movement is y-symmetrical, so the xz plane is considered. The xy plane coincides with the equilibrium position of a phase boundary. The medium above the boundary layer ($z > 0$) is given the index 1, the medium below it ($z < 0$) is given the index 2. The media are barotropic and incompressible. At time $t = 0$ the flow field will be through

$$U_1 > 0, \quad U_2 > 0, \quad V_1 = V_2 = W_1 = W_2 = 0 \quad (16.377)$$

described. The Coriolis force is neglected. It applies

$$\nabla \times \mathbf{v}_1 = \nabla \times \mathbf{v}_2 = 0. \quad (16.378)$$

Due to the circulation law in the form Eq. (15.39) this also applies to $t > 0$ as long as the media does not mix. Therefore the velocity fields are described by two current functions

$$\psi_1 = U_1 x + \psi'_1, \quad \psi_2 = U_2 x + \psi'_2, \quad (16.379)$$

where the deleted variables stand for the disturbances. Because of the lack of divergence,

$$\Delta \psi'_1 = \Delta \psi'_2 = 0. \quad (16.380)$$

The deflection of the phase boundary is denoted by ζ . With $\mathbf{n}$ as the normal vector of the surface and ζ as the surface deflection, the kinematic boundary condition applies

$$\mathbf{n} \cdot \nabla \psi_1 = \mathbf{n} \cdot \left(\frac{\partial \zeta}{\partial t} \mathbf{e}_z \right) = \mathbf{n} \cdot \nabla \psi_2 \text{ bei } z = \zeta. \quad (16.381)$$

Neglecting the surface tension, the dynamic boundary condition follows

$$p_1 = p_2 \text{ bei } z = \zeta. \quad (16.382)$$

For the normal vector $\mathbf{n}$ applies

$$\mathbf{n} = \frac{\mathbf{I}}{\sqrt{\mathbf{I} + \left(\frac{\partial \zeta}{\partial x}\right)^2}} \begin{pmatrix} -\frac{\partial \zeta}{\partial x} \\ \mathbf{I} \end{pmatrix}. \quad (16.383)$$

The kinematic boundary condition Eq. (16.381) becomes

$$-\left(U_1 + \frac{\partial \psi'_1}{\partial x}\right) \frac{\partial \zeta}{\partial x} + \frac{\partial \psi'_1}{\partial z} = \frac{\partial \zeta}{\partial t} = -\left(U_2 + \frac{\partial \psi'_2}{\partial x}\right) \frac{\partial \zeta}{\partial x} + \frac{\partial \psi'_2}{\partial z} \text{ bei } z = \zeta, \quad (16.384)$$

where the root expression was multiplied out. To linearize this expression, apply it at $z = 0$ and neglect quadratic terms:

$$-U_1 \frac{\partial \zeta}{\partial x} + \frac{\partial \psi'_1}{\partial z} = \frac{\partial \zeta}{\partial t} = -U_2 \frac{\partial \zeta}{\partial x} + \frac{\partial \psi'_2}{\partial z} \text{ bei } z = 0 \quad (16.385)$$

Since the flow field is rotation-free and one also assumes an ideal fluid, one can use the time-dependent Bernoulli equations (see equation (15.122)) of the two layers

$$\frac{\partial \psi_1}{\partial t} + \frac{1}{2} |\nabla \psi_1|^2 + \frac{p_1}{\rho_1} + gz = C, \quad (16.386)$$

$$\frac{\partial \psi_2}{\partial t} + \frac{1}{2} |\nabla \psi_2|^2 + \frac{p_2}{\rho_2} + gz = C_2 \quad (16.387)$$

with real constants C, C_2 . The dynamic boundary condition Eq. (16.382) implies identity at $z = \zeta$

$$\rho_1 \left(C - \frac{\partial \psi_1}{\partial t} - \frac{1}{2} |\nabla \psi_1|^2 - gz \right) = \rho_2 \left(C_2 - \frac{\partial \psi_2}{\partial t} - \frac{1}{2} |\nabla \psi_2|^2 - gz \right). \quad (16.388)$$

Without disruption applies

$$\rho_1 \left(C - \frac{1}{2} U_1^2 \right) = \rho_2 \left(C_2 - \frac{1}{2} U_2^2 \right). \quad (16.389)$$

Subtracting Eq. (16.389) from Eq. (16.388) leads to

$$\rho_1 \left(-\frac{\partial \psi_1}{\partial t} + \frac{1}{2} U_1^2 - \frac{1}{2} |\nabla \psi_1|^2 - gz \right) = \rho_2 \left(-\frac{\partial \psi_2}{\partial t} + \frac{1}{2} U_2^2 - \frac{1}{2} |\nabla \psi_2|^2 - gz \right), \quad (16.390)$$

which applies at $z = \zeta$. With the equations (16.379) - (16.379) follows

$$\frac{1}{2} |\nabla \psi_j|^2 = \frac{1}{2} \left(U_j^2 + \left(\frac{\partial \psi'_j}{\partial x} \right)^2 + 2 U_j \frac{\partial \psi'_j}{\partial x} + \left(\frac{\partial \psi'_j}{\partial z} \right)^2 \right) \quad (16.391)$$

for $j = 1, 2$. Putting this into Eq. (16.390), you get

$$\begin{aligned} & \rho_1 \left(-\frac{\partial \psi_1}{\partial t} - \frac{1}{2} \left(\frac{\partial \psi'_1}{\partial x} \right)^2 - U_1 \frac{\partial \psi'_1}{\partial x} - \frac{1}{2} \left(\frac{\partial \psi'_1}{\partial z} \right)^2 - gz \right) \\ &= \rho_2 \left(-\frac{\partial \psi_2}{\partial t} - \frac{1}{2} \left(\frac{\partial \psi'_2}{\partial x} \right)^2 - U_2 \frac{\partial \psi'_2}{\partial x} - \frac{1}{2} \left(\frac{\partial \psi'_2}{\partial z} \right)^2 - gz \right), \end{aligned} \quad (16.392)$$

at $z = \zeta$. This equation is linearized by evaluating it at $z = 0$ and neglecting the quadratic terms:

$$\rho_1 \left(\frac{\partial \psi_1}{\partial t} + U_1 \frac{\partial \psi_1'}{\partial x} + g\zeta \right) = \rho_2 \left(\frac{\partial \psi_2}{\partial t} + U_2 \frac{\partial \psi_1'}{\partial x} + g\zeta \right) \quad (16.393)$$

Now you do the approach for $j = 1, 2$

$$\psi_j' = A_j(z) \exp(ikx - i\omega t). \quad (16.394)$$

With the Laplace equations Eq. (16.380) follows

$$-k^2 A_j + \frac{d^2 A_j}{dz^2} = 0. \quad (16.395)$$

The solutions are of the form

$$A_j(z) = A_{\pm} \exp(\pm kz). \quad (16.396)$$

With the specifications

$$\lim_{z \rightarrow \infty} \psi_1' = 0, \quad \lim_{z \rightarrow -\infty} \psi_2' = 0, \quad (16.397)$$

which mean that the disturbance should disappear into infinity, follow

$$\psi_1' = A_- \exp[ikx - i\omega t - kz], \quad \psi_2' = A_+ \exp[ikx - i\omega t + kz]. \quad (16.398)$$

The surface deflection is taken accordingly

$$\zeta = \zeta_0 \exp(ikx - i\omega t) \quad (16.399)$$

to. If you insert this into the equations (16.385) and (16.393), you get

$$-U_1 ik \zeta_0 - k A_- = -i\omega \zeta_0 = -U_2 ik \zeta_0 + k A_+, \quad (16.400)$$

$$\rho_1 (-i\omega A_- + ik U_1 A_- + g\zeta_0) = \rho_2 (-i\omega A_+ + ik U_2 A_+ + g\zeta_0). \quad (16.401)$$

Eq. (16.400) implied

$$A_- = \frac{i}{k} \zeta_0 (\omega - U_1 k), \quad A_+ = \frac{i}{k} \zeta_0 (U_2 k - \omega). \quad (16.402)$$

Putting this into Eq. (16.401), follows

$$\begin{aligned} \rho_1 \left(-i\omega \frac{i}{k} \zeta_0 (\omega - U_1 k) + ik U_1 \frac{i}{k} \zeta_0 (\omega - U_1 k) + g\zeta_0 \right) &= \rho_2 \left(-i\omega \frac{i}{k} \zeta_0 (U_2 k - \omega) + ik U_2 \frac{i}{k} \zeta_0 (U_2 k - \omega) + g\zeta_0 \right) \\ \Leftrightarrow \rho_1 \left(\frac{\omega}{k} (\omega - U_1 k) - U_1 (\omega - U_1 k) + g \right) &= \rho_2 \left(\frac{\omega}{k} (U_2 k - \omega) - U_2 (U_2 k - \omega) + g \right) \\ \Leftrightarrow \rho_1 (\omega (\omega - U_1 k) - k U_1 (\omega - U_1 k) + kg) &= \rho_2 (\omega (U_2 k - \omega) - U_2 k (U_2 k - \omega) + kg). \end{aligned} \quad (16.403)$$

This is a quadratic equation for ω , i.e. a dispersion relation. Further algebraic transformation results

$$\omega^2 - 2k\omega \frac{\rho_1 U_1 + \rho_2 U_2}{\rho_1 + \rho_2} - kg \frac{\rho_2 - \rho_1}{\rho_1 + \rho_2} + k^2 \frac{U_1^2 \rho_1 + U_2^2 \rho_2}{\rho_1 + \rho_2} = 0. \quad (16.404)$$

This gives two solutions for the angular frequency:

$$\omega_{\pm} = \frac{\rho_1 U_1 k + \rho_2 U_2 k}{\rho_1 + \rho_2} \pm \left[kg \frac{\rho_2 - \rho_1}{\rho_1 + \rho_2} - k^2 \frac{U_1^2 \rho_1 \rho_2 + U_2^2 \rho_1 \rho_2 - 2 \rho_1 \rho_2 U_1 U_2}{(\rho_1 + \rho_2)^2} \right]^{1/2}$$

$$\Leftrightarrow \omega_{\pm} = \frac{\rho_1 U_1 k + \rho_2 U_2 k}{\rho_1 + \rho_2} \pm \left[kg \frac{\rho_2 - \rho_1}{\rho_1 + \rho_2} - k^2 \rho_1 \rho_2 \frac{(U_1 - U_2)^2}{(\rho_1 + \rho_2)^2} \right]^{1/2} \quad (16.405)$$

Instability exists in the case

$$kg \frac{\rho_2 - \rho_1}{\rho_1 + \rho_2} - k^2 \rho_1 \rho_2 \frac{(U_1 - U_2)^2}{(\rho_1 + \rho_2)^2} < 0$$

$$\Leftrightarrow kg \frac{\rho_2 - \rho_1}{\rho_1 + \rho_2} < k^2 \rho_1 \rho_2 \frac{(U_1 - U_2)^2}{(\rho_1 + \rho_2)^2}$$

$$\Leftrightarrow g(\rho_2^2 - \rho_1^2) < k \rho_1 \rho_2 (U_1 - U_2)^2, \quad (16.406)$$

so if

- the density difference is small enough,
- the wave is short enough or the
- speed difference is large enough.

An example is the formation of water surface waves under the influence of wind. One can assume that there are almost always spectral components in the wind field that satisfy the condition Eq. (16.406). The further development of the system over time can look different, e.g. B. this depends on whether the media can mix or not.

16.7.2.2 In continuous layering

Consider the xz plane again and ignore the Coriolis acceleration. You also do the Boussinesq approximation (see section 13.6). The momentum, continuity equations and the first law of thermodynamics read with σ as the potential density

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x}, \quad (16.407)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g, \quad (16.408)$$

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0, \quad (16.409)$$

$$\frac{\partial \sigma}{\partial t} + u \frac{\partial \sigma}{\partial x} + w \frac{\partial \sigma}{\partial z} = 0. \quad (16.410)$$

Now one assumes a vertically sheared background wind field $\bar{u}(z) = u(x, z, t) - u'(x, z, t)$, the vertical background wind $\bar{w}$ disappears. The background density $\bar{\rho}(z) = \rho(x, z, t) - \rho'(x, z, t)$ is in hydrostatic balance with the background pressure field $\bar{p}(z) = p(x, z, t) - p'(x, z, t)$, i.e

$$\frac{\partial \bar{p}}{\partial z} = -g \bar{\rho}. \quad (16.411)$$

Plugging this into the equations and linearizing them, you get

$$\frac{\partial u'}{\partial t} + \bar{u} \frac{\partial u'}{\partial x} + w \frac{\partial \bar{u}}{\partial z} = -\frac{1}{\rho} \frac{\partial p'}{\partial x} \approx -\frac{1}{\tilde{\rho}} \frac{\partial p'}{\partial x}, \quad (16.412)$$

$$\frac{\partial w}{\partial t} + \bar{u} \frac{\partial w}{\partial x} = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g \approx -\frac{1}{\tilde{\rho}} \frac{\partial p}{\partial z} - \frac{g\tilde{\rho}}{\tilde{\rho}} = -\frac{1}{\tilde{\rho}} \frac{\partial p'}{\partial z} - \frac{g\tilde{\rho}'}{\tilde{\rho}}, \quad (16.413)$$

$$\frac{\partial u'}{\partial x} + \frac{\partial w}{\partial z} = 0, \quad (16.414)$$

$$\frac{\partial \sigma'}{\partial t} + \bar{u} \frac{\partial \sigma'}{\partial x} + w \frac{\partial \bar{\sigma}}{\partial z} = 0. \quad (16.415)$$

In the x-component of the momentum equation, $\rho \rightarrow \tilde{\rho}$ was replaced in the denominator of the pressure gradient term, where $\tilde{\rho}$ denotes an average density assumed to be homogeneous; in the z-component, the right-hand side was multiplied by $\frac{\tilde{\rho}}{\rho}$ before Eq. (16.411) was used. The disturbance of the flow is divergence-free, so a current function $\psi = \psi(x, z, t)$ is used

$$u' = \frac{\partial \psi}{\partial z}, \quad w = -\frac{\partial \psi}{\partial x} \quad (16.416)$$

to. This means that the continuity equation is automatically fulfilled. The remaining three equations are

$$\frac{\partial^2 \psi}{\partial t \partial z} + \bar{u} \frac{\partial^2 \psi}{\partial z \partial x} - \frac{\partial \psi}{\partial x} \frac{\partial \bar{u}}{\partial z} = -\frac{1}{\tilde{\rho}} \frac{\partial p'}{\partial x}, \quad (16.417)$$

$$-\frac{\partial^2 \psi}{\partial t \partial x} - \bar{u} \frac{\partial^2 \psi}{\partial x^2} = -\frac{1}{\tilde{\rho}} \frac{\partial p'}{\partial z} - \frac{g\tilde{\rho}'}{\tilde{\rho}}, \quad (16.418)$$

$$\frac{\partial \sigma'}{\partial t} + \bar{u} \frac{\partial \sigma'}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial \bar{\sigma}}{\partial z} = 0. \quad (16.419)$$

Now you continue to do the approaches

$$\psi(x, z, t) = \psi_0(z) \exp[ik(x - ct)], \quad p'(x, z, t) = p_0(z) \exp[ik(x - ct)], \quad (16.420)$$

$$\rho'(x, z, t) = \rho_0(z) \exp[ik(x - ct)], \quad \sigma'(x, z, t) = \sigma_0(z) \exp[ik(x - ct)]. \quad (16.421)$$

It follows

$$-ikc \frac{d\psi_0}{dz} + \bar{u} ik \frac{d\psi_0}{dz} - ik\psi_0 \frac{\partial \bar{u}}{\partial z} = -ik \frac{p_0}{\tilde{\rho}}, \quad (16.422)$$

$$-k^2 c \psi_0 + \bar{u} k^2 \psi_0 = -\frac{1}{\tilde{\rho}} \frac{dp_0}{dz} - g \frac{\rho_0}{\tilde{\rho}}, \quad (16.423)$$

$$-ikc \sigma_0 + \bar{u} ik \sigma_0 - ik\psi_0 \frac{d\bar{\sigma}}{dz} = 0. \quad (16.424)$$

This results in simplification

$$-c \frac{d\psi_0}{dz} + \bar{u} \frac{d\psi_0}{dz} - \psi_0 \frac{\partial \bar{u}}{\partial z} = -\frac{p_0}{\tilde{\rho}}, \quad (16.425)$$

$$\psi_0 k^2 (\bar{u} - c) = -\frac{1}{\tilde{\rho}} \frac{dp_0}{dz} - g \frac{\rho_0}{\tilde{\rho}}, \quad (16.426)$$

$$\sigma_0 (\bar{u} - c) - \psi_0 \frac{d\bar{\sigma}}{dz} = 0. \quad (16.427)$$

If you differentiate the first equation according to z , you get

$$\frac{d^2 \psi_0}{dz^2} (\bar{u} - c) - \psi_0 \frac{d^2 \bar{u}}{dz^2} = -\frac{1}{\tilde{\rho}} \frac{dp_0}{dz}. \quad (16.428)$$

If you put Eq. (16.426), follows

$$(\bar{u} - c) \left[\frac{d^2 \psi_o}{dz^2} - k^2 \psi_o \right] - \psi_o \frac{d^2 \bar{u}}{dz^2} - g \frac{\rho_o}{\bar{\rho}} = 0. \quad (16.429)$$

To eliminate ρ_o , one first sets Eq. (16.427) to σ_o and gets

$$\sigma_o = \frac{\psi_o}{\bar{u} - c} \frac{d\bar{\sigma}}{dz}. \quad (16.430)$$

O.B.d. A. you can place the reference level in the level you are currently considering and use $\rho_o = \sigma_o$. This results in used

$$(\bar{u} - c) \left[\frac{d^2 \psi_o}{dz^2} - k^2 \psi_o \right] - \psi_o \frac{d^2 \bar{u}}{dz^2} - \frac{\psi_o}{\bar{u} - c} \frac{g}{\bar{\rho}} \frac{d\bar{\sigma}}{dz} = 0. \quad (16.431)$$

Here you set the Brunt-Väisälä frequency

$$N^2 := -\frac{g}{\bar{\rho}} \frac{d\bar{\sigma}}{dz} \quad (16.432)$$

one and receives

$$(\bar{u} - c) \left(\frac{d^2}{dz^2} - k^2 \right) \psi + \left(\frac{N^2}{\bar{u} - c} - \frac{d^2 \bar{u}}{dz^2} \right) \psi = 0. \quad (16.433)$$

This equation is called *Taylor-Goldstein equation*. It is an eigenvalue problem $\{\psi, c\}$ for the function ψ with the eigenvalue c depending on $\bar{u}(z)$. If $\{\psi, c\}$ is a solution, then $\{\psi^*, c^*\}$ is also a solution. A positive imaginary part of c means that ψ is an unstable solution. A shear $\bar{u} = \bar{u}(z)$ is stable if and only if all solutions of Eq. (16.433) have real eigenvalues. It is now further assumed that at $z = 0, H$ the boundary conditions $w = 0$ apply, from which it follows

$$\psi(0) = \psi(H) = 0. \quad (16.434)$$

Now define φ by

$$\psi = \sqrt{\bar{u} - c} \varphi. \quad (16.435)$$

Differentiating according to z gives

$$\frac{d\psi}{dz} = \frac{1}{2} \frac{1}{\sqrt{\bar{u} - c}} \varphi \frac{d\bar{u}}{dz} + \sqrt{\bar{u} - c} \frac{d\varphi}{dz}, \quad (16.436)$$

$$\Rightarrow \frac{d^2 \psi}{dz^2} = \frac{1}{\sqrt{\bar{u} - c}} \frac{d\bar{u}}{dz} \frac{d\varphi}{dz} - \frac{1}{4} \frac{1}{\sqrt{\bar{u} - c}^3} \varphi \left(\frac{d\bar{u}}{dz} \right)^2 + \frac{1}{2} \frac{1}{\sqrt{\bar{u} - c}} \frac{d^2 \bar{u}}{dz^2} \varphi + \sqrt{\bar{u} - c} \frac{d^2 \varphi}{dz^2}. \quad (16.437)$$

Putting this into Eq. (16.433) and dividing by $\sqrt{\bar{u} - c}$, you get

$$\frac{d}{dz} \left[(\bar{u} - c) \frac{d\varphi}{dz} \right] - \left[k^2 (\bar{u} - c) + \frac{1}{2} \frac{d^2 \bar{u}}{dz^2} + \frac{1}{\bar{u} - c} \left(\frac{1}{4} \left(\frac{d\bar{u}}{dz} \right)^2 - N^2 \right) \right] \varphi = 0. \quad (16.438)$$

The boundary conditions remain under the assumption $c \neq \bar{u}$

$$\varphi(0) = \varphi(H) = 0. \quad (16.439)$$

The Eq. (16.438) is now multiplied by φ^* :

$$\varphi^\star \frac{d}{dz} \left[(\bar{u} - c) \frac{d\varphi}{dz} \right] - \left[k^2 (\bar{u} - c) + \frac{1}{2} \frac{d^2 \bar{u}}{dz^2} + \frac{1}{\bar{u} - c} \left(\frac{1}{4} \left(\frac{d\bar{u}}{dz} \right)^2 - N^2 \right) \right] |\varphi|^2 = 0. \quad (16.440)$$

If you integrate the first term from 0 to H , it follows using partial integration

$$\int_0^H \varphi^\star \frac{d}{dz} \left[(\bar{u} - c) \frac{d\varphi}{dz} \right] dz = - \int_0^H (\bar{u} - c) \left| \frac{d\varphi}{dz} \right|^2 dz. \quad (16.441)$$

Eq. (16.440) is now integrated from 0 to H :

$$\int_0^H \left[N^2 - \frac{1}{4} \left(\frac{d\bar{u}}{dz} \right)^2 \right] \frac{|\varphi|^2}{\bar{u} - c} dz = \int_0^H (\bar{u} - c) \left(\left| \frac{d\varphi}{dz} \right|^2 + k^2 |\varphi|^2 \right) + \frac{1}{2} \frac{d^2 \bar{u}}{dz^2} |\varphi|^2 dz. \quad (16.442)$$

Now write for the phase velocity

$$c = c_r + ic_i \quad (16.443)$$

with $c_r, c_i \in \mathbb{R}$. The imaginary part of Eq. (16.442) is written as

$$\begin{aligned} c_i \int_0^H \left[N^2 - \frac{1}{4} \left(\frac{d\bar{u}}{dz} \right)^2 \right] \frac{|\varphi|^2}{|\bar{u} - c|^2} dz &= -c_i \int_0^H \left(\left| \frac{d\varphi}{dz} \right|^2 + k^2 |\varphi|^2 \right) dz \\ \Rightarrow c_i \int_0^H \left[N^2 - \frac{1}{4} \left(\frac{d\bar{u}}{dz} \right)^2 \right] \frac{|\varphi|^2}{|\bar{u} - c|^2} + \left| \frac{d\varphi}{dz} \right|^2 + k^2 |\varphi|^2 dz &= 0. \end{aligned} \quad (16.444)$$

If $N^2 - \frac{1}{4} \left(\frac{d\bar{u}}{dz} \right)^2 > 0$ everywhere in the interval $(0, H)$, then $c_i = 0$. One defines the *Richardson number* R_i by

$$R_i := \frac{N^2}{\left(\frac{d\bar{u}}{dz} \right)^2}. \quad (16.445)$$

The frequency

$$M := \frac{d\bar{u}}{dz} \quad (16.446)$$

is called *Prandtl frequency*. The condition

$$R_i > \frac{1}{4} \text{ überall in } (0, H) \quad (16.447)$$

is sufficient for stability.

16.7.3 Barotropic instability

Assume a western base current $U > 0$ that depends only on y

$$U = U(y) \quad (16.448)$$

and a disorder

$$\mathbf{v}'_h = (u, v)^T = \mathbf{k} \times \nabla \psi \quad (16.449)$$

with a current function ψ . Consider a zonal channel of extent $2b$ with $b > 0$, the line $y = 0$ lies in the middle of this channel. The boundary conditions are $\omega = 0$ at $p = 0$ and $p = p_0$ and $v = 0$ at $y = \pm b$. Then the horizontal wind is divergence-free and the *barotropic vorticity equation* can be applied,

$$\frac{\partial \zeta}{\partial t} + \beta v + u \frac{\partial \zeta}{\partial x} + v \frac{\partial \zeta}{\partial y} = 0. \quad (16.450)$$

Let β be homogeneous, see section 13.9.2. If you do a perturbation approach according to Sect. 16.3, you get

$$\frac{\partial \zeta'}{\partial t} + \beta v + U \frac{\partial \zeta'}{\partial x} + v \frac{\partial \bar{\zeta}}{\partial y} = 0. \quad (16.451)$$

Here the vorticity was written $\zeta = \bar{\zeta} + \zeta'$ with $\bar{\zeta}$ as the vorticity of U and ζ' as the vorticity of ψ'_h . Set ψ for the perturbation

$$\psi(x, y, t) = Y(y) \psi_0 e^{i(kx - \omega t)} \quad (16.452)$$

to. With $Y(\pm b) \stackrel{!}{=} 0$ the boundary conditions on v are satisfied, one also obtains

$$v = \frac{\partial \psi}{\partial x} = ik\psi, \quad (16.453)$$

$$\zeta' = \Delta \psi = -k^2 \psi + Y'' \psi_0 e^{i(kx - \omega t)}, \quad (16.454)$$

$$\frac{\partial \zeta'}{\partial x} = -ik^3 \psi + Y'' \psi_0 ik e^{i(kx - \omega t)}. \quad (16.455)$$

$$(16.456)$$

Plugging this into the barotropic vorticity equation and subtracting $\psi_0 e^{i(kx - \omega t)}$, you get

$$\begin{aligned} i\omega k^2 Y - i\omega Y'' + \beta ikY - Uik^3 Y + Y'' ikU - ikY \frac{d^2 U}{dy^2} &= 0 \\ \Leftrightarrow \omega k^2 Y - \omega Y'' + \beta kY - Uk^3 Y + Y'' kU - kY \frac{d^2 U}{dy^2} &= 0. \end{aligned} \quad (16.457)$$

Instability means that ω is not purely real,

$$\omega = \omega_r + i\omega_c, \quad (16.458)$$

with $\omega_r, \omega_c \in \mathbb{R} \setminus \{0\}$. Inserting into Eq. (16.457) returns

$$k^2 Y(\omega_r + i\omega_c) - Y''(\omega_r + i\omega_c) + \beta kY - Uk^3 Y + Y'' kU = 0. \quad (16.459)$$

The imaginary part of this is

$$k^2 Y\omega_c - Y''\omega_c = 0 \Leftrightarrow Y'' = k^2 Y. \quad (16.460)$$

Substituting this into the real part, you get

$$k^2 Y\omega_r - k^2 Y\omega_r + \beta kY - Uk^3 Y + Uk^3 Y - kY \frac{d^2 U}{dy^2} = 0 \Rightarrow \frac{d^2 U}{dy^2} = \beta. \quad (16.461)$$

this is a necessary condition. If you put Eq. (16.461), Eq. (16.457) (we don't yet know whether ω is real)

$$\omega k^2 Y - \omega Y'' - Uk^3 Y + Y'' kU = 0. \quad (16.462)$$

Assuming a jet-shaped background wind

$$U(y) = U_{\min} + \frac{\mathbf{I}}{2} (U_{\max} - U_{\min}) \left(\mathbf{I} + e^{i\frac{y\pi}{b}} \right) \quad (16.463)$$

with $U_{\min}, U_{\max} > 0$, one obtains in the imaginary part of Eq. (16.462)

$$k^3 Y \frac{\mathbf{I}}{2} (U_{\max} - U_{\min}) \sin\left(\frac{y\pi}{b}\right) = Y'' k \frac{\mathbf{I}}{2} (U_{\max} - U_{\min}) \sin\left(\frac{y\pi}{b}\right), \quad (16.464)$$

so is

$$Y'' = k^2 Y. \quad (16.465)$$

The fact that a state is unstable does not necessarily mean that it will collapse. However, an arbitrarily small initial deflection v is sufficient to generate an exponentially increasing disturbance. In reality one can assume the existence of such a very small initial disturbance, so that instability in reality always leads to the collapse of the basic state.

16.7.4 Baroclinic instability

For the expression under the root in Eq. (16.311) now becomes an abbreviation

$$g = g(\bar{u}_T, k) := \frac{\beta^2 K^4}{4k^2} + \bar{u}_T^2 k^2 (k^4 - K^4) \quad (16.466)$$

defined. In the case $g < 0$ applies

$$\omega = \omega_r + i \frac{\mathbf{I}}{k^2 + K^2} \omega'_i \quad (16.467)$$

with

$$\omega'_i := \pm \sqrt{|g(\bar{u}_T, k)|}. \quad (16.468)$$

This means that in the case of the negative sign the amplitude increases exponentially, so there is instability. Define

$$N := \frac{\omega'_i}{k^2 + K^2} = \frac{\sqrt{|g(\bar{u}_T, k)|}}{k^2 + K^2}, \quad (16.469)$$

this is the growth constant of the disorder. So it applies in the unstable case

$$N^2 + \frac{g}{(k^2 + K^2)^2} = N^2 + \frac{\frac{\beta^2 K^4}{4k^2} + \bar{u}_T^2 k^2 (k^4 - K^4)}{(k^2 + K^2)^2} = 0. \quad (16.470)$$

At this point a dimensionless circular wave number is defined

$$\kappa := \frac{k}{K}, \quad (16.471)$$

that follows

$$\begin{aligned} N^2 + \frac{\frac{\beta^2}{4k^2} + \bar{u}_T^2 k^2 (\kappa^2 + \mathbf{I})(\kappa^2 - \mathbf{I})}{(\kappa^2 + \mathbf{I})^2} &= N^2 + \frac{\beta^2}{4k^2 (\kappa^2 + \mathbf{I})^2} + \bar{u}_T^2 k^2 \frac{\kappa^2 - \mathbf{I}}{\kappa^2 + \mathbf{I}} = 0 \\ \Rightarrow N^2 + \frac{\beta^2}{4k^2 (\kappa^2 + \mathbf{I})^2} + \frac{\beta^2}{K^2} \bar{u}_T^2 \kappa^2 \frac{\kappa^2 - \mathbf{I}}{\kappa^2 + \mathbf{I}} &= 0 \end{aligned} \quad (16.472)$$

with a dimensionless thermal wind

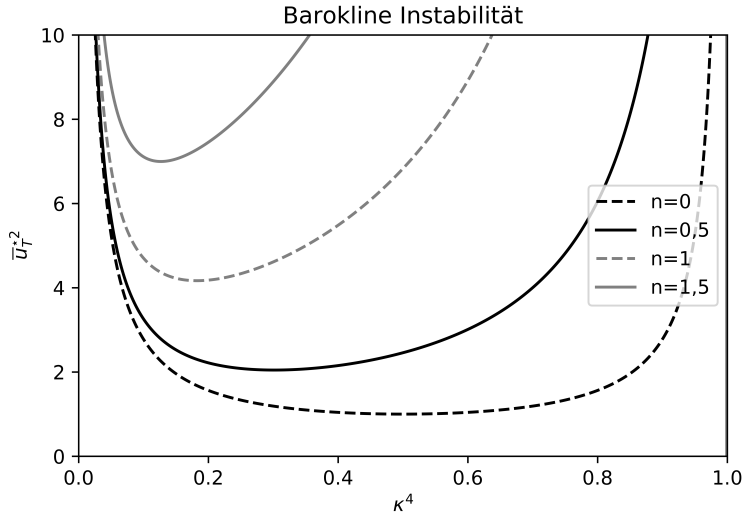


Figure 16.7: The wind shear required for certain growth rates as a function of wave number.

$$\bar{u}_T^* := \frac{\bar{u}_T K^2}{\beta}. \quad (16.473)$$

From this it follows

$$\frac{N^2 K^2}{\kappa^2 \beta^2} + \frac{1}{4\kappa^4 (\kappa^2 + 1)^2} + \bar{u}_T^{*2} \frac{\kappa^2 - 1}{\kappa^2 + 1} = 0 \quad (16.474)$$

With the dimensionless growth rate

$$n := \frac{NK}{\kappa\beta} \quad (16.475)$$

you can do this as

$$n^2 + \frac{1}{4\kappa^4 (\kappa^2 + 1)^2} + \bar{u}_T^{*2} \frac{\kappa^2 - 1}{\kappa^2 + 1} = 0 \quad (16.476)$$

note down. If you convert this to $\bar{u}_T^{*2}$, it follows

$$\bar{u}_T^{*2} = n^2 \frac{1 + \kappa^2}{1 - \kappa^2} + \frac{1}{4\kappa^4 (1 - \kappa^4)}. \quad (16.477)$$

Fig. 16.7 shows the thermal wind shear required for different wave numbers and growth rates. From the definitions of κ and $\bar{u}_T^*$ it is clear that as thermal stability decreases, one moves to the top left in this representation, i.e. towards baroclinic lability.

In baroclinic instability, potential energy of the stratification, which is continually generated by the radiation field, is converted into kinetic energy of the horizontal wind before it is dissipated.

There is no mathematically exact definition of whether a flow field is turbulent or not. It can be assumed that any flow field, if viewed from a sufficiently large distance, will appear turbulent. However, if you zoom in far enough, you will usually find a scale on which the field makes a *laminar* impression, which is understood as the opposite of turbulence. If this scale is the molecular scale, *full turbulence* is present.

17.1 Basics

Define an averaging operator by

$$\bar{f} := \frac{1}{\mu(\Omega)} \int_{\Omega} f d\omega, \quad (17.1)$$

where Ω should be an arbitrary spatial and/or temporal quantity, $\mu(\Omega)$ its measure, f an arbitrary function of space and time and $d\omega$ a suitable differential. Now you can use f in the form

$$f \equiv \bar{f} + f' \quad (17.2)$$

dismantle; For this purpose, the fluctuation or turbulence is defined by

$$f' := f - \bar{f}. \quad (17.3)$$

If the statements

$$\overline{\frac{\partial f}{\partial x_i}} = \frac{\partial \bar{f}}{\partial x_i}, \quad (17.4)$$

$$\frac{\partial \bar{f}}{\partial t} = \frac{\partial \bar{f}}{\partial t}, \quad (17.5)$$

$$\overline{f'g} = 0 \quad (17.6)$$

with an arbitrary field g , $\bar{f}$ is called *Reynolds operator* and the corresponding averaging is called *Reynolds averaging*. It is easy to realize that this also results in the two statements

$$\bar{f'} = 0, \quad \bar{\bar{f}} = \bar{f} \quad (17.7)$$

consequences. At this point we don't care about what such an operator could actually look like; in Section 17.1.2 it will be stated that the usual averaging operators are not Reynolds operators. From now on, however, Eq. (17.1) is used, instead the *Hesselberg mean*

$$\langle f \rangle := \frac{1}{\int_{\Omega} \varrho d\omega} \int_{\Omega} \varrho f d\omega \quad (17.8)$$

used, where ϱ is the density. You now write for the fluctuation

$$f'' := f - \langle f \rangle. \quad (17.9)$$

It is now assumed that the Hesselberg mean is a Reynolds operator. Applying this to the dry adiabatic system of equations follows

$$\frac{\partial \bar{\mathbf{v}}}{\partial t} = -(\bar{\mathbf{v}} \cdot \nabla) \bar{\mathbf{v}} - \overline{(\mathbf{v}'' \cdot \nabla) \mathbf{v}''} - \bar{a} \frac{\partial \bar{p}}{\partial x} - \overline{a'' \frac{\partial p'}{\partial x}} - \mathbf{f} \times \bar{\mathbf{v}} + \mathbf{g}, \quad (17.10)$$

$$\frac{\partial \bar{\theta}}{\partial t} = -\bar{\mathbf{v}} \cdot \nabla \bar{\theta} - \overline{\mathbf{v}'' \cdot \nabla \theta''}, \quad (17.11)$$

$$\frac{\partial \bar{\rho}}{\partial t} = -\bar{\rho} \nabla \cdot \bar{\mathbf{v}} - \bar{\mathbf{v}} \cdot \nabla \bar{\rho} - \overline{\rho'' \nabla \cdot \mathbf{v}''} - \overline{\mathbf{v}'' \cdot \nabla \rho''}, \quad (17.12)$$

$$\bar{p}a = R_d \bar{T} - \overline{p'' a''}. \quad (17.13)$$

The prognostic equations of the averaged fields are therefore corrected compared to those of the unaveraged fields by terms of the form $\overline{f''g''}$, where f, g are linear in the fields and their derivatives. These terms are referred to as the convergences of the *turbulent correlation flow*. These of course depend on the size of the quantity being averaged over, i.e. h. in the case of a numerical model, it depends on the resolution. As the averaging amount becomes smaller and smaller, the covariance terms become less important until they finally disappear completely.

However, there are no prognostic equations for the turbulent quantities, which is referred to as the *closure problem*. To further specify the correlation terms in the momentum equation, one applies the Reynolds averaging operator to Eq. (8.15), you get like this

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla p + \nabla \cdot \Pi - \rho \mathbf{g} + \nabla \cdot \tilde{\Pi} = 0, \quad (17.14)$$

where the horizontal lines have been omitted for clarity. Furthermore, the *turbulence correlation tensor* $\tilde{\Pi}$ is through

$$\tilde{\Pi} := \rho \begin{pmatrix} \overline{u''u''} & \overline{u''v''} & \overline{u''w''} \\ \overline{v''u''} & \overline{v''v''} & \overline{v''w''} \\ \overline{w''u''} & \overline{w''v''} & \overline{w''w''} \end{pmatrix} =: \begin{pmatrix} \tilde{\Pi}_{x,x} & \tilde{\Pi}_{x,y} & \tilde{\Pi}_{x,z} \\ \tilde{\Pi}_{y,x} & \tilde{\Pi}_{y,y} & \tilde{\Pi}_{y,z} \\ \tilde{\Pi}_{z,x} & \tilde{\Pi}_{z,y} & \tilde{\Pi}_{z,z} \end{pmatrix} \quad (17.15)$$

defined. It was justified by the assumption

$$\left| \frac{\rho''}{\bar{\rho}} \right| \ll \left| \frac{u''}{\bar{u}} \right| \quad (17.16)$$

went out. $-\nabla \cdot \tilde{\Pi}$ provides the *Eddy stress terms*, which are reflected in the momentum equation and instead of the $-\overline{(\mathbf{v}'' \cdot \nabla) \mathbf{v}''} - \overline{a'' \frac{\partial p'}{\partial x}}$ can be used.

17.1.1 Turbulent dissipation

Analogous to the molecular dissipation ε (see equation (8.66)), one can have a *turbulent dissipation* associated with the turbulence

$$\varepsilon_{\text{turb}} := \frac{1}{\rho} \sum_{i,j=1}^3 -\tilde{\Pi}_{i,j} S_{i,j} = \frac{1}{\rho} \sum_{i,j=1}^3 -\tilde{\Pi}_{i,j} \frac{\partial v_j}{\partial x_i} \quad (17.17)$$

define. Since there is no explicit formula for $\tilde{\Pi}$, one cannot find a turbulent analogue to Eq. Find (8.90): The sign of $\varepsilon_{\text{turb}}$ remains undetermined.

17.1.2 Concrete averaging operators

Let f be a scalar or vector function of position and time. A general averaging operator $\bar{f}$ is defined by

$$\bar{f}(x_i) := \frac{\int_{\Omega} f(x_i) h(x_i) dx_1 \dots dx_n}{\int_{\Omega} h(x_i) dx_1 \dots dx_n}, \quad (17.18)$$

where the time t should be understood as one of the x_i and h represents a weighting function.

17.1.2.1 Moving time average

The *moving time average* with the averaging length T is obtained from Eq. (17.18) with $\Omega = (t - \frac{T}{2}, t + \frac{T}{2})$ and $h = 1$, so

$$\bar{f}(\mathbf{r}, t) = \frac{1}{T} \int_{t-\frac{T}{2}}^{t+\frac{T}{2}} f(\mathbf{r}, t') dt'. \quad (17.19)$$

One now checks whether this operator fulfills the properties of a Reynolds operator equations (17.4) - (17.6). First of all

$$\frac{\partial \bar{f}}{\partial x_i} = \frac{1}{T} \int_{t-\frac{T}{2}}^{t+\frac{T}{2}} \frac{\partial f}{\partial x_i}(\mathbf{r}, t') dt' = \overline{\frac{\partial f}{\partial x_i}}, \quad (17.20)$$

Eq. (17.4) is therefore fulfilled. The verification of the fulfillment of Eq. (17.5) is done using the main theorem of differential and integral calculus:

$$\frac{\partial \bar{f}}{\partial t} = \frac{f(\mathbf{r}, t + \frac{T}{2}) - f(\mathbf{r}, t - \frac{T}{2})}{T} = \frac{1}{T} \int_{t-\frac{T}{2}}^{t+\frac{T}{2}} \frac{\partial f}{\partial t'}(\mathbf{r}, t') dt' = \overline{\frac{\partial f}{\partial t}} \quad (17.21)$$

The first two properties are therefore fulfilled. For the third one calculates with $g = 1$

$$\bar{\bar{f}} = \frac{1}{T} \int_{t-\frac{T}{2}}^{t+\frac{T}{2}} f(\mathbf{r}, t') - \bar{f}(\mathbf{r}, t') dt' \stackrel{!}{=} 0. \quad (17.22)$$

This should apply to any point in time, so it follows from this

$$\bar{\bar{f}} = f \quad (17.23)$$

at all times as a criterion for the validity of Eq. (17.6) for the simple case $g = 1$, which is only the case for linear functions f .

17.1.2.2 Hesselberg means

If you put in Eq. (17.18) the case $h = \rho$, one obtains the Hesselberg mean already mentioned in the introduction. For this you note the decomposition

$$f = \langle f \rangle + f'', \quad (17.24)$$

to use the Hesselberg mean from other averages such as B. the moving time average or a general Reynolds operator.

17.1.2.3 Low pass

The Fourier transform $\tilde{f}(k)$ of a field $f = f(x)$ is

$$\tilde{f}(k) \stackrel{\text{Glg. (C.3)}}{=} C \int_{-\infty}^{\infty} f(x) \exp(-ikx) dx. \quad (17.25)$$

The inverse Fourier transformation is according to Eq. (C.6) given by

$$f(x) = \tilde{C} \int_{-\infty}^{\infty} \tilde{f}(k) \exp(ikx) dk, \quad (17.26)$$

where according to Eq. (C.9) pay attention to $C\tilde{C} = 1/(2\pi)$. A low pass with the cutoff wave number $k^* > 0$ is given by the equation

$$\bar{f}(x) = \tilde{C} \int_{-k^*}^{k^*} f(x) \exp(ikx) dk \quad (17.27)$$

set. As already indicated by the notation $\bar{f}$, this is also a type of averaging operator. For the fluctuation f' one obtains

$$\begin{aligned} f'(x) &:= f(x) - \bar{f}(x) = \tilde{C} \int_{-\infty}^{\infty} f(x) \exp(ikx) dk - \tilde{C} \int_{-k^*}^{k^*} f(x) \exp(ikx) dk \\ &= \tilde{C} \int_{-\infty}^{-k^*} f(x) \exp(ikx) dk + \tilde{C} \int_{k^*}^{\infty} f(x) \exp(ikx) dk. \end{aligned} \quad (17.28)$$

17.2 Mixing path approach

However, the $\tau_{i,j}$ are still unknown quantities. In order to parameterize them (see also section 17.9), one uses the *mixing path approach*. It is assumed that the pressure gradient and Coriolis force do not play a significant role, which is why

$$\frac{D\mathbf{v}}{Dt} = 0 \quad (17.29)$$

follows what is called *Burgers equation*. Accordingly, every fluid particle moves along a straight, uniform path. However, this is not a completely sensible approach, but it does provide a useful way to parameterize the u'' , v'' , w'' . If a particle moves from z to $z + l$ while maintaining its horizontal velocity $\mathbf{v}_h$, Eq. (17.29)

$$\mathbf{v}_h''(z + l) = \mathbf{v}_h(z + l) - \overline{\mathbf{v}_h}(z + l) = \overline{\mathbf{v}_h}(z) - \overline{\mathbf{v}_h}(z + l) = \overline{\mathbf{v}_h}(z + l) - l \frac{\partial \overline{\mathbf{v}_h}}{\partial z} - \overline{\mathbf{v}_h}(z + l) = -l \frac{\partial \overline{\mathbf{v}_h}}{\partial z} \quad (17.30)$$

Please also note the sign of l , which must be understood as negative in the case of downward movement. This follows, for example:

$$\tau_{x,z} = -\overline{\rho u'' w''} = \overline{\rho w'' l} \frac{\partial \bar{u}}{\partial z}. \quad (17.31)$$

In the case of an indifferently layered atmosphere, $|w''|$ applies $\sim |\mathbf{v}_h''|$, which corresponds to the fact that in this case the horizontal scale of the vortices is the same size as the vertical one, one therefore sets

$$w'' = l \left| \frac{\partial \overline{\mathbf{v}_h}}{\partial z} \right|. \quad (17.32)$$

It follows

$$\tau_{x,z} = -\overline{\rho u' w'} = \rho \bar{l}^2 \left| \frac{\partial \overline{\mathbf{v}_h}}{\partial z} \right| \frac{\partial \bar{u}}{\partial z} \equiv A_z \frac{\partial \bar{u}}{\partial z}. \quad (17.33)$$

The coefficient

$$A_z := \rho \bar{l}^2 \left| \frac{\partial \overline{\mathbf{v}_h}}{\partial z} \right| \quad (17.34)$$

is called *Eddy exchange coefficient*.

17.2.1 Planetary boundary layer

The *planetary boundary layer* is defined as the lower layer of the atmosphere in which the *ground friction*, i.e. h. the existence of the earth's surface has an influence. This is where the balance of power comes in

$$-fv = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{1}{\rho} \frac{\partial \tau_{x,z}}{\partial z}, \quad (17.35)$$

$$fu = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{1}{\rho} \frac{\partial \tau_{y,z}}{\partial z}. \quad (17.36)$$

where the averaging operators have been omitted again for the sake of clarity. The horizontal correlation flows were also omitted at this point. If one also assumes that the density varies only slightly within the altitude interval under consideration, it follows

$$-fv = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{\partial}{\partial z} \left(\frac{\tau_{x,z}}{\rho} \right), \quad (17.37)$$

$$fu = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{\partial}{\partial z} \left(\frac{\tau_{y,z}}{\rho} \right). \quad (17.38)$$

One now assumes that the movement has only one x component and defines the so-called *frictional velocity* $u_\star > 0$ by

$$u_\star^2 := \frac{\tau_{x,z}}{\rho} = \frac{A_z}{\rho} \frac{\partial \bar{u}}{\partial z}. \quad (17.39)$$

So far it was assumed that the mixing path length l is independent of altitude. Very close to the Earth's surface, however, it can be expected that the vertical extent of the vortices increases with height, which is what can be seen in the simplest case

$$l(z) = kz \quad (17.40)$$

can express, where the number $k > 0$ is called *von Karman constant*. This has a typical value of 0.4. Eq. (17.40) is only valid up to a certain height. Thus follows

$$u_\star^2 = k^2 z^2 \left| \frac{\partial \bar{u}}{\partial z} \right|^2, \quad (17.41)$$

so in the case $\frac{\partial \bar{u}}{\partial z} > 0$

$$u_\star = kz \frac{\partial \bar{u}}{\partial z}. \quad (17.42)$$

The solution for $\bar{u}(z)$ is the logarithmic wind profile

$$\bar{u}(z) = \frac{u_\star}{k} \ln \left(\frac{z}{z_o} \right). \quad (17.43)$$

The constant $z_o > 0$ is the *roughness length*, $\bar{u}(z_o) = 0$. Eq. (17.43) should only be used for $z > z_o$.

The layer in which Eq. (17.40) is a good approximation, is called *Prandtl layer*. It typically has dimensions of one to two free mixing path lengths l . At the bottom it is limited by the *laminar sublayer*, which is $\sim 1 \text{ mm}$ thick and in which molecular diffusion predominates. Laminar sublayer and Prandtl layer taken together form the *surface layer*. The surface layer is bounded at the top by the *Ekman layer*.

17.2.1.1 Friction speed

For the friction speed $u_\star$ applies

$$\bar{u}(z_\star) \stackrel{!}{=} u_\star \Leftrightarrow 1 = \frac{1}{k} \ln \left(\frac{z_\star}{z_o} \right) \Leftrightarrow z_\star = z_o \exp(k). \quad (17.44)$$

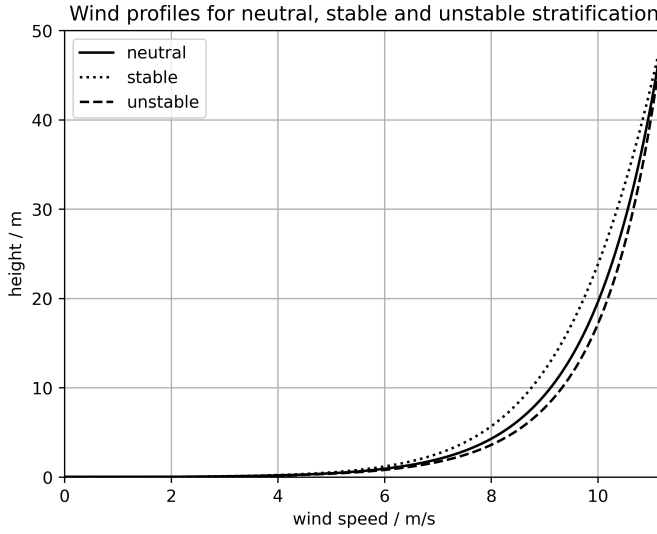


Figure 17.1: Wind profiles at a given wind speed at a height of 50 m.

The friction speed is therefore the wind speed that prevails at the height $z_* = z_o e^k \approx 1.5 z_o$. If you know the wind U at height z (for example the lowest layer of a model), the friction speed can be calculated from Eq. (17.43) determine:

$$U = \frac{u_*}{k} \ln \left(\frac{z}{z_o} \right) \Leftrightarrow u_* = \frac{Uk}{\ln \left(\frac{z}{z_o} \right)}. \quad (17.45)$$

17.2.1.2 Stable or unstable stratification

The previous derivations in this section were based on the assumption of indifferent stratification. In the case of unstable or stable stratification, the mixing path length is no longer simply given by Eq. (17.40) given. In the case of unstable stratification, the particles can oscillate further vertically, i.e. $l > \kappa z$, in the case of unstable stratification they can oscillate less, i.e. $l < \kappa z$. In [30], expressions for this are derived from small-scale simulations, which are:

$$l = \begin{cases} \frac{\kappa z}{3.7}, & \zeta \geq 1, \\ \frac{\kappa z}{1+2.7\zeta}, & 0 \leq \zeta < 1, \\ \kappa z (1 - 1.00\zeta)^{0.2}, & \zeta < 0 \end{cases} \quad (17.46)$$

with

$$\zeta := \frac{z}{L}, \quad (17.47)$$

here L is the Monin-Obukhov length.

We further generalize Eq. (17.43)

$$\bar{u}(z) = \frac{u_*}{k} \left[\ln \left(\frac{z}{z_o} \right) - \psi_m(\zeta) \right], \quad (17.48)$$

ψ_m is an auxiliary function that modifies the logarithmic wind profile. In the case of indifferent stratification $\psi_m = 0$. Fig. 17.1 shows with Eq. (17.48) calculated wind profiles.

The friction speed results from this:

$$u_* = \frac{Uk}{\ln \left(\frac{z}{z_o} \right) - \psi_m \left(\frac{z}{L} \right)}. \quad (17.49)$$

17.3 Ekman transport

The *Ekman transport* occurs wherever a geostrophic medium meets a horizontal boundary at which the adhesion condition applies. Define the *eddy viscosity coefficient* K by

$$K := \frac{A_z}{\rho}, \quad (17.50)$$

is written Eq. (17.33) as

$$\tau_{x,z} = K\rho \frac{\partial \bar{u}}{\partial z}. \quad (17.51)$$

Under the assumption $\frac{\partial}{\partial z}(K\rho) = 0$, which is only a useful assumption above the Prandtl layer, holds

$$\frac{1}{\rho} \frac{\partial \tau_{x,z}}{\partial z} = K \frac{\partial^2 \bar{u}}{\partial z^2}. \quad (17.52)$$

The equations (17.35) - (17.36) then become

$$0 = f\tilde{v} + K \frac{\partial^2 \bar{u}}{\partial z^2}, \quad 0 = -f\tilde{u} + K \frac{\partial^2 \bar{v}}{\partial z^2}. \quad (17.53)$$

It became the definition

$$\tilde{u} := \bar{u} - u_g, \quad \tilde{v} := \bar{v} - v_g \quad (17.54)$$

with $\mathbf{v}_{h,g} = (u_g, v_g)^T$ used as the geostrophic wind. If you neglect the thermal wind, it follows

$$0 = f\tilde{v} + K \frac{\partial^2 \tilde{u}}{\partial z^2}, \quad 0 = -f\tilde{u} + K \frac{\partial^2 \tilde{v}}{\partial z^2} \quad \Rightarrow \quad \frac{if}{K}(\tilde{u} + i\tilde{v}) = \frac{\partial^2 (\tilde{u} + i\tilde{v})}{\partial z^2}. \quad (17.55)$$

This is solved by

$$\tilde{u} + i\tilde{v} = C \exp\left(\sqrt{\frac{if}{K}}z\right) + C_2 \exp\left(-\sqrt{\frac{if}{K}}z\right) \quad (17.56)$$

with $C, C_2 \in \mathbb{C}$. In the case of the lower limit of the atmosphere, the boundary conditions apply in the Northern Hemisphere

$$\lim_{z \rightarrow \infty} \tilde{u} + i\tilde{v} = 0 \Rightarrow C = 0, \quad (17.57)$$

$$(\tilde{u} + i\tilde{v})(z = 0) = -u_g - iv_g \Rightarrow C_2 = -u_g - iv_g, \quad (17.58)$$

and in the southern hemisphere

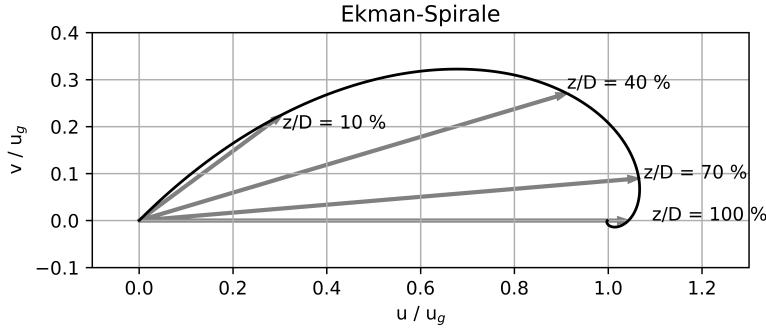
$$\lim_{z \rightarrow \infty} \tilde{u} + i\tilde{v} = 0 \Rightarrow C_2 = 0, \quad (17.59)$$

$$(\tilde{u} + i\tilde{v})(z = 0) = -u_g - iv_g \Rightarrow C = -u_g - iv_g, \quad (17.60)$$

so the solution is north of the equator

$$\tilde{u} + i\tilde{v} = -(u_g + iv_g) \exp\left(-\sqrt{\frac{if}{K}}z\right) = -(u_g + iv_g) \exp\left(-\sqrt{\frac{f}{2K}}z\right) \exp\left(-i\sqrt{\frac{f}{2K}}z\right) \quad (17.61)$$

and south of it

Figure 17.2: The Ekman spiral, it is $v_g = 0$.

$$\tilde{u} + i\tilde{v} = -(u_g + iv_g) \exp\left(-\sqrt{\frac{|f|}{2K}}z\right) = -(u_g + iv_g) \exp\left(-\sqrt{\frac{|f|}{2K}}z\right) \exp\left(i\sqrt{\frac{|f|}{2K}}z\right). \quad (17.62)$$

This can be generalized to:

$$\bar{u} = u_g - \left[\text{sign}(f) v_g \sin\left(\sqrt{\frac{|f|}{2K}}z\right) + u_g \cos\left(\sqrt{\frac{|f|}{2K}}z\right) \right] \exp\left(-\sqrt{\frac{|f|}{2K}}z\right), \quad (17.63)$$

$$\bar{v} = v_g + \left[\text{sign}(f) u_g \sin\left(\sqrt{\frac{|f|}{2K}}z\right) - v_g \cos\left(\sqrt{\frac{|f|}{2K}}z\right) \right] \exp\left(-\sqrt{\frac{|f|}{2K}}z\right). \quad (17.64)$$

You can o. B. d. A. Assuming $u_g > 0, v_g = 0$, then the following applies

$$\bar{u} = u_g - u_g \cos\left(\sqrt{\frac{|f|}{2K}}z\right) \exp\left(-\sqrt{\frac{|f|}{2K}}z\right), \quad (17.65)$$

$$\bar{v} = \text{sign}(f) u_g \sin\left(\sqrt{\frac{|f|}{2K}}z\right) \exp\left(-\sqrt{\frac{|f|}{2K}}z\right). \quad (17.66)$$

$\text{sign}(f) \rho \bar{v}$ is the mass flux density into the deep, so double partial integration is used

$$\begin{aligned} \int_0^\infty \sin(az) \exp(-\beta z) dz &= \frac{a}{\beta} \int_0^\infty \cos(az) \exp(-\beta z) dz = \frac{a}{\beta^2} - \frac{a^2}{\beta^2} \int_0^\infty \sin(az) \exp(-\beta z) dz \\ \Rightarrow \int_0^\infty \sin(az) \exp(-\beta z) dz &= \frac{\frac{a}{\beta^2}}{1 + \frac{a^2}{\beta^2}} = \frac{a}{\beta^2 + a^2}. \end{aligned} \quad (17.67)$$

In an isothermal atmosphere applies

$$a = \sqrt{\frac{|f|}{2K}}, \quad \beta = -\sqrt{\frac{|f|}{2K}} - \frac{1}{H} \quad (17.68)$$

$$\Rightarrow a^2 + \beta^2 = \frac{|f|}{K} + \frac{1}{H^2} + \sqrt{\frac{2|f|}{KH^2}} \Rightarrow \frac{a}{\beta^2 + a^2} = \frac{1}{\sqrt{\frac{2|f|}{K}} + \sqrt{\frac{2K}{|f|H^4}} + \frac{2}{H}} = \frac{H}{2 + H\sqrt{\frac{2|f|}{K}} + \sqrt{\frac{2K}{|f|H^2}}} \quad (17.69)$$

with $H \approx 8$ km as the scale height. From this it follows

$$\text{sign}(f) \int_0^\infty \rho \bar{v} dz = \frac{H}{2 + H \sqrt{\frac{2|f|}{K}} + \sqrt{\frac{2K}{fH}}} \quad (17.70)$$

for the mass flux density into the deep. The height D at which the wind is parallel to the geostrophic wind is often used as a technical definition of *Boundary layer thickness*. It applies

$$D = \sqrt{\frac{2K}{|f|}} \pi \quad (17.71)$$

There the wind speed is slightly higher than the geostrophic speed, which is why this height is also referred to as *gradient wind height*.

This allows the system of equations (17.65) - (17.66) to be written in the form

$$\bar{u} = u_g - u_g \cos\left(\frac{\pi}{D} z\right) \exp\left(-\frac{\pi}{D} z\right), \quad (17.72)$$

$$\bar{v} = \text{sign}(f) u_g \sin\left(\frac{\pi}{D} z\right) \exp\left(-\frac{\pi}{D} z\right). \quad (17.73)$$

note down. From observations we know that at a height of approx. 1 km the wind strives for its geostrophic value, and it follows from this

$$K \approx \frac{|f| D^2}{2\pi^2} \approx 5 \text{ m}^2/\text{s}. \quad (17.74)$$

This is over five orders of magnitude above the kinematic viscosity value of $1.5 \cdot 10^{-5} \text{ m}^2/\text{s}$. With Eq. (17.34) follows for the mixing path length

$$l = \sqrt{\frac{K}{\left|\frac{\partial \bar{v}_h}{\partial z}\right|}} \sim \sqrt{\frac{KD}{u_g}} \sim 2 \cdot 10^1 \text{ m}. \quad (17.75)$$

This corresponds to the expectation that $l \ll D$ must be for the mixing path concept to be meaningful in the planetary boundary layer. It follows from Eq. (17.40) a height D_P of the Prandtl layer of approx.

$$D_P = \frac{l}{k} = 50 \text{ m} \quad (17.76)$$

with $k = 0.4$. One defines the *Ekman number* Ek as the ratio of friction to Coriolis terms, i.e

$$\text{Ek} := \frac{KU}{H^2 f U} = \frac{K}{f H^2}, \quad (17.77)$$

where H is the characteristic vertical extent of the phenomenon. At small Ekman numbers, the friction force can be balanced by the Coriolis force. In the boundary layer one obtains an Ekman number of $\text{Ek} \sim 5\%$.

For a cyclone with radius R , the Ekman spiral leads to a pressure tendency $\frac{\partial p}{\partial t}$ of the order of magnitude

$$\frac{\partial p}{\partial t} \sim \frac{2g}{R} \frac{u_g \rho_0 a}{\beta^2 + \alpha^2}. \quad (17.78)$$

With $u_g \sim 10 \text{ m/s}$, $\rho_0 \approx 1.2 \text{ kg/m}^3$ and $R \sim 500 \text{ km}$

$$\frac{\partial p}{\partial t} \sim 2, 6 \frac{\text{hPa}}{\text{hr}}. \quad (17.79)$$

This is significantly lower than the value estimated in Sect. 13.10.2. The upper limit of the boundary layer is also the upper limit of the Ekman layer.

17.3.1 Importance of Eddy Viscosity

Eddy exchange coefficients A_{ij} and mixing path lengths l_x, l_y, l_z were introduced to examine the effects of turbulence, i.e. h. the subscale variability, to describe the resolved (averaged) fields. It is questionable how fundamental these quantities are, i.e. whether these are material properties or rather auxiliary variables.

First of all, it can be stated that at very fine resolution the diffusion coefficients describe the molecular flows, i.e. converge to the molecular physical diffusion coefficients. At a coarser resolution, however, the diffusive terms also contain turbulent components. However, in this chapter no explicit assumptions were made about the spatial or temporal scope of the averaging operators. On the other hand, it was implicitly assumed that the averaging operator is a Reynolds operator. This is only a realistic assumption if the turbulent fluctuations are small compared to the size of the averaging, but the averaging is not so extensive that synoptic-scale processes are affected. Such an averaging is, in a sense, superior to others, and so are the eddy exchange coefficients and mixing path lengths obtained with it.

17.3.2 Monin-Obukhov length

The length

$$L := -\frac{\bar{\theta} u_*^3}{kg(\overline{w'\theta'})} \quad (17.80)$$

is called *Monin-Obukhov length*.

17.3.3 Spin down

If one assumes time independence of the density, it follows from the continuity equation

$$\frac{\partial}{\partial z} (\rho w) = -\frac{\partial}{\partial x} (\rho u) - \frac{\partial}{\partial y} (\rho v). \quad (17.81)$$

Integrating this from $z = 0$ to $z = D$ under the assumption $w(z = 0) = 0$ gives

$$(\rho w)_D = -\int_0^D \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) dz. \quad (17.82)$$

If you put Eq. (17.73), you get

$$(\rho w)_D = -\text{sign}(f) \frac{\partial}{\partial y} \int_0^D \rho u_g \sin\left(\frac{\pi}{D} z\right) \exp\left(-\frac{\pi}{D} z\right) dz. \quad (17.83)$$

If you assume a homogeneous density, you get from this

$$w(D) = -\text{sign}(f) \frac{\partial u_g}{\partial y} \int_0^D \sin\left(\frac{\pi}{D} z\right) \exp\left(-\frac{\pi}{D} z\right) dz. \quad (17.84)$$

$\zeta_g = -\frac{\partial u_g}{\partial y}$ is the geostrophic vorticity, thus follows

$$w(D) = \text{sign}(f) \zeta_g \int_0^D \sin\left(\frac{\pi}{D} z\right) \exp\left(-\frac{\pi}{D} z\right) dz. \quad (17.85)$$

Again using partial integration one obtains

$$\begin{aligned}
\int_0^D \sin\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right) dz &= -\left[\frac{D}{\pi} \cos\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right)\right]_0^D - \int_0^D \cos\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right) dz \\
&= \frac{D}{\pi} (1 + e^{-\pi}) - \int_0^D \cos\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right) dz \\
&= \frac{D}{\pi} (1 + e^{-\pi}) - \left[\frac{D}{\pi} \sin\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right)\right]_0^D - \int_0^D \sin\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right) dz \\
\Rightarrow \int_0^D \sin\left(\frac{\pi}{D}z\right) \exp\left(-\frac{\pi}{D}z\right) dz &= \frac{D}{2\pi} (1 + e^{-\pi}) \approx \frac{D}{2\pi} = \sqrt{\frac{K}{2f}}.
\end{aligned} \tag{17.86}$$

This implies neglecting the approximately sign

$$w(D) = \text{sign}(f) \zeta_g \sqrt{\frac{K}{2|f|}}. \tag{17.87}$$

If you substitute $\zeta_g \sim 10^{-5}$, $f \sim 10^{-4}$, $K \sim 2$ in SI units, you get

$$w \sim 0, 1 \text{ cm/s}. \tag{17.88}$$

The quasi-geostrophic vorticity equation Eq. (13.219) is with a transformation into the z system, neglecting advection

$$\frac{\partial \zeta_g}{\partial t} = f \frac{\partial w}{\partial z}. \tag{17.89}$$

If you integrate this from D to the tropopause height z_T , you get $w(z = z_T) = 0$ under the assumption

$$\int_D^{z_T} \frac{\partial \zeta_g}{\partial t} dz = -f w(D). \tag{17.90}$$

Assuming that the geostrophic relative vorticity is height independent,

$$\frac{\partial \zeta_g}{\partial t} = -\frac{f}{z_T - D} w(D). \tag{17.91}$$

If you put Eq. (17.87), you get

$$\frac{\partial \zeta_g}{\partial t} = -\frac{\zeta_g}{z_T - D} \sqrt{\frac{K|f|}{2}} \approx -\zeta_g \sqrt{\frac{K|f|}{2z_T^2}}. \tag{17.92}$$

From this it follows, again ignoring the approximately sign,

$$\zeta_g(t) = \zeta_g(0) \exp\left(-\sqrt{\frac{K|f|}{2z_T^2}} t\right) = \zeta_g(0) \exp\left(-\frac{t}{\tau}\right) \tag{17.93}$$

with the *spin-down time*

$$\tau := z_T \sqrt{\frac{2}{K|f|}}. \tag{17.94}$$

If you substitute $z_T \sim 10^4$, $f \sim 10^{-4}$, $K \sim 2$ in SI units, you get

$$\tau \sim 10^6 \text{ s} \sim 10 \text{ d.} \quad (17.95)$$

17.4 Isotropic turbulence

17.4.1 Spectral form of the Navier-Stokes equations

For the Fourier transformation $\tilde{\mathbf{v}}(\mathbf{k}, t)$ of a velocity field $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$ applies

$$\tilde{\mathbf{v}}(\mathbf{k}, t) = C^3 \int_{\mathbb{R}^3} \mathbf{v}(\mathbf{r}, t) \exp(-i\mathbf{k} \cdot \mathbf{r}) d^3 r. \quad (17.96)$$

The inverse Fourier transform is

$$\mathbf{v}(\mathbf{r}, t) = \tilde{C}^3 \int_{\mathbb{R}^3} \tilde{\mathbf{v}}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k. \quad (17.97)$$

At this point you set $\tilde{C} = 1 \stackrel{\text{Eq. (C.9)}}{\Leftrightarrow} C = \frac{1}{2\pi}$ to shorten the notation and neglects the $\mathbb{R}^3$ on the integral. The incompressible momentum equation is:

$$\frac{\partial \mathbf{v}}{\partial t} = -\nabla \pi - \nabla \varphi - (\mathbf{v} \cdot \nabla) \mathbf{v} + r \Delta \mathbf{v}, \quad (17.98)$$

where the abbreviation

$$\pi := \frac{p}{\rho} \quad (17.99)$$

was used. The inverse Fourier transformations of the other occurring fields are:

$$\pi(\mathbf{r}, t) = \int \tilde{\pi}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k, \quad (17.100)$$

$$\varphi(\mathbf{r}) = \int \tilde{\varphi}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k. \quad (17.101)$$

This also applies to the application of the differential operators to the fields

$$\frac{\partial \mathbf{v}}{\partial t} = \int \frac{\partial \tilde{\mathbf{v}}(\mathbf{k}, t)}{\partial t} \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k, \quad (17.102)$$

$$-\nabla \pi = -i \int \mathbf{k} \tilde{\pi}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k, \quad (17.103)$$

$$-\nabla \varphi = -i \int \mathbf{k} \tilde{\varphi}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k, \quad (17.104)$$

$$\Delta \mathbf{v} = - \int \mathbf{k}^2 \tilde{\mathbf{v}}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3 k. \quad (17.105)$$

applies to momentum advection

$$\begin{aligned}
(\mathbf{v} \cdot \nabla) \mathbf{v} &= \left(\int \tilde{\mathbf{v}}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k \cdot \nabla \right) \int \tilde{\mathbf{v}}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k \\
&= \left(\int \tilde{\mathbf{v}}(\mathbf{k}', t) \exp(i\mathbf{k}' \cdot \mathbf{r}) d^3k' \cdot \nabla \right) \int \tilde{\mathbf{v}}(\mathbf{k}'', t) \exp(i\mathbf{k}'' \cdot \mathbf{r}) d^3k'' \\
&= \int \int \exp(i\mathbf{k}' \cdot \mathbf{r}) [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \nabla] [\tilde{\mathbf{v}}(\mathbf{k}'', t) \exp(i\mathbf{k}'' \cdot \mathbf{r})] d^3k' d^3k'' \\
&= i \int \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \mathbf{k}''] \tilde{\mathbf{v}}(\mathbf{k}'', t) \exp[i(\mathbf{k}' + \mathbf{k}'') \cdot \mathbf{r}] d^3k' d^3k''.
\end{aligned} \tag{17.106}$$

This implies

$$\begin{aligned}
\left[\widetilde{(\mathbf{v} \cdot \nabla) \mathbf{v}} \right](\mathbf{k}) &= \frac{i}{(2\pi)^3} \int \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \mathbf{k}'] \tilde{\mathbf{v}}(\mathbf{k}'', t) \exp[i(-\mathbf{k} + \mathbf{k}' + \mathbf{k}'') \cdot \mathbf{r}] d^3k' d^3k'' \\
&\stackrel{\text{Glg. (A.84)}}{=} i \int \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \mathbf{k}'] \tilde{\mathbf{v}}(\mathbf{k}'', t) \delta(\mathbf{k}' + \mathbf{k}'' - \mathbf{k}) d^3k' d^3k'' \\
&= i \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot (\mathbf{k} - \mathbf{k}')] \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) d^3k'
\end{aligned} \tag{17.107}$$

From the incompressible continuity equation

$$\nabla \cdot \mathbf{v} = 0 \tag{17.108}$$

follows

$$\mathbf{k} \cdot \tilde{\mathbf{v}}(\mathbf{k}, t) = 0. \tag{17.109}$$

This gives you

$$\left[\widetilde{(\mathbf{v} \cdot \nabla) \mathbf{v}} \right](\mathbf{k}) = i \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \mathbf{k}] \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) d^3k' \tag{17.110}$$

From the previous calculations one can put together the development of the momentum equation with respect to plane waves:

$$\begin{aligned}
&\int \left(\frac{\partial}{\partial t} + \nu \mathbf{k}^2 \right) \tilde{\mathbf{v}}(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k \\
&= i \int \left\{ -\mathbf{k} \tilde{\pi}(\mathbf{k}, t) - \mathbf{k} \tilde{\varphi}(\mathbf{k}) - \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \mathbf{k}] \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) d^3k' \right\} \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k
\end{aligned} \tag{17.111}$$

This must apply at every point in spectral space, so

$$\left(\frac{\partial}{\partial t} + \nu \mathbf{k}^2 \right) \tilde{\mathbf{v}}(\mathbf{k}, t) = -i\mathbf{k} \tilde{\pi}(\mathbf{k}, t) - i\mathbf{k} \tilde{\varphi}(\mathbf{k}) - i \int [\tilde{\mathbf{v}}(\mathbf{k}', t) \cdot \mathbf{k}] \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) d^3k'. \tag{17.112}$$

This is the spectral form of the incompressible momentum equation. From this it can be seen that the only term that contains interactions between scales is momentum advection.

17.4.2 Energy transfer function

How to get from the Parseval identity Eq. (C.31) can conclude, the specific kinetic energy with the wave vector $\mathbf{k}$ is determined by the size

$$\tilde{e}(\mathbf{k}, t) = \frac{1}{2} \tilde{v}(\mathbf{k}, t) \tilde{v}(-\mathbf{k}, t) \quad (17.113)$$

described. If you write down Eq. (17.112) with the substitution $\mathbf{k} \rightarrow -\mathbf{k}$, one obtains

$$\left(\frac{\partial}{\partial t} + r\mathbf{k}^2 \right) \tilde{v}(-\mathbf{k}, t) = i\mathbf{k}\tilde{\pi}(-\mathbf{k}, t) + i\mathbf{k}\tilde{\varphi}(-\mathbf{k}) + i \int [\tilde{v}(\mathbf{k}', t) \cdot \mathbf{k}] \tilde{v}(-\mathbf{k} - \mathbf{k}', t) d^3k'. \quad (17.114)$$

If you multiply Eq. (17.114) with $\tilde{v}(\mathbf{k}, t)$ and takes Eq. (17.109), you get

$$\tilde{v}(\mathbf{k}, t) \cdot \left(\frac{\partial}{\partial t} + r\mathbf{k}^2 \right) \tilde{v}(-\mathbf{k}, t) = i \int [\tilde{v}(\mathbf{k}', t) \cdot \mathbf{k}] [\tilde{v}(\mathbf{k}, t) \cdot \tilde{v}(-\mathbf{k} - \mathbf{k}', t)] d^3k'. \quad (17.115)$$

If you multiply analogously to Eq. (17.112) with $\tilde{v}(-\mathbf{k}, t)$, one obtains

$$\tilde{v}(-\mathbf{k}, t) \cdot \left(\frac{\partial}{\partial t} + r\mathbf{k}^2 \right) \tilde{v}(\mathbf{k}, t) = -i \int [\tilde{v}(\mathbf{k}', t) \cdot \mathbf{k}] [\tilde{v}(-\mathbf{k}, t) \cdot \tilde{v}(\mathbf{k} - \mathbf{k}', t)] d^3k' \quad (17.116)$$

If you add the equations (17.115) and (17.116) and divide by two, you get

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + 2r\mathbf{k}^2 \right) \tilde{e}(\mathbf{k}, t) \\ &= \frac{i}{2} \int [\tilde{v}(\mathbf{k}', t) \cdot \mathbf{k}] [\tilde{v}(\mathbf{k}, t) \cdot \tilde{v}(-\mathbf{k} - \mathbf{k}', t)] d^3k' - \frac{i}{2} \int [\tilde{v}(\mathbf{k}', t) \cdot \mathbf{k}] [\tilde{v}(-\mathbf{k}, t) \cdot \tilde{v}(\mathbf{k} - \mathbf{k}', t)] d^3k'. \end{aligned} \quad (17.117)$$

If you substitute in the first integral with $\mathbf{f}(\mathbf{k}') = \mathbf{k}' - \mathbf{k}$ and in the second integral with $\mathbf{f}(\mathbf{k}') = \mathbf{k} - \mathbf{k}'$, you get

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + 2r\mathbf{k}^2 \right) \tilde{e}(\mathbf{k}, t) \\ &= \frac{i}{2} \int \{ [\tilde{v}(\mathbf{k}' - \mathbf{k}, t) \cdot \mathbf{k}] [\tilde{v}(\mathbf{k}, t) \cdot \tilde{v}(-\mathbf{k}', t)] - [\tilde{v}(\mathbf{k} - \mathbf{k}', t) \cdot \mathbf{k}] [\tilde{v}(-\mathbf{k}, t) \cdot \tilde{v}(\mathbf{k}', t)] \} d^3k'. \end{aligned} \quad (17.118)$$

In the second integral, it should be noted that the minus sign that results from exchanging the integration limits cancels out the one that results from the derivation of the substituted function. One defines the *energy transfer function* $W = W(\mathbf{k}, \mathbf{k}', t)$ by

$$W(\mathbf{k}, \mathbf{k}', t) := \frac{i\mathbf{k}}{2} \cdot \{ \tilde{v}(\mathbf{k}' - \mathbf{k}, t) [\tilde{v}(\mathbf{k}, t) \cdot \tilde{v}(-\mathbf{k}', t)] - \tilde{v}(\mathbf{k} - \mathbf{k}', t) [\tilde{v}(-\mathbf{k}, t) \cdot \tilde{v}(\mathbf{k}', t)] \}. \quad (17.119)$$

This gives you the balance equation of the kinetic energy in spectral form

$$\left(\frac{\partial}{\partial t} + 2r\mathbf{k}^2 \right) \tilde{e}(\mathbf{k}, t) = \int W(\mathbf{k}, \mathbf{k}', t) d^3k'. \quad (17.120)$$

This shows that the friction $\propto \frac{1}{L^2}$ is scale-sensitive and in any case reduces the spectral specific kinetic energy. For the energy transfer function applies

$$\begin{aligned} W(\mathbf{k}', \mathbf{k}, t) &= \frac{i\mathbf{k}'}{2} \cdot \{ \tilde{v}(\mathbf{k} - \mathbf{k}', t) [\tilde{v}(\mathbf{k}', t) \cdot \tilde{v}(-\mathbf{k}, t)] - \tilde{v}(\mathbf{k}' - \mathbf{k}, t) [\tilde{v}(-\mathbf{k}', t) \cdot \tilde{v}(\mathbf{k}, t)] \} \\ &= -\frac{i\mathbf{k}'}{2} \cdot \{ \tilde{v}(\mathbf{k}' - \mathbf{k}, t) [\tilde{v}(-\mathbf{k}', t) \cdot \tilde{v}(\mathbf{k}, t)] - \tilde{v}(\mathbf{k} - \mathbf{k}', t) [\tilde{v}(\mathbf{k}', t) \cdot \tilde{v}(-\mathbf{k}, t)] \} \\ &= -\frac{i\mathbf{k}'}{2} \cdot \{ \tilde{v}(\mathbf{k}' - \mathbf{k}, t) [\tilde{v}(\mathbf{k}, t) \cdot \tilde{v}(-\mathbf{k}', t)] - \tilde{v}(\mathbf{k} - \mathbf{k}', t) [\tilde{v}(-\mathbf{k}, t) \cdot \tilde{v}(\mathbf{k}', t)] \} \end{aligned} \quad (17.121)$$

From this it follows

$$\begin{aligned}
& W(\mathbf{k}', \mathbf{k}, t) + W(\mathbf{k}, \mathbf{k}', t) \\
&= \frac{i\mathbf{k}}{2} \cdot \{ \tilde{\mathbf{v}}(\mathbf{k}' - \mathbf{k}, t) [\tilde{\mathbf{v}}(\mathbf{k}, t) \cdot \tilde{\mathbf{v}}(-\mathbf{k}', t)] - \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) [\tilde{\mathbf{v}}(-\mathbf{k}, t) \cdot \tilde{\mathbf{v}}(\mathbf{k}', t)] \} \\
&- \frac{i\mathbf{k}'}{2} \cdot \{ \tilde{\mathbf{v}}(\mathbf{k}' - \mathbf{k}, t) [\tilde{\mathbf{v}}(\mathbf{k}, t) \cdot \tilde{\mathbf{v}}(-\mathbf{k}', t)] - \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) [\tilde{\mathbf{v}}(-\mathbf{k}, t) \cdot \tilde{\mathbf{v}}(\mathbf{k}', t)] \} \\
&= \frac{i}{2} [\tilde{\mathbf{v}}(\mathbf{k}, t) \cdot \tilde{\mathbf{v}}(-\mathbf{k}', t)] \tilde{\mathbf{v}}(\mathbf{k}' - \mathbf{k}, t) \cdot (\mathbf{k} - \mathbf{k}') \\
&- \frac{i}{2} [\tilde{\mathbf{v}}(-\mathbf{k}, t) \cdot \tilde{\mathbf{v}}(\mathbf{k}', t)] \tilde{\mathbf{v}}(\mathbf{k} - \mathbf{k}', t) \cdot (\mathbf{k} - \mathbf{k}') \\
&\stackrel{\text{Glg. (17.109)}}{=} 0.
\end{aligned} \tag{17.122}$$

The energy transfer function is therefore antisymmetric:

$$W(k, k', t) = -W(k', k, t) \tag{17.123}$$

This is related to the conservation of energy: the energy gain of component $\mathbf{k}$ at the expense of component $\mathbf{k}'$ is equal to the energy loss of component $\mathbf{k}'$ due to component $\mathbf{k}$.

17.4.2.1 Isotropic form

Now one makes the assumption of isotropy, i.e. h. It is assumed that spectral properties do not depend on the three components of the vector $\mathbf{k}$, but only on the magnitude of k , i.e

$$e(\mathbf{k}, t) \rightarrow \frac{\tilde{e}(k, t)}{4\pi k^2}, \quad W(\mathbf{k}, \mathbf{k}', t) \rightarrow \frac{W(k, k', t)}{4\pi k'^2 4\pi k^2}. \tag{17.124}$$

The geometry of the spherical coordinates was corrected. Thus, Eq. (17.120) to

$$\left(\frac{\partial}{\partial t} + 2rk^2 \right) \frac{\tilde{e}(k, t)}{4\pi k^2} = \int \frac{W(k, k', t)}{4\pi k'^2 4\pi k^2} 4\pi k'^2 dk'$$

$$\Rightarrow \left(\frac{\partial}{\partial t} + 2rk^2 \right) \tilde{e}(k, t) = \int W(k, k', t) dk'. \tag{17.125}$$

17.4.3 Heisenberg approach

The *Heisenberg approach* initially assumes stationarity, i.e

$$2rk^2 \tilde{e}(k) = \int W(k, k') dk'. \tag{17.126}$$

Furthermore, it is assumed that there is a cutoff wave number k^* , which divides the spectrum into two regions:

- The region $k < k^*$ (larger wavelengths) is referred to as region 1. For geometric reasons, no isotropy can be assumed here. The Heisenberg approach makes no statements about this area.
- The region $k \geq k^*$ (smaller wavelengths) is called *universality region*. Isotropy can be assumed here and the flow is little influenced by boundary conditions.

The Heisenberg approach refers exclusively to the universality region. It is assumed that the smaller scales have a similar effect on the larger scales as the viscosity has on the smallest-scale vortices: they diffuse momentum. This is justified because it can be assumed that the smaller-scale vortices diffuse momentum on average (reduce the gradient of the velocity field). The Heisenberg approach is the formula

$$W(k, k') = -2\kappa_H k^2 \tilde{e}(k) g(k', \tilde{e}(k')), \quad (17.127)$$

where $k, k' \geq k^*$ and $k' > k$ are assumed.

$$\kappa_H = 0,5 \pm 0,03 \quad (17.128)$$

[41] is a kind of dimensionless viscosity, the so-called *Heisenberg constant*. This formula is analogous to the molecular dissipative term $-2r k^2 \tilde{e}(k)$. The function $g(k', \tilde{e}(k'))$ describes how the smaller scale k' acts on the scale k , whereby an explicit dependence on the energy $\tilde{e}(k')$ present at k' was included. Apply in the SI system

$$[\tilde{e}] = \frac{\text{J}}{\text{kg/m}} = \frac{\text{Jm}}{\text{kg}} = \frac{\text{Nm}^2}{\text{kg}} = \frac{\text{m}^3}{\text{s}^2} \quad (17.129)$$

$$\Rightarrow \left[\frac{\partial \tilde{e}}{\partial t} \right] = \frac{\text{m}^3}{\text{s}^3}, \quad [W] = \frac{\text{m}^4}{\text{s}^3}, \quad \Rightarrow [k^2 \tilde{e}(k)] = \frac{\text{m}}{\text{s}^2} \quad \Rightarrow [g(k', \tilde{e}(k'))] = \frac{\text{m}^3}{\text{s}}. \quad (17.130)$$

The approach for g is now chosen

$$g(k', \tilde{e}(k')) = (k')^a \tilde{e}(k')^\beta. \quad (17.131)$$

This implies

$$\beta = \frac{1}{2}, a = -\frac{3}{2} \quad (17.132)$$

$$\Rightarrow g(k', \tilde{e}(k')) = (k')^{-3/2} \tilde{e}(k')^{1/2} = \sqrt{\frac{\tilde{e}(k')}{(k')^3}}. \quad (17.133)$$

In summary, the Heisenberg approach is

$$T(k, k') = \begin{cases} -2\kappa_H k^2 \tilde{e}(k) \tilde{e}(k')^{1/2} (k')^{-3/2}, & \text{falls } k' \geq k \text{ gilt (Energieverlust an kleinere Skala),} \\ 2\kappa_H k^2 \tilde{e}(k) \tilde{e}(k')^{1/2} (k')^{-3/2}, & \text{falls } k' < k \text{ gilt (Energiegewinn von größerer Skala).} \end{cases} \quad (17.134)$$

In the context of stationarity, the kinetic energy lost through dissipation is compensated by the supply from the larger scales. The larger scales therefore have an energy loss to the smaller scales, which must be compensated for by a production $\sigma(k)$ of kinetic energy. The mechanism through which this happens is left open here. However, one assumes $\sigma(k) = 0$ for $k > k^*$ in order to simplify the considerations in the universality region. Eq. (17.126) becomes

$$2r k^2 \tilde{e}(k) = \int W(k, k') dk' + \sigma(k). \quad (17.135)$$

17.4.4 Energy spectrum

If you integrate Eq. (17.135) up to a wave number $k > k^*$, one obtains

$$2r \int_0^k (k')^2 \tilde{e}(k') dk' = \int_0^k \int_0^\infty W(k', k'') dk'' dk' + \int_0^k \sigma(k') dk'. \quad (17.136)$$

For $k = \infty$ one obtains

$$2r \int_0^\infty (k')^2 \tilde{e}(k') dk' = \int_0^\infty \int_0^\infty W(k', k'') dk'' dk' + \int_0^\infty \sigma(k') dk'. \quad (17.137)$$

Due to the antisymmetry of the energy transfer function $W(k', k'') = -W(k'', k')$ holds

$$\int_0^\infty \int_0^\infty W(k', k'') dk'' dk' = 0. \quad (17.138)$$

This corresponds to the fact that the energy transfer function redistributes kinetic energy, but does not produce or destroy kinetic energy. This leads to

$$2r \int_0^\infty (k')^2 \tilde{e}(k') dk' = \int_0^\infty \sigma(k') dk'. \quad (17.139)$$

This corresponds to the fact that under stationary conditions the energy input is equal to the energy loss. The energy loss is equal to the dissipation:

$$\varepsilon = 2r \int_0^\infty (k')^2 \tilde{e}(k') dk' \quad (17.140)$$

Because $k > k^*$ and $\sigma(k') = 0$ for $k' > k^*$ holds

$$\int_0^k \sigma(k') dk' = \int_0^\infty \sigma(k') dk'. \quad (17.141)$$

Thus, one can use Eq. (17.136) in the form

$$2r \int_0^k (k')^2 \tilde{e}(k') dk' = \int_0^k \int_0^\infty W(k', k'') dk'' dk' + \varepsilon \quad (17.142)$$

write down. Again because of the antisymmetry $W(k', k'') = -W(k'', k')$ holds

$$\int_0^k \int_0^k W(k', k'') dk'' dk' = 0. \quad (17.143)$$

Therefore applies

$$\begin{aligned} 2r \int_0^k (k')^2 \tilde{e}(k') dk' &= \int_0^k \int_k^\infty W(k', k'') dk'' dk' + \varepsilon \\ \Leftrightarrow \varepsilon &= 2r \int_0^k (k')^2 \tilde{e}(k') dk' - \int_0^k \int_k^\infty W(k', k'') dk'' dk'. \end{aligned} \quad (17.144)$$

If you put Eq. (17.134) and consider $k'' > k'$, you get

$$\begin{aligned} \varepsilon &= 2r \int_0^k (k')^2 \tilde{e}(k') dk' - \int_0^k \int_k^\infty -2\kappa_H (k')^2 \tilde{e}(k') \tilde{e}(k'')^{1/2} (k'')^{-3/2} dk'' dk' \\ \Leftrightarrow \varepsilon &= 2r \int_0^k (k')^2 \tilde{e}(k') dk' + 2\kappa_H \int_0^k \int_k^\infty (k')^2 \tilde{e}(k') \tilde{e}(k'')^{1/2} (k'')^{-3/2} dk'' dk' \\ \Leftrightarrow \varepsilon &= 2r \int_0^k (k')^2 \tilde{e}(k') dk' + 2\kappa_H \int_k^\infty \tilde{e}(k'')^{1/2} (k'')^{-3/2} dk'' \int_0^k (k')^2 \tilde{e}(k') dk' \\ \Leftrightarrow \varepsilon &= 2r \int_0^k (k')^2 \tilde{e}(k') dk' + 2\kappa_H \int_k^\infty \sqrt{\frac{\tilde{e}(k'')}{(k'')^3}} dk'' \int_0^k (k')^2 \tilde{e}(k') dk' \\ \Leftrightarrow \varepsilon &= \left(2r + 2\kappa_H \int_k^\infty \sqrt{\frac{\tilde{e}(k'')}{(k'')^3}} dk'' \right) \int_0^k (k')^2 \tilde{e}(k') dk' \\ \Leftrightarrow \varepsilon &= \left(r + \kappa_H \int_k^\infty \sqrt{\frac{\tilde{e}(k'')}{(k'')^3}} dk'' \right) \int_0^k 2 (k')^2 \tilde{e}(k') dk'. \end{aligned} \quad (17.145)$$

The size

$$K := \kappa_H \int_k^\infty \sqrt{\frac{\tilde{e}(k')}{(k')^3}} dk' \quad (17.146)$$

has the dimension of a viscosity and is called *Heisenberg's exchange coefficient*.

You now define an auxiliary function

$$f(k) := \int_0^k (k')^2 \tilde{e}(k') dk' \Rightarrow f'(k) = k^2 \tilde{e}(k). \quad (17.147)$$

This allows Eq. (17.145) in the form

$$\frac{\varepsilon}{f(k)} = r + \kappa_H \int_k^\infty \sqrt{\frac{\tilde{e}(k')}{(k')^3}} dk' = r + \kappa_H \int_k^\infty \sqrt{\frac{f'(k')}{k'^5}} dk' \quad (17.148)$$

note down. If you differentiate this equation, you get

$$-\frac{\varepsilon f'(k)}{f(k)^2} = -\kappa_H \sqrt{\frac{f'(k)}{2k^5}} \Rightarrow \frac{\varepsilon^2 f'(k)^2}{f(k)^4} = \kappa_H^2 \frac{f'(k)}{2k^5} \Leftrightarrow \frac{\varepsilon^2 f'(k)}{f(k)^4} = \frac{\kappa_H^2}{2k^5}. \quad (17.149)$$

If you integrate both sides over k , you get

$$-\frac{\varepsilon^2}{3f(k)^3} + C = -\frac{\kappa_H^2}{8k^4} \Leftrightarrow \frac{\varepsilon^2}{3f(k)^3} = C + \frac{\kappa_H^2}{8k^4} \quad (17.150)$$

with an integration constant C . To determine this, consider Eq. (17.150) for $k \rightarrow \infty$:

$$C = \frac{\varepsilon^2}{3f(\infty)^3} \quad (17.151)$$

To determine $f(\infty)$, evaluate Eq. (17.148) for $k \rightarrow \infty$ from:

$$\begin{aligned} \frac{\varepsilon}{f(\infty)} &= r \Rightarrow f(\infty) = \frac{\varepsilon}{r} \\ \Rightarrow C &= \frac{\varepsilon^2}{3f(\infty)^3} = \frac{r^3}{3\varepsilon} \end{aligned} \quad (17.152)$$

Putting this into Eq. (17.150), you get

$$\begin{aligned} \frac{\varepsilon^2}{3f(k)^3} &= \frac{r^3}{3\varepsilon} + \frac{\kappa_H^2}{8k^4} \\ \Rightarrow f(k)^3 &= \frac{\varepsilon^2}{3} \left(\frac{\kappa_H^2}{8k^4} + \frac{r^3}{3\varepsilon} \right)^{-1} \\ \Rightarrow f(k) &= \frac{\varepsilon^{2/3}}{3^{1/3}} \left(\frac{\kappa_H^2}{8k^4} + \frac{r^3}{3\varepsilon} \right)^{-1/3}. \end{aligned} \quad (17.153)$$

If you differentiate this by k , you get

$$f'(k) = \frac{\varepsilon^{2/3}}{3^{1/3}} \frac{4}{3} \frac{\kappa_H^2}{8k^5} \left(\frac{\kappa_H^2}{8k^4} + \frac{r^3}{3\varepsilon} \right)^{-4/3}. \quad (17.154)$$

If you put Eq. (17.147), you get

$$\begin{aligned}
2k^2 \tilde{e}(k) &= \frac{\varepsilon^{2/3}}{3^{1/3}} \frac{4}{3} \frac{\varkappa_H^2}{8k^5} \left(\frac{\varkappa_H^2}{8k^4} + \frac{r^3}{3\varepsilon} \right)^{-4/3} \\
\Leftrightarrow \tilde{e}(k) &= \frac{\varepsilon^{2/3}}{3^{1/3}} \frac{2}{3k^3} \frac{\varkappa_H^2}{8k^4} \left(\frac{\varkappa_H^2}{8k^4} + \frac{r^3}{3\varepsilon} \right)^{-4/3} \\
\Leftrightarrow \tilde{e}(k) &= \frac{\varepsilon^{2/3}}{3^{1/3}} \frac{2}{3k^3} \left(\frac{\varkappa_H^2}{8k^4} \right)^{-1/3} \left(\frac{8k^4}{\varkappa_H^2} \right)^{-4/3} \left(\frac{\varkappa_H^2}{8k^4} + \frac{r^3}{3\varepsilon} \right)^{-4/3} \\
\Leftrightarrow \tilde{e}(k) &= \frac{\varepsilon^{2/3}}{3^{1/3}} \frac{2}{3k^3} \left(\frac{\varkappa_H^2}{8k^4} \right)^{-1/3} \left(\mathbf{1} + \frac{8r^3k^4}{3\varepsilon\varkappa_H^2} \right)^{-4/3} \\
\Leftrightarrow \tilde{e}(k) &= \frac{\varepsilon^{2/3}}{3^{1/3}} \frac{2}{3} \left(\frac{\varkappa_H^2}{8} \right)^{-1/3} k^{-5/3} \left(\mathbf{1} + \frac{8r^3k^4}{3\varepsilon\varkappa_H^2} \right)^{-4/3} \\
\Leftrightarrow \tilde{e}(k) &= \left(\frac{8^2}{3^4\varkappa_H^2} \right)^{1/3} \varepsilon^{2/3} k^{-5/3} \left(\mathbf{1} + \frac{8r^3k^4}{3\varepsilon\varkappa_H^2} \right)^{-4/3}
\end{aligned}$$

$$\Leftrightarrow \tilde{e}(k) = \left(\frac{8}{9\varkappa_H} \right)^{2/3} \varepsilon^{2/3} k^{-5/3} \left(\mathbf{1} + \frac{8r^3k^4}{3\varepsilon\varkappa_H^2} \right)^{-4/3}. \quad (17.155)$$

17.4.5 Definitions and approximations

The starting point of this section is Eq. (17.155). First you define some abbreviations. First you define

$$k_c := \left(\frac{\varepsilon}{r^3} \right)^{1/4}. \quad (17.156)$$

This makes Eq. (17.157) to

$$\tilde{e}(k) = \left(\frac{8}{9\varkappa_H} \right)^{2/3} \varepsilon^{2/3} k^{-5/3} \left(\mathbf{1} + \frac{8k^4}{3\varkappa_H^2 k_c^4} \right)^{-4/3}. \quad (17.157)$$

Furthermore, one defines the *Kolmogorov constant* $\varkappa_K$ by

$$\varkappa_K := \left(\frac{8}{9\varkappa_H} \right)^{2/3}, \quad (17.158)$$

the *characteristic length* l_c through

$$l_c := \left(\frac{r^3}{\varepsilon} \right)^{1/4} \quad (17.159)$$

as well as the *characteristic time* t_c

$$t_c := \left(\frac{r}{\varepsilon} \right)^{1/2}. \quad (17.160)$$

From this it follows

$$k_c = \frac{\mathbf{1}}{l_c}. \quad (17.161)$$

Putting this into Eq. (17.157), you get

$$\tilde{e}(k) = \kappa_K \varepsilon^{2/3} k^{-5/3} \left(1 + \frac{8k^4 l_c^4}{3\kappa_H^2} \right)^{-4/3} = \kappa_K \varepsilon^{2/3} k^{-5/3} \left(1 + \frac{8k^4}{3\kappa_H^2 k_c^4} \right)^{-4/3}. \quad (17.162)$$

Two important borderline cases can be derived from this. For $k > \sqrt{\kappa_H} k_c$ applies

$$\begin{aligned} \tilde{e}(k) &\approx \left(\frac{8}{9\kappa_H} \right)^{2/3} \varepsilon^{2/3} k^{-5/3} \left(\frac{8k^4 l_c^4}{3\kappa_H^2} \right)^{-4/3} = \left(\frac{8\varepsilon}{9\kappa_H} \right)^{2/3} \left(\frac{8r^3}{3\varepsilon\kappa_H^2} \right)^{-4/3} k^{-7} \\ &= \left(\frac{8\varepsilon}{9\kappa_H} \right)^{2/3} \left(\frac{3\varepsilon\kappa_H^2}{8r^3} \right)^{4/3} k^{-7} \end{aligned}$$

$$\Leftrightarrow \tilde{e}(k) \approx \left(\frac{\kappa_H \varepsilon}{2r^2} \right)^2 k^{-7}. \quad (17.163)$$

This region of the spectrum ($k > k_c$) is called *dissipative range*. In this range, the viscosity leads to a steep drop in the spectrum. In the case $k^* < k \ll k_c$ applies

$$\tilde{e}(k) \approx \kappa_K \varepsilon^{2/3} k^{-5/3}. \quad (17.164)$$

This region of the spectrum ($k^* < k \ll k_c$) is called *inertial subrange*.

17.5 Classic Smagorinsky model

The simplest approach to calculate the turbulent horizontal diffusion coefficient K is the so-called *classic Smagorinsky model (CSM)*. The starting point for the derivation is Eq. (17.146), where the just resolved circular wave number $\frac{\pi}{2\Delta} = \frac{\pi}{\Delta}$ is used for k :

$$K := \kappa_H \int_{\frac{\pi}{\Delta}}^{\infty} \sqrt{\frac{\tilde{e}(k)}{k^3}} dk \quad (17.165)$$

The relevant scale range of turbulent diffusion in the atmosphere is the inertial subrange ($k^* < k \ll k_c$), in which Eq. (17.164). From this it follows

$$\begin{aligned} K &= \kappa_H \int_{\frac{\pi}{\Delta}}^{\infty} \sqrt{\frac{\kappa_K \varepsilon^{2/3} k^{-5/3}}{k^3}} dk = \kappa_H \sqrt{\kappa_K \varepsilon^{1/3}} \int_{\frac{\pi}{\Delta}}^{\infty} \sqrt{k^{-14/3}} dk \\ \Leftrightarrow K &= \kappa_H \sqrt{\kappa_K \varepsilon^{1/3}} \int_{\frac{\pi}{\Delta}}^{\infty} k^{-7/3} dk = \kappa_H \sqrt{\kappa_K \varepsilon^{1/3}} \left[-\frac{3}{4} k^{-4/3} \right]_{\frac{\pi}{\Delta}}^{\infty} \\ \Leftrightarrow K &= \frac{3}{4} \kappa_H \sqrt{\kappa_K \varepsilon^{1/3}} \left(\frac{\pi}{\Delta} \right)^{-4/3} = \frac{3}{4} \kappa_H \sqrt{\kappa_K \varepsilon^{1/3}} \left(\frac{\Delta}{\pi} \right)^{4/3}. \end{aligned} \quad (17.166)$$

This result cannot yet be used directly for a numerical model because ε is not known. To determine an expression for ε , one starts from Eq. (17.145) from:

$$\varepsilon = (r + K) \int_0^{\frac{\pi}{\Delta}} 2k^2 \tilde{e}(k) dk. \quad (17.167)$$

Comparing this with Eq. , follows

$$\varepsilon = (r + K) S^2.$$

Because $\Delta \gg l_c$ is a good approximation

$$\varepsilon = KS^2 \Rightarrow \varepsilon^{\frac{1}{3}} = K^{\frac{1}{3}} S^{\frac{2}{3}}. \quad (17.168)$$

Putting this into Eq. (17.166), you get

$$\begin{aligned} K &= \frac{3}{4} \kappa_H \sqrt{\kappa_K} K^{\frac{1}{3}} S^{\frac{2}{3}} \left(\frac{\Delta}{\pi} \right)^{4/3} \\ \Leftrightarrow K^{\frac{2}{3}} &= \frac{3}{4} \kappa_H \sqrt{\kappa_K} S^{\frac{2}{3}} \left(\frac{\Delta}{\pi} \right)^{4/3} \\ \Leftrightarrow K &= \kappa_K^{\frac{3}{4}} \left(\frac{3}{4} \kappa_H \right)^{\frac{3}{2}} S \left(\frac{\Delta}{\pi} \right)^2 \\ \Leftrightarrow K &= \frac{1}{\pi^2} \kappa_K^{\frac{3}{4}} \left(\frac{3}{4} \kappa_H \right)^{\frac{3}{2}} \Delta^2 S. \end{aligned} \quad (17.169)$$

With the definition

$$\begin{aligned} c_S^2 &:= \frac{1}{\pi^2} \kappa_K^{\frac{3}{4}} \left(\frac{3}{4} \kappa_H \right)^{\frac{3}{2}} \stackrel{\text{Glg. (17.158)}}{=} \frac{1}{\pi^2} \left(\frac{8}{9 \kappa_H} \right)^{1/2} \left(\frac{3}{4} \kappa_H \right)^{\frac{3}{2}} = \frac{\kappa_H}{\pi^2} \left(\frac{8}{9} \right)^{1/2} \left(\frac{3}{4} \right)^{\frac{3}{2}} = \frac{\kappa_H}{\pi^2} \left(\frac{8 \cdot 9}{9 \cdot 16} \right)^{1/2} \left(\frac{3}{4} \right)^{\frac{1}{2}} \\ &= \frac{\sqrt{3} \kappa_H}{2 \sqrt{2} \pi^2} \stackrel{\text{Glg. (17.128)}}{\approx} \frac{\sqrt{3}}{4 \sqrt{2} \pi^2} \approx 0,03 \\ \Leftrightarrow c_S &= \left(\frac{3}{8} \right)^{1/4} \frac{\sqrt{\kappa_H}}{\pi} \approx \left(\frac{3}{8} \right)^{1/4} \frac{1}{\sqrt{2} \pi} \approx 0,176 \end{aligned} \quad (17.170)$$

you can do this in the form

$$K = c_S^2 \Delta^2 S \quad (17.171)$$

note down. This follows in the case of two-dimensional flow

$$K = \rho r \Delta = \rho c_S^2 \Delta^2 \sqrt{\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2} = \rho c_S^2 \Delta^2 \sqrt{E^2 + F^2}. \quad (17.172)$$

From Eq. (17.166) an expression for the dissipation can also be derived if the diffusion coefficient is known:

$$\begin{aligned} \frac{3}{4} \kappa_H \sqrt{\kappa_K} \varepsilon^{1/3} \left(\frac{\Delta}{\pi} \right)^{4/3} &= K \\ \Leftrightarrow \varepsilon^{1/3} &= \frac{4}{3 \kappa_H \sqrt{\kappa_K}} \left(\frac{\pi}{\Delta} \right)^{4/3} K \\ \Leftrightarrow \varepsilon &= \left(\frac{4}{3 \kappa_H \sqrt{\kappa_K}} \right)^3 \left(\frac{\pi}{\Delta} \right)^4 K^3 \approx 1039 \cdot \frac{K^3}{\Delta^4} \end{aligned} \quad (17.173)$$

17.6 Turbulent kinetic energy

The so-called specific *turbulent kinetic energy* k_s is the subscale part of the kinetic energy, in contrast to the resolved part, which is denoted here by k_m . A prognostic equation should be derived for this size. You start by first calculating the specific kinetic energy equation Eq. (14.8) noted again:

$$\frac{\partial k}{\partial t} = \frac{1}{2} \frac{\partial}{\partial t} (u^2 + v^2 + w^2) = -\mathbf{v} \cdot \nabla k - \frac{1}{\rho} \mathbf{v} \cdot \nabla p - wg - \varepsilon = - \sum_{i,j=1}^3 u_i u_j \frac{\partial u_j}{\partial x_i} - \frac{1}{\rho} \mathbf{v} \cdot \nabla p - wg - \varepsilon. \quad (17.174)$$

The pressure gradient is expressed using the Exner pressure:

$$\frac{\partial k}{\partial t} = - \sum_{i,j=1}^3 u_i u_j \frac{\partial u_j}{\partial x_i} - c^{(p)} \theta \mathbf{v} \cdot \nabla \Pi - w g - \varepsilon. \quad (17.175)$$

Furthermore, write down the momentum equation without friction:

$$\frac{\partial u_i}{\partial t} = - \sum_{j=1}^3 u_j \frac{\partial u_i}{\partial x_j} - c^{(p)} \theta \frac{\partial \Pi}{\partial x_i} - g_i. \quad (17.176)$$

If you carry out Reynolds averaging here, you get

$$\frac{\partial \bar{u}_i}{\partial t} = - \sum_{j=1}^3 \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} - \sum_{j=1}^3 \overline{u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{\theta} \frac{\partial \bar{\Pi}}{\partial x_i} - c^{(p)} \overline{\theta' \frac{\partial \Pi'}{\partial x_i}} - g_i. \quad (17.177)$$

Multiplying this equation by $\bar{u}_i$ gives

$$\bar{u}_i \frac{\partial \bar{u}_i}{\partial t} = - \bar{u}_i \sum_{j=1}^3 \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} - \bar{u}_i \sum_{j=1}^3 \overline{u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{u}_i \bar{\theta} \frac{\partial \bar{\Pi}}{\partial x_i} - c^{(p)} \overline{\bar{u}_i \theta' \frac{\partial \Pi'}{\partial x_i}} - \bar{u}_i g_i. \quad (17.178)$$

Summing this equation over i we get

$$\begin{aligned} \frac{\partial k_m}{\partial t} &= - \sum_{i,j=1}^3 \bar{u}_i u_j \frac{\partial \bar{u}_i}{\partial x_j} - \sum_{i,j=1}^3 \overline{\bar{u}_i u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{\theta} \bar{\mathbf{v}} \cdot \nabla \bar{\Pi} - c^{(p)} \bar{\mathbf{v}} \cdot \overline{\theta' \nabla \Pi'} + \bar{\mathbf{v}} \cdot \mathbf{g} \\ &= - \sum_{j=1}^3 \bar{u}_j \sum_{i=1}^3 \bar{u}_i \frac{\partial \bar{u}_i}{\partial x_j} - \sum_{i,j=1}^3 \overline{\bar{u}_i u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{\theta} \bar{\mathbf{v}} \cdot \nabla \bar{\Pi} - c^{(p)} \bar{\mathbf{v}} \cdot \overline{\theta' \nabla \Pi'} + \bar{\mathbf{v}} \cdot \mathbf{g} \\ &= - \sum_{j=1}^3 \bar{u}_j \frac{\partial k_m}{\partial x_j} - \sum_{i,j=1}^3 \overline{\bar{u}_i u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{\theta} \bar{\mathbf{v}} \cdot \nabla \bar{\Pi} - c^{(p)} \bar{\mathbf{v}} \cdot \overline{\theta' \nabla \Pi'} + \bar{\mathbf{v}} \cdot \mathbf{g} \\ &= - \bar{\mathbf{v}} \cdot \nabla k_m - \sum_{i,j=1}^3 \overline{\bar{u}_i u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{\theta} \bar{\mathbf{v}} \cdot \nabla \bar{\Pi} - c^{(p)} \bar{\mathbf{v}} \cdot \overline{\theta' \nabla \Pi'} + \bar{\mathbf{v}} \cdot \mathbf{g}. \end{aligned} \quad (17.179)$$

Here is

$$k_m := \frac{1}{2} (\bar{u}^2 + \bar{v}^2 + \bar{w}^2) \quad (17.180)$$

the average kinetic energy. If one further assumes that the background state is hydrostatically balanced, i.e. $-c^{(p)} \bar{\theta} \nabla \bar{\Pi} + \mathbf{g} = \mathbf{0}$, it follows

$$\frac{\partial k_m}{\partial t} = - \bar{\mathbf{v}} \cdot \nabla k_m - \sum_{i,j=1}^3 \overline{\bar{u}_i u'_j \frac{\partial u'_i}{\partial x_j}} - c^{(p)} \bar{\mathbf{v}} \cdot \overline{\theta' \nabla \Pi'}. \quad (17.181)$$

The subscale or turbulent kinetic energy is

$$k_s := k' = \frac{1}{2} \frac{\partial}{\partial t} (u'^2 + v'^2 + w'^2). \quad (17.182)$$

Putting this into Eq. (17.175), you get

$$\frac{\partial k_m}{\partial t} + \frac{\partial k_s}{\partial t} = - \sum_{i,j=1}^3 u_i u_j \frac{\partial u_j}{\partial x_i} - c^{(p)} \theta \mathbf{v} \cdot \nabla \Pi - w g - \varepsilon. \quad (17.183)$$

If you carry out Reynolds averaging here, you get

$$\begin{aligned}
\frac{\partial k_m}{\partial t} + \frac{\partial k_s}{\partial t} &= -\bar{\mathbf{v}} \cdot \nabla k_m - \sum_{i,j=1}^3 \overline{u_i' u_j'} \frac{\partial u_i'}{\partial x_j} - c^{(p)} \bar{\mathbf{v}} \cdot \bar{\theta'} \nabla \Pi' \\
&\quad - \sum_{i,j=1}^3 \overline{u_i' u_j'} \frac{\partial \bar{u}_i}{\partial x_j} - \sum_{i,j=1}^3 \overline{u_j' u_i'} \frac{\partial u_i'}{\partial x_j} - c^{(p)} \bar{\theta'} \bar{\mathbf{v}}' \cdot \nabla \bar{\Pi} - c^{(p)} \bar{\theta} \bar{\mathbf{v}}' \cdot \nabla \Pi' - \bar{\varepsilon} \\
&= -\bar{\mathbf{v}} \cdot \nabla k_m - \sum_{i,j=1}^3 \overline{u_i' u_j'} \frac{\partial u_i'}{\partial x_j} - c^{(p)} \bar{\mathbf{v}} \cdot \bar{\theta'} \nabla \Pi' \\
&\quad - \sum_{i,j=1}^3 \overline{u_i' u_j'} \frac{\partial \bar{u}_i}{\partial x_j} - \bar{\mathbf{v}} \cdot \nabla k_s - c^{(p)} \bar{\theta'} \bar{w}' \frac{\partial \bar{\Pi}}{\partial z} - c^{(p)} \bar{\theta} \bar{\mathbf{v}}' \cdot \nabla \Pi' - \bar{\varepsilon}.
\end{aligned} \tag{17.184}$$

If you take Eq. (17.181), you get the so-called *TKE equation*:

$$\frac{\partial k_s}{\partial t} = -\bar{\mathbf{v}} \cdot \nabla k_s - \sum_{i,j=1}^3 \overline{u_i' u_j'} \frac{\partial \bar{u}_i}{\partial x_j} - c^{(p)} \bar{\theta'} \bar{w}' \frac{\partial \bar{\Pi}}{\partial z} - c^{(p)} \bar{\theta} \bar{\mathbf{v}}' \cdot \nabla \Pi' - \bar{\varepsilon} \tag{17.185}$$

With

$$-c^{(p)} \bar{\theta} \frac{\partial \bar{\Pi}}{\partial z} = g \tag{17.186}$$

you can rephrase this as:

$$\frac{\partial k_s}{\partial t} + \bar{\mathbf{v}} \cdot \nabla k_s = \underbrace{- \sum_{i,j=1}^3 \overline{u_i' u_j'} \frac{\partial \bar{u}_i}{\partial x_j}}_{\text{dynamische Produktion}} + \underbrace{g \frac{\bar{\theta'}}{\bar{\theta}} \bar{w}'}_{\text{buoyancy flux}} - c^{(p)} \bar{\theta} \bar{\mathbf{v}}' \cdot \nabla \Pi' - \bar{\varepsilon}. \tag{17.187}$$

Dynamic production describes the production of TKE through dissipation of large-scale movements.

In the dynamic production term, only the vertical shear terms of the horizontal wind are usually taken into account. The third term, which represents the correlation between velocity and pressure fluctuations, is usually neglected. This leads to

$$\frac{\partial k_s}{\partial t} + \bar{\mathbf{v}} \cdot \nabla k_s = -\overline{u' w'} \frac{\partial \bar{u}}{\partial z} - \overline{v' w'} \frac{\partial \bar{v}}{\partial z} + g \frac{\bar{\theta'}}{\bar{\theta}} \bar{w}' - \bar{\varepsilon}. \tag{17.188}$$

If you multiply this equation by ρ and the continuity equation by k_s and add the results, you get the TKE equation in flow form:

$$\frac{\partial (\rho k_s)}{\partial t} + \nabla \cdot (\rho k_s \bar{\mathbf{v}}) = -\rho \overline{u' w'} \frac{\partial \bar{u}}{\partial z} - \rho \overline{v' w'} \frac{\partial \bar{v}}{\partial z} + \rho g \frac{\bar{\theta'}}{\bar{\theta}} \bar{w}' - \rho \bar{\varepsilon}. \tag{17.189}$$

17.7 Geostrophic turbulence

If you apply the operator $\nabla \times$ to Eq. (17.97) in two dimensions is obtained

$$\begin{aligned}
\zeta &= \mathbf{e}_z \cdot \nabla \times \mathbf{v} = \mathbf{e}_z \cdot \nabla \times \int_{\mathbb{R}^2} \tilde{\mathbf{v}}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^2 r = \mathbf{e}_z \cdot \int_{\mathbb{R}^2} \nabla \times [\tilde{\mathbf{v}}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r})] d^2 r \\
&\stackrel{\text{Glg. (B.60)}}{=} \mathbf{e}_z \cdot \int_{\mathbb{R}^2} i \tilde{\mathbf{v}}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) \times \mathbf{k} d^2 r = \int_{\mathbb{R}^2} \mathbf{e}_z \cdot [i \tilde{\mathbf{v}}(\mathbf{k}) \times \mathbf{k}] \exp(i\mathbf{k} \cdot \mathbf{r}) d^2 r.
\end{aligned} \tag{17.190}$$

From this it follows

$$\tilde{\zeta}(\mathbf{k}) = \mathbf{e}_z \cdot [\mathbf{i} \tilde{\mathbf{v}}(\mathbf{k}) \times \mathbf{k}]. \quad (17.191)$$

From the Parseval identity Eq. (C.31) is obtained

$$\begin{aligned} \tilde{\zeta}^2(\mathbf{k}) &= -4\pi^2 \mathbf{i} (\tilde{\mathbf{v}}(-\mathbf{k}) \times \mathbf{k}) \cdot \mathbf{i} (\tilde{\mathbf{v}}(\mathbf{k}) \times \mathbf{k}) = 4\pi^2 (\tilde{\mathbf{v}}(-\mathbf{k}) \times \mathbf{k}) \cdot (\tilde{\mathbf{v}}(\mathbf{k}) \times \mathbf{k}) \\ &= 4\pi^2 (\tilde{\mathbf{v}}(\mathbf{k})^* \times \mathbf{k}) \cdot (\tilde{\mathbf{v}}(\mathbf{k}) \times \mathbf{k}) \end{aligned} \quad (17.192)$$

In polar coordinates this gives

$$\tilde{\zeta}^2(k, \varphi) = 4\pi^2 \tilde{\mathbf{v}}(k, \varphi)^* k \sin(\varphi) \tilde{\mathbf{v}}(k, \varphi) k \sin(\varphi) = 4\pi^2 |\tilde{\mathbf{v}}(k, \varphi)|^2 k^2 \sin^2(\varphi). \quad (17.193)$$

For isotropy $(\tilde{\mathbf{v}}(k, \varphi) \rightarrow \tilde{\mathbf{v}}(k))$ applies

$$\int_0^{2\pi} 4\pi^2 |\tilde{\mathbf{v}}(k)|^2 k^2 \sin^2(\varphi) d\varphi = 4\pi^2 |\tilde{\mathbf{v}}(k)|^2 k^2 \int_0^{2\pi} \sin^2(\varphi) d\varphi = 4\pi^2 |\tilde{\mathbf{v}}(k)|^2 k^2 \pi = 4\pi^3 |\tilde{\mathbf{v}}(k)|^2 k^2. \quad (17.194)$$

This means for enstrophy

$$|\Omega \subseteq \mathbb{R}^2| \overline{\zeta^2} = \int_{\Omega} \zeta^2 d^2 r = \int_{\mathbb{R}^2} \tilde{\zeta}^2(k_x, k_y) d^2 k = \int_0^\infty 4\pi^3 |\tilde{\mathbf{v}}(k)|^2 k^2 dk. \quad (17.195)$$

17.8 Energy cascade

17.9 Parameterizations

Estimating the effects of subscale variability on the averaged variables is called *parameterization*. In another convention, everything that goes beyond the dry adiabatic system of equations is referred to as parameterization, or „physics“ (in contrast to „dynamics“). This convention is not used here.

17.9.1 Scalar advection

Nature diffuses the quantities temperature T and gas densities ρ_i . Let ψ be such a quantity. The diffusion occurs through a diffusion coefficient κ_ψ that depends on the thermodynamic state variables and therefore depends on location and time. You take notes

$$\frac{\partial \psi}{\partial t} = \dots + \nabla \cdot (\kappa_\psi \nabla \psi). \quad (17.196)$$

κ_ψ is first of all of molecular origin. The covariance terms of scalar advection $-\overline{\mathbf{v}'' \cdot \nabla \psi''}$ arising in nonlinear systems when averaging are usefully parameterized in such a way that one starts

$$\kappa_{\psi, \Delta} = \kappa_\psi + \kappa_{\psi, S}, \quad (17.197)$$

where the index Δ represents the diffusion coefficient to be used in the discretization and the index S represents the effect of the subscale. In this way, physical self-consistency is guaranteed. As $\Delta x, \Delta t$ becomes smaller, i.e. with higher resolution, $\kappa_{\psi, \Delta}$ converges to κ_ψ . At low resolution, a good approximation is $\kappa_{\psi, \Delta} = \kappa_{\psi, S}$. Since the vertical grid point spacing is usually significantly smaller than the horizontal one, $\kappa_{\psi, S}$ can be assumed to be direction-dependent, i.e

$$\kappa_{\psi, \Delta} \nabla \psi \rightarrow \kappa_{\psi, \Delta, H} \nabla_h \psi + \kappa_{\psi, \Delta, z} \frac{\partial \psi}{\partial z} \mathbf{k}. \quad (17.198)$$

The horizontal diffusion coefficient is greater than the vertical one.

17.9.2 Impulse advection

In order to derive an approach for the parameterization of momentum advection, analogous to the case of scalar advection in the previous section, one starts from the approach that the subscale variability becomes isotropic Diffusion leads. This also corresponds to the mixing path approach described in section 17.2. It was assumed that the fluid transports its properties unchanged over a certain length, the so-called mixing path length, before it adapts to the environment. This is also the case with molecular diffusion, and thus also with friction as a special case. First, remember Eq. (8.52) for the frictional acceleration $\mathbf{f}_R$:

$$\begin{aligned}\mathbf{f}_R &= r\Delta\mathbf{v} + \left(\frac{\mu_v}{\rho} + \frac{r}{3}\right) \nabla(\nabla \cdot \mathbf{v}) \stackrel{\text{Glg. (B.54)}}{=} \left(\frac{\mu_v}{\rho} + \frac{4r}{3}\right) \nabla(\nabla \cdot \mathbf{v}) - r\nabla \times (\nabla \times \mathbf{v}) \\ &= \left(\frac{\mu_v}{\rho} + \frac{4r}{3}\right) \nabla D - r\nabla \times \boldsymbol{\xi}\end{aligned}\quad (17.199)$$

The following analogy can be used as a modified justification for this approach: The Maxwell distribution Eq. (5.191) is isotropic. Atoms and molecules are subscale within the Navier-Stokes equations. Their isotropic momentum distribution is superimposed on the wind speed $\mathbf{v}$. This has the physical effect of the existence of the frictional acceleration Eq. (8.52) and the dissipation Eq. (8.66). If the turbulent (subscale) motion is isotropic, one can assume that the turbulence has similar effects on the averaged quantities. This analogy also applies to the diffusive approaches to subscale transport of scalar quantities.

However, the effective viscosities remain to be determined. In a discretization one now uses analogous to Eq. (17.197)

$$K = r + r_S, \quad K_v = \mu_v + \mu_{v,S} \quad (17.200)$$

to. This follows for the effective frictional acceleration

$$\mathbf{f}_R = \left(\frac{K_v}{\rho} + \frac{4K}{3}\right) \nabla D - K\nabla \times \boldsymbol{\xi}. \quad (17.201)$$

17.9.3 Phase transitions

Let ρ_v be the density of water vapor, the advection equation for this quantity is

$$\frac{\partial \rho_v}{\partial t} = -\nabla \cdot (\rho_v \mathbf{v}) + s_v, \quad (17.202)$$

here s_v is the source density of the water vapor. If you integrate this equation over a set $\Omega \subseteq \mathbb{R}^3$, you get Gauss' theorem

$$\int_{\Omega} \frac{\partial \rho_v}{\partial t} d^3r = - \int_{\Omega} \nabla \cdot (\rho_v \mathbf{v}) d^3r = - \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} + \int_{\Omega} s_v d^3r dt'. \quad (17.203)$$

If one further integrates over a time interval $[t, t + \Delta t]$, it follows

$$\begin{aligned}& \int_t^{t+\Delta t} \int_{\Omega} \frac{\partial \rho_v}{\partial t} d^3r dt' = - \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + \int_t^{t+\Delta t} \int_{\Omega} s_v d^3r dt' \\ \Leftrightarrow & \int_{\Omega} \rho_v(t + \Delta t) - \rho_v(t) d^3r = - \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + \int_t^{t+\Delta t} \int_{\Omega} s_v d^3r dt' \\ \Leftrightarrow & V[\bar{\rho}_v(t + \Delta t) - \bar{\rho}_v(t)] = - \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + \int_t^{t+\Delta t} \int_{\Omega} s_v d^3r dt' \\ \Leftrightarrow & \bar{\rho}_v(t + \Delta t) = \bar{\rho}_v(t) - \frac{1}{V} \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + \int_t^{t+\Delta t} \int_{\Omega} s_v d^3r dt' \\ \Leftrightarrow & \bar{\rho}_v(t + \Delta t) = \bar{\rho}_v(t) - \frac{1}{V} \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + \int_{\Omega} \int_t^{t+\Delta t} s_v dt' d^3r.\end{aligned}\quad (17.204)$$

For the sake of simplicity, it is assumed at this point that there are no condensates at time t and that no phase transitions in the direction of water vapor take place during the time interval $[t, t + \Delta t]$. In this case applies

$$\int_t^{t+\Delta t} s_v dt' = -\Theta \left[\rho_v(t+\Delta t) - \rho_v^{(\text{sat})}(t+\Delta t) \right] \left[\rho_v(t+\Delta t) - \rho_v^{(\text{sat})}(t+\Delta t) \right] \leq \mathfrak{o}. \quad (17.205)$$

So it applies

$$Q_v := \int_{\Omega} \int_t^{t+\Delta t} s_v dt' d^3r = - \int_{\Omega} \Theta \left[\rho_v(t+\Delta t) - \rho_v^{(\text{sat})}(t+\Delta t) \right] \left[\rho_v(t+\Delta t) - \rho_v^{(\text{sat})}(t+\Delta t) \right] d^3r \leq \mathfrak{o}. \quad (17.206)$$

Now define

$$\tilde{Q}_v := -\Theta \left\{ \bar{\rho}_v(t+\Delta t) - \rho_v^{(\text{sat})}[\bar{T}(t+\Delta t), \bar{p}(t+\Delta t)] \right\} \left\{ \rho_v(t+\Delta t) - \rho_v^{(\text{sat})}[\bar{T}(t+\Delta t), \bar{p}(t+\Delta t)] \right\} \leq \mathfrak{o} \quad (17.207)$$

This is the source term that would result if the phase transition were calculated from the averaged thermodynamic quantities (in a model these would be the values in the grid boxes). It applies

$$Q_v \leq \tilde{Q}_v. \quad (17.208)$$

Now define the difference between the actual phase transition and the one calculated from the averaged quantities

$$\Delta Q_v := Q_v - \tilde{Q}_v \leq \mathfrak{o}. \quad (17.209)$$

This allows Eq. (17.204) in the form

$$\begin{aligned} \bar{\rho}_v(t+\Delta t) &= \bar{\rho}_v(t) - \frac{1}{V} \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + Q_v \\ &= \bar{\rho}_v(t) - \frac{1}{V} \int_t^{t+\Delta t} \int_{\partial\Omega} \rho_v \mathbf{v} \cdot d\mathbf{n} dt' + \tilde{Q}_v + \Delta Q_v. \end{aligned} \quad (17.210)$$

The source term Q_v is therefore composed of two parts:

- The term $\tilde{Q}_v \leq \mathfrak{o}$ corresponds to the resolved part.
- The term $\Delta Q_v \leq \mathfrak{o}$ corresponds to the subscale part.

A model would initially only have knowledge of the resolved portion $\tilde{Q}_v$ and would therefore underestimate the overall phase transition Q_v . In particular, there can be situations with $\tilde{Q}_v = \mathfrak{o}$ and $\Delta Q_v < \mathfrak{o}$. One can now derive approaches for the term ΔQ_v from derived or measured spectral properties of the fields.

This section continues that all types of parameterizations ultimately have to do with subscale variability. In the case $\Omega, \Delta t \rightarrow \mathfrak{o}$, ΔQ_v approaches zero, which is also the case for all parameterizations.

17.9.4 convection

Convection occurs locally in the presence of thermal instability, i.e. in the fall

$$N^2 < \mathfrak{o}. \quad (17.211)$$

However, if one averages over a base area $\mathcal{A} \subseteq \mathbb{R}^2$, due to the variability of N , i.e

$$N_{\min}^2 \leq \overline{N^2}, \quad (17.212)$$

Eq. (17.211) locally satisfied somewhere within $\mathcal{A}$ before the criterion is satisfied on average.

17.10 Flow resistances

The concept of *flow resistance* will first be explained using the horizontal momentum. The friction acceleration is general

$$\frac{\partial v_{N_L}}{\partial t} = \frac{1}{\rho} \frac{\tau_{N_L} - \tau_{N_L+1}}{\Delta z_{N_L}}. \quad (17.213)$$

Here N_L is the number of layers. Now note the turbulent flow on the surface

$$\tau_{N_L+1} \stackrel{!}{=} \rho \frac{v_{N_L+1}}{r_M}. \quad (17.214)$$

This is the defining equation for the flow resistance of the pulse r_M . So from this you get

$$r_M = \rho \frac{v_{N_L+1}}{\tau_{N_L+1}}. \quad (17.215)$$

From the definition equation of the friction velocity Eq. (17.39) is obtained

$$\tau_{N_L+1} = \rho u_*^2. \quad (17.216)$$

This is followed by

$$r_M = \frac{v_{N_L+1}}{u_*^2}. \quad (17.217)$$

If the stratification is indifferent, the logarithmic wind profile according to Eq. (17.43), from this it follows

$$r_M = \frac{u_*}{k u_*^2} \ln \left(\frac{z_{N_L+1}}{z_o} \right) = \frac{1}{k u_*} \ln \left(\frac{z_{N_L+1}}{z_o} \right). \quad (17.218)$$

The relationships discussed in Section 17.9.3 are often also dealt with in the context of convection parameterizations.

17.10.1 Evaporation rates

Evaporation occurs on water surfaces. This applies to the net mass flow into the atmosphere

$$\text{Netto-Massenfluss} = \text{Verdunstung} - \text{Kondensation}. \quad (17.219)$$

If the vapor pressure is equal to the saturation vapor pressure, the two terms on the right cancel each other and the net evaporation rate is zero. The exact calculation of the two terms on the right-hand side for given conditions (p_v, T) will not be discussed here. From now on, the term *evaporation rate* Q will be used for the net evaporation rate.

It can be assumed that the air in the laminar lower layer is saturated, as it only exchanges molecularly-diffusively and therefore slowly with the air above. The question is therefore important for an atmospheric model

How quickly does water vapor pass through the upper boundary of the laminar sublayer?

The answer to this could be determined from the diffusion laws, but after averaging turbulent covariance terms arise which have to be parameterized.

First you take notes

$$Q = \frac{\rho_v^{(s)} - \rho_v}{r_H}, \quad (17.220)$$

Here $\rho_v^{(s)}$ is the absolute saturation humidity at SST (sea surface temperature), ρ_v is the actual absolute humidity in the lowest model layer and r_H is the flow resistance of the sensible heat.

Part IV

Applications of dynamics

The areas between the *Tropics*, which lie at latitudes $\pm\beta$, are called *Tropics*, the areas outside this strip as *Extratropics*. The areas at latitudes beyond the *Arctic Circles* that are located at latitudes $\pm\left(\frac{\pi}{2} - \beta\right)$ are called *high latitudes*. The areas between the tropics and the high latitudes are called *middle latitudes*. The dynamics of the extratropics differ significantly from those of the tropics, since in the former the diabatic fluxes are smaller due to weaker convection and radiation and the geostrophic assumption is more justified. The dynamics of the tropics therefore contain certain difficulties and are therefore discussed separately in Chap. 20 investigated.

18.1 Cyclogenesis

Geostrophy applies to zero order on the synoptic scale in the extratropics, consequences of which were discussed in Sect. 13.10.1. In Section 13.11 the quasi-geostrophic equation system, consisting of the trend equation Eq. (13.226) and ω -equation Eq. (13.231), which can be applied to zonal channels in the extratropics whose meridional extent allows application of the β -plane approximation. In Section 16.7.4 it was shown that the baroclinic waves found as solutions of a quasi-geostrophic linearized two-layer model are unstable. The process triggered by this is cyclogenesis, which will be discussed in more detail here.

18.1.1 Tendency equation

First you define the *geopotential tendency* by

$$\mathcal{X} := \frac{\partial \Phi}{\partial t}. \quad (18.1)$$

Eq. (13.226) was

$$\begin{aligned} \frac{\partial}{\partial t} \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) + \mathbf{v}_{h,g} \cdot \nabla \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) &= 0 \\ \Leftrightarrow \frac{\partial}{\partial t} \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) &= -\mathbf{v}_{h,g} \cdot \nabla \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) \\ \Leftrightarrow \frac{\partial}{\partial t} \left(\Delta + \frac{f_o}{\sigma} \frac{\partial^2}{\partial p^2} \right) \psi &= -\mathbf{v}_{h,g} \cdot \nabla \left(f + \Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right) \\ \Leftrightarrow \frac{\partial}{\partial t} \left(\Delta + \frac{f_o}{\sigma} \frac{\partial^2}{\partial p^2} \right) \psi &= -v_g \beta - \mathbf{v}_{h,g} \cdot \nabla \left(\Delta \psi + \frac{f_o}{\sigma} \frac{\partial^2 \psi}{\partial p^2} \right). \end{aligned} \quad (18.2)$$

Multiplying this by f_o gives

$$\frac{\partial}{\partial t} \left(\Delta + \frac{f_o}{\sigma} \frac{\partial^2}{\partial p^2} \right) (f_o \psi) = -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla \left[\Delta (f_o \psi) + \frac{f_o}{\sigma} \frac{\partial^2 (f_o \psi)}{\partial p^2} \right]. \quad (18.3)$$

Due to Eq. (13.221) is

$$\psi = \frac{\Phi}{f_o}, \quad (18.4)$$

so it applies

$$\begin{aligned} \frac{\partial}{\partial t} \left(\Delta + \frac{f_o}{\sigma} \frac{\partial^2}{\partial p^2} \right) \Phi &= -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla \left(\Delta \Phi + \frac{f_o}{\sigma} \frac{\partial^2 \Phi}{\partial p^2} \right) \\ \Leftrightarrow \frac{\partial}{\partial t} \left(\Delta + \frac{f_o}{\sigma} \frac{\partial^2}{\partial p^2} \right) \Phi &= -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla (\Delta \Phi) - \mathbf{v}_{h,g} \cdot \nabla \left(\frac{f_o}{\sigma} \frac{\partial^2 \Phi}{\partial p^2} \right). \end{aligned} \quad (18.5)$$

Assuming a homogeneous static stability parameter σ , it follows

$$\begin{aligned} \left(\Delta + \frac{f_o^2}{\sigma} \frac{\partial^2}{\partial p^2} \right) \frac{\partial \Phi}{\partial t} &= -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla (\Delta \Phi) - \frac{f_o^2}{\sigma} \mathbf{v}_{h,g} \cdot \nabla \frac{\partial^2 \Phi}{\partial p^2} \\ \Leftrightarrow \left(\Delta + \frac{f_o^2}{\sigma} \frac{\partial^2}{\partial p^2} \right) \frac{\partial \Phi}{\partial t} &= -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla (\Delta \Phi) - \frac{f_o^2}{\sigma} \mathbf{v}_{h,g} \cdot \frac{\partial}{\partial p} \left(\nabla \frac{\partial \Phi}{\partial p} \right). \end{aligned} \quad (18.6)$$

From Eq. (13.191) follows

$$\nabla \frac{\partial \Phi}{\partial p} \cdot \frac{\partial \mathbf{v}_{h,g}}{\partial p} = \nabla \frac{\partial \Phi}{\partial p} \cdot \left(\mathbf{k} \times \frac{1}{f_o} \nabla \frac{\partial \Phi}{\partial p} \right) = \frac{1}{f_o} \nabla \frac{\partial \Phi}{\partial p} \cdot \left(\mathbf{k} \times \nabla \frac{\partial \Phi}{\partial p} \right) = 0, \quad (18.7)$$

therefore you can too

$$\begin{aligned} \Leftrightarrow \left(\Delta + \frac{f_o^2}{\sigma} \frac{\partial^2}{\partial p^2} \right) \frac{\partial \Phi}{\partial t} &= -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla (\Delta \Phi) - \frac{f_o^2}{\sigma} \mathbf{v}_{h,g} \cdot \frac{\partial}{\partial p} \left(\nabla \frac{\partial \Phi}{\partial p} \right) - \frac{f_o^2}{\sigma} \left(\nabla \frac{\partial \Phi}{\partial p} \right) \cdot \frac{\partial \mathbf{v}_{h,g}}{\partial p} \\ \Leftrightarrow \left(\Delta + \frac{f_o^2}{\sigma} \frac{\partial^2}{\partial p^2} \right) \frac{\partial \Phi}{\partial t} &= -f_o v_g \beta - \mathbf{v}_{h,g} \cdot \nabla (\Delta \Phi) - \frac{f_o^2}{\sigma} \frac{\partial}{\partial p} \left(\mathbf{v}_{h,g} \cdot \nabla \frac{\partial \Phi}{\partial p} \right) \end{aligned} \quad (18.8)$$

write. With Eq. (18.1) you can put this in the form

$$\boxed{\underbrace{\left(\Delta + \frac{f_o^2}{\sigma} \frac{\partial^2}{\partial p^2} \right) \chi}_{=:A} = \underbrace{-f_o v_g \beta}_{=:B} \underbrace{- \mathbf{v}_{h,g} \cdot \nabla (\Delta \Phi)}_{=:C} \underbrace{- \frac{f_o^2}{\sigma} \frac{\partial}{\partial p} \left(\mathbf{v}_{h,g} \cdot \nabla \frac{\partial \Phi}{\partial p} \right)}_{=:D}} \quad (18.9)$$

bring.

This equation will now be examined conceptually. Assuming that χ consists of only a single Fourier component in three-dimensional space, it follows

$$A \sim -\chi \sim \text{Zyklogenese}, \quad (18.10)$$

whereby cyclogenesis means a decrease in the pressure surface. In the extratropics, meridional waves are often found, which are superimposed on a zonal base current U . Therefore, the approach is made for the geopotential Φ

$$\Phi(x, y, p) = -U f_o y + \frac{\hat{v} f_o L}{2\pi} \sin\left(\frac{2\pi}{L} x\right) \sin(ap + b) + \Phi_o(p), \quad (18.11)$$

where $\hat{v}$ denotes the velocity amplitude of the meridional oscillation. The linear function $ap + b$ allows the disturbance to phase shift with height; Φ_o represents a background state.

In this case one finds for the term B

$$B = -f_o \beta \hat{v} \cos\left(\frac{2\pi}{L} x\right). \quad (18.12)$$

This term therefore leads to cyclogenesis wherever v_g is negative, i.e. upstream of the trough and downstream of the ridge. So it contributes to retrograde progression. Term B is the advection of planetary vorticity.

For the expression C , which is the advection of relative vorticity, one first calculates

$$\Delta \Phi = -\frac{2\pi}{L} \hat{v} f_o \sin\left(\frac{2\pi}{L} x\right), \quad (18.13)$$

whereby it should be remembered that $\Delta \Phi$ here only refers to the horizontal. From this it follows

$$C = U \frac{4\pi^2}{L^2} \hat{v} f_o \cos\left(\frac{2\pi}{L} x\right) = -\frac{2\pi U}{L \beta} B. \quad (18.14)$$

This term therefore leads to cyclogenesis downstream of the trough and upstream of the ridge, and to anticyclogenesis elsewhere. So it contributes to normal progression and decreases with wavelength. At a cutoff wavelength

$$\tilde{L} = \frac{2\pi U}{\beta} \quad (18.15)$$

B and C compensate each other, the wave is stationary. Even longer waves propagate retrogradely. Both terms B and C disappear at the axes of the pressure structures, so they only contribute to their displacement, but not to their deepening. The term D is responsible for this. The dot product $\mathbf{v}_h \cdot \nabla \frac{\partial \Phi}{\partial p}$ is the horizontal temperature advection, as can be seen from the basic hydrostatic equation in the form Eq. (13.124) results. Therefore D is also referred to as negative *differential temperature advection*. It applies

$$D = \begin{cases} \text{positiv, falls Kaltluftadvektion mit der Tiefe zunimmt,} \\ \text{negativ, falls Warmluftadvektion mit der Tiefe zunimmt.} \end{cases} \quad (18.16)$$

Warm air advection at altitude and cold air advection at depth therefore lead to cyclogenesis, while cold air advection at altitude and warm air advection at depth lead to anticyclonogenesis. This is illustrative because warmer air has a larger specific volume.

18.1.2 ω –equation

18.2 Frontogenesis

18.2.1 Quasigeostrophic frontogenesis

18.2.2 Semigeostrophic frontogenesis

18.3 PV thinking

In Section 16.7.4 it is shown that a strong thermal wind is a prerequisite for the formation of synoptic disturbances in the middle latitudes. In reality, it is found that there are latitudes with particularly strong baroclinicity in which a jet exists in the tropopause region. These frontal zones are therefore classic areas where low pressure areas form (see chapter 18). However, it is unclear why these air mass boundaries exist at all. Intuitively, it would be more obvious to assume that such zones of strong gradients are broken down by some mechanism, at the latest by diffusion. The aim of this chapter is to clear up this ambiguity.

Statistical variables of the Earth system are called *climate*, compilations of such characteristics are called *climatologies*. Typically, 30-year funds are formed. This chapter is about zonal resources

$$\overline{\psi}(\varphi, z) := \frac{1}{2\pi} \int_{\lambda=0}^{2\pi} \psi(\varphi, \lambda, t) d\lambda \quad (19.1)$$

of sizes ψ , where λ is the geographical longitude. These funds meet the rules

$$\frac{\partial \overline{\psi}}{\partial t} = \frac{1}{2\pi} \frac{\partial}{\partial t} \int_{\lambda=0}^{2\pi} \psi d\lambda = \frac{1}{2\pi} \int_{\lambda=0}^{2\pi} \frac{\partial \psi}{\partial t} d\lambda = \overline{\frac{\partial \psi}{\partial t}}, \quad (19.2)$$

$$\frac{\partial \overline{\psi}}{\partial x} = \frac{1}{2\pi} \int_{\lambda=0}^{2\pi} \frac{\partial \psi}{\partial x} d\lambda = \frac{1}{2\pi} [\psi]_0^{2\pi} = \frac{1}{2\pi} [\psi]_0^0 = 0, \quad (19.3)$$

$$\frac{\partial \overline{\psi}}{\partial y} = \frac{1}{2\pi} \frac{\partial}{\partial y} \int_{\lambda=0}^{2\pi} \psi d\lambda = \frac{1}{2\pi} \int_{\lambda=0}^{2\pi} \frac{\partial \psi}{\partial y} d\lambda = \overline{\frac{\partial \psi}{\partial y}}, \quad (19.4)$$

$$\overline{\overline{\psi}} = \frac{1}{2\pi} \int_{\lambda=0}^{2\pi} \overline{\psi} d\lambda = \overline{\psi}. \quad (19.5)$$

They are assumed to be independent of time, so it is of

$$\frac{\partial \overline{\psi}}{\partial t} = 0 \quad (19.6)$$

went out. For deviations, write down $\psi' := \psi - \overline{\psi}$, which therefore applies to the complete field

$$\psi(\varphi, \lambda, z, t) = \overline{\psi}(\varphi, \lambda) + \psi'(\varphi, \lambda, z, t). \quad (19.7)$$

Meet these deviations

$$\overline{\psi'} = \overline{\psi - \overline{\psi}} = \overline{\psi} - \overline{\overline{\psi}} \stackrel{\text{Glg. (19.5)}}{=} \overline{\psi} - \overline{\psi} = 0. \quad (19.8)$$

By comparing with the equations (17.4) - (17.6) one finds that zonal means are Reynolds means. Here one limits oneself to $\psi = p, T, u, v, w$. Asymmetries in the properties of the earth's surface (orography, roughness, radiation properties) lead to asymmetries in the climatology; such effects are not taken into account here.

19.1 Hadley circulation

Imagine an earth without obliquity, i.e. an earth without seasons. This would have an energy supply in the short wave range in the tropics

$$S_{\text{in}} = \frac{S_0}{4\pi} \cos(\varphi) > 0. \quad (19.9)$$

Here S_{in} is the vertical radiation flux density in the short-wave range and φ is, as usual, the width. All variables are considered as climatological averages. Exactly at the poles, the vertical shortwave radiation flux density would be zero, barring scattering and other weak effects. In the long-wave range, the radiation S_{out} at the poles would be weaker than in the tropics, but not zero. Since the global integral over the short-wave incoming radiation is equal to the global integral over the long-wave outgoing radiation,

$$\int_{\varphi=-\pi/2}^{\pi/2} \int_{\lambda=0}^{2\pi} S_o \Theta[\cos(\lambda)] \cos(\varphi) a^2 \cos(\varphi) d\lambda d\varphi = a^2 S_o \int_{\varphi=-\pi/2}^{\pi/2} \cos(\varphi)^2 \int_{\lambda=0}^{2\pi} \Theta[\cos(\lambda)] d\lambda d\varphi$$

$$a^2 S_o \int_{\varphi=-\pi/2}^{\pi/2} \cos(\varphi)^2 d\varphi = a^2 S_o \int_{\varphi=-\pi/2}^{\pi/2} \cos(\varphi)^2 d\varphi = \pi a^2 S_o \quad (19.10)$$

$$\Rightarrow \int_{\varphi=-\pi/2}^{\pi/2} \int_{\lambda=0}^{2\pi} S_{out} \cos(\varphi) d\varphi d\lambda = \pi a^2 S_o, \quad (19.11)$$

The radiation balance is positive in the tropics and negative in the polar regions. This is called *differential heating*. If one assumes a stationary temperature field, it follows for

$$\text{Konvergenz der Strahlungsflussdichte} + \text{Konvergenz der Flussdichte innerer Energie} = 0 \quad (19.12)$$

$$\Rightarrow \text{Konvergenz der Strahlungsflussdichte} = \text{Divergenz der Flussdichte innerer Energie}, \quad (19.13)$$

$$\Rightarrow S_{in} - S_{out} = \text{Divergenz der Flussdichte innerer Energie} \quad (19.14)$$

$$\Rightarrow S_{in} - S_{out} = \frac{c^{(V)}}{a} \left[\frac{\partial V}{\partial \varphi} - V \tan(\varphi) \right]. \quad (19.15)$$

Here is

$$V := \int_0^\infty \rho T v dz \quad (19.16)$$

the vertically integrated meridional flux density of internal energy. If you put in Eq. (19.15)

$$S_{in} = \frac{S_o}{4\pi} \cos(\varphi) \quad (19.17)$$

as well as the approximation

$$S_{out} = \frac{S_o}{4} \quad (19.18)$$

one, you get

$$\frac{S_o}{4\pi} \cos(\varphi) - \frac{S_o}{4} = \frac{c^{(V)}}{a} \left[\frac{\partial V(\varphi)}{\partial \varphi} - V(\varphi) \tan(\varphi) \right]$$

$$\Rightarrow \cos(\varphi) - \pi = \frac{4\pi c^{(V)}}{S_o a} \left[\frac{\partial V(\varphi)}{\partial \varphi} - V(\varphi) \tan(\varphi) \right]. \quad (19.19)$$

This is a differential equation for the function $V = V(\varphi)$.

The interaction of radiation with the atmosphere essentially takes place via the earth's surface. The atmosphere is warmed from below in the tropics and thus becomes unstable, and in the polar regions it is cooled from below and thus stabilized. This leads to positive vertical motion in the tropics and negative vertical motion at the poles. For reasons of mass conservation, the flow in the upper troposphere must run towards the poles and in the lower troposphere towards the equator.

Assuming homogeneous ground pressure, the higher temperature in the tropics leads to an increase in the geopotential in this area. This induces a geostrophic zonal flow directed in the direction of the planet's rotation in both hemispheres.

Such meridional circulations are called *Hadley circulation*. The three important points of the Hadley circulation are summarized again:

- Differential heating leads to instability in the tropics and stabilization in the polar regions.
- This leads to a meridional circulation: the vertical velocity is positive in the tropics and negative at the poles. Air flows toward the poles in the upper troposphere and toward the equator in the lower troposphere.
- This leads to a geostrophic zonal flow, which is directed in the direction of the planet's rotation.

19.1.1 Entropy perspective

In the climatological average, both the energy and the entropy of the atmosphere are constant. Radiation adds heat q in the tropics over a climatological time interval, which is released again in the polar regions. Since the temperature at the poles is lower, the amount of entropy released is greater than that absorbed. The interaction with the Earth leads to an increase in entropy for the rest of the universe. In order for the entropy of the Earth itself not to decrease, entropy must be produced in the atmosphere and ocean. This happens via irreversible processes, especially friction.

19.1.2 The atmosphere as a heat engine

The atmosphere is supplied with heat from space via radiation. Some of this heat is used to generate kinetic energy (wind). This energy is ultimately dissipated, producing entropy. The same amount of heat that the atmosphere has absorbed is finally released back into space, only this time this is associated with a higher entropy flow. So the universe puts energy into the earth, which produces kinetic energy, and gets the energy back in dissipated form. This corresponds to a heat engine.

19.2 Zonally averaged equations

19.2.1 Linear shallow water equations

First, the linearized shallow water equations Equations (13.173) - (13.174) are assumed. These are in components

$$\frac{\partial u}{\partial t} = -g \frac{\partial d}{\partial x} + f v, \quad (19.20)$$

$$\frac{\partial v}{\partial t} = -g \frac{\partial d}{\partial y} - f u, \quad (19.21)$$

$$\frac{\partial d}{\partial t} = -D \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} - v \frac{\tan(\varphi)}{a} \right). \quad (19.22)$$

Zonal means of zonal gradients disappear, thus one obtains

$$\frac{\partial \bar{u}}{\partial t} = f \bar{v}, \quad (19.23)$$

$$\frac{\partial \bar{v}}{\partial t} = -g \frac{\partial \bar{d}}{\partial y} - f \bar{u}, \quad (19.24)$$

$$\frac{\partial \bar{d}}{\partial t} = -D \left(\frac{\partial \bar{v}}{\partial y} - \bar{v} \frac{\tan(\varphi)}{a} \right). \quad (19.25)$$

If one assumes constant averaged sizes, it follows

$$0 = f \bar{v}, \quad (19.26)$$

$$0 = -g \frac{\partial \bar{d}}{\partial y} - f \bar{u}, \quad (19.27)$$

$$0 = -D \left(\frac{\partial \bar{v}}{\partial y} - \bar{v} \frac{\tan(\varphi)}{a} \right). \quad (19.28)$$

From Eq. (19.26) follows $\bar{v} = 0$, so all that remains of the entire system of equations is

$$f \bar{u} = -g \frac{\partial \bar{d}}{\partial y}. \quad (19.29)$$

left, $\bar{u}$ is geostrophically balanced.

19.2.2 Nonlinear shallow water equations

If you write down the momentum equation of the nonlinear shallow water equations Eq. (15.166) component-wise, you get

$$\frac{\partial u}{\partial t} = -\frac{\partial (gh + gb + k)}{\partial x} + ghv = -g \frac{\partial (h + b + k)}{\cos(\varphi) \partial \lambda} - \nabla k + (f + \zeta) v, \quad (19.30)$$

$$\frac{\partial v}{\partial t} = -\frac{\partial (gh + gb + k)}{\partial y} - (f + \zeta) u. \quad (19.31)$$

Zonal averaging performs

$$\frac{\partial \bar{u}}{\partial t} = f\bar{v} + \bar{\zeta}\bar{v} = (f + \bar{\zeta})\bar{v} + \overline{\zeta'v'}, \quad (19.32)$$

$$\frac{\partial \bar{v}}{\partial t} = -\frac{\partial (g\bar{h} + g\bar{b} + \bar{k})}{\partial y} - (f + \bar{\zeta})\bar{u} - \overline{\zeta'u'}. \quad (19.33)$$

Zonal means are assumed to be constant, from which it follows

$$0 = (f + \bar{\zeta})\bar{v} + \overline{\zeta'v'}, \quad (19.34)$$

$$0 = -\frac{\partial (g\bar{h} + g\bar{b} + \bar{k})}{\partial y} - (f + \bar{\zeta})\bar{u} - \overline{\zeta'u'}. \quad (19.35)$$

For mass conservation reasons applies

$$\bar{v} = 0, \quad (19.36)$$

from which immediately

$$\overline{\zeta'v'} = 0 \quad (19.37)$$

follows. In the context of the shallow water equations, there is no turbulent meridional transport of relative vorticity. Furthermore, it follows from Eq. (19.36)

$$\bar{\zeta} = -\frac{\partial \bar{u}}{\partial y} + \frac{\bar{u}}{a} \tan(\varphi), \quad (19.38)$$

$$\begin{aligned} \bar{k} = \frac{1}{2}\bar{u}^2 + \frac{1}{2}\bar{v}^2 &\Rightarrow \frac{\partial \bar{k}}{\partial y} = \bar{u} \frac{\partial \bar{u}}{\partial y} + \bar{v} \frac{\partial \bar{v}}{\partial y} = \bar{u} \frac{\partial \bar{u}}{\partial y} + \bar{v} \frac{\partial \bar{v}}{\partial y} + \overline{u' \frac{\partial u'}{\partial y}} + \overline{v' \frac{\partial v'}{\partial y}} \\ &= \bar{u} \frac{\partial \bar{u}}{\partial y} + \overline{u' \frac{\partial u'}{\partial y}} + \overline{v' \frac{\partial v'}{\partial y}}. \end{aligned} \quad (19.39)$$

Putting this into Eq. (19.35), follows

$$g \frac{\partial (\bar{h} + \bar{b})}{\partial y} = -f\bar{u} - \frac{\bar{u}}{a} \tan(\varphi) \bar{u} - \overline{u' \frac{\partial u'}{\partial y}} - \overline{v' \frac{\partial v'}{\partial y}} - \overline{\zeta'u'}. \quad (19.40)$$

With

$$\zeta' = \frac{\partial v'}{\partial x} - \frac{\partial u'}{\partial y} + \frac{v'}{a} \tan(\varphi) \quad (19.41)$$

Can this be further transformed to

$$\begin{aligned}
g \frac{\partial (\bar{h} + \bar{b})}{\partial y} &= -f\bar{u} - \frac{\bar{u}}{a} \tan(\varphi) \bar{u} - \overline{u' \frac{\partial u'}{\partial y}} - \overline{v' \frac{\partial v'}{\partial y}} - \overline{\left(\frac{\partial v'}{\partial x} - \frac{\partial u'}{\partial y} + \frac{v'}{a} \tan(\varphi) \right) u'} \\
\Leftrightarrow g \frac{\partial (\bar{h} + \bar{b})}{\partial y} &= -f\bar{u} - \frac{\bar{u}}{a} \tan(\varphi) \bar{u} - \overline{v' \frac{\partial v'}{\partial y}} - \overline{\left(\frac{\partial v'}{\partial x} + \frac{v'}{a} \tan(\varphi) \right) u'} \\
\Leftrightarrow g \frac{\partial (\bar{h} + \bar{b})}{\partial y} &= -f\bar{u} - \overline{v' \frac{\partial v'}{\partial y}} - \overline{u' \frac{\partial v'}{\partial x}} + \overline{\frac{u' v'}{a} \tan(\varphi)} - \frac{\bar{u}^2}{a} \tan(\varphi). \tag{19.42}
\end{aligned}$$

The **red** marked terms contain the geostrophic balance, the **blue** marked parts are metric terms. The black terms are the turbulent momentum advection.

19.2.3 Quasigeostrophy

The application of the quasigeostrophic theory is limited to the β level and is therefore not possible globally (see section 13.11). Nevertheless, the quasi-geostrophic equations should also be zonally averaged here.

19.2.4 Semigeostrophy

Frontal zones and jets can be better understood with the semi-geostrophic system of equations than with the quasi-geostrophic one.

Between the tropics, the baroclinicity is generally significantly smaller than in the middle latitudes. The diurnal cycle is strong and dominated by convection.

20.1 Scale analysis

20.2 Cyclogenesis

21.1 Wind-driven circulation

The derivation of the Ekman spiral carried out in Section 17.3 can be transferred to a flat ocean floor without modifications. On the ocean surface, however, the adhesion condition $\lim_{r \rightarrow \partial V} \mathbf{v} = \mathbf{o}$ is missing; rather, it would make sense to assume that on the ocean surface wind speed and current speed converge towards a common limit value. The Ekman spiral would then have to be solved simultaneously in the ocean and atmosphere. However, there is an easier way to fundamentally study the influence of wind on ocean circulation. To do this, first set the balance of forces in the equations (17.35) - (17.36):

$$f\mathbf{k} \times \mathbf{v}_h = -\nabla\varphi + \frac{1}{\rho_o} \frac{\partial \boldsymbol{\tau}}{\partial z} \quad (21.1)$$

It is now assumed that the vertical density gradients are so small that the term $\frac{1}{\rho_o}$ can be included in the partial derivative, i.e

$$f\mathbf{k} \times \mathbf{v}_h = -\nabla\varphi + \frac{\partial}{\partial z} \left(\frac{\boldsymbol{\tau}}{\rho_o} \right). \quad (21.2)$$

From here you now apply the rotation, so

$$\nabla \times f\mathbf{k} \times \mathbf{v}_h = \nabla \times \frac{\partial}{\partial z} \left(\frac{\boldsymbol{\tau}}{\rho_o} \right). \quad (21.3)$$

With Eq. (B.53) follows

$$\nabla \times f\mathbf{k} \times \mathbf{v}_h = (\mathbf{v}_h \cdot \nabla) f\mathbf{k} - \mathbf{v}_h (\nabla \cdot f\mathbf{k}) + f\mathbf{k} \nabla \cdot \mathbf{v}_h - (f\mathbf{k} \cdot \nabla) \mathbf{v}_h \quad (21.4)$$

Projection onto the vertical direction results

$$\begin{aligned} \mathbf{k} \cdot \nabla \times f\mathbf{k} \times \mathbf{v}_h &= \mathbf{k} \cdot (\mathbf{v}_h \cdot \nabla) f\mathbf{k} + f \nabla \cdot \mathbf{v}_h \\ \Rightarrow \mathbf{k} \cdot \nabla \times f\mathbf{k} \times \mathbf{v}_h &= v\beta - f \frac{\partial w}{\partial z}. \end{aligned} \quad (21.5)$$

Integration over the height interval $[z_B, z_T]$ thus yields

$$\beta \int_{z_B}^{z_T} v dz - f(w_T - w_B) = \mathbf{k} \cdot \frac{1}{\rho_o} \nabla \times (\boldsymbol{\tau}_T - \boldsymbol{\tau}_B). \quad (21.6)$$

With the definitions

$$D := z_T - z_B, \quad \bar{v} := \frac{1}{D} \int_{z_B}^{z_T} v dz \quad (21.7)$$

you can do this shorter than

$$\beta D \bar{v} - f(w_T - w_B) = \mathbf{k} \cdot \frac{1}{\rho_o} \nabla \times (\boldsymbol{\tau}_T - \boldsymbol{\tau}_B) \quad (21.8)$$

note down. Since this concerns the entire water column, one can use the simple boundary condition

$$w_T = w_B = \mathbf{o} \quad (21.9)$$

apply. This gives you

$$\beta D \bar{v} = \mathbf{k} \cdot \frac{1}{\rho_o} \nabla \times (\boldsymbol{\tau}_T - \boldsymbol{\tau}_B) \quad (21.10)$$

To parameterize the friction term at the bottom, one uses the *Stommel model*, which reads

$$\boldsymbol{\tau}_B = r \overline{\boldsymbol{v}_h} \quad (21.11)$$

with a constant $r > 0$. With $w = 0$ we also have $\nabla \cdot \boldsymbol{v}_h = 0$, which is why the average wind can be expressed by a current function ψ :

$$\bar{u} = -\frac{\partial \psi}{\partial y}, \quad \bar{v} = \frac{\partial \psi}{\partial x} \quad (21.12)$$

So you can take notes

$$\begin{aligned} \beta D \frac{\partial \psi}{\partial x} + \boldsymbol{k} \cdot \frac{1}{\rho_0} \nabla \times \boldsymbol{\tau}_B &= \boldsymbol{k} \cdot \frac{1}{\rho_0} \nabla \times \boldsymbol{\tau}_T \\ \Leftrightarrow \beta D \frac{\partial \psi}{\partial x} + \frac{r}{\rho_0} \Delta \psi &= \boldsymbol{k} \cdot \frac{1}{\rho_0} \nabla \times \boldsymbol{\tau}_T \\ \Leftrightarrow \frac{\partial \psi}{\partial x} + \frac{r}{\rho_0 \beta D} \Delta \psi &= \frac{1}{\rho_0 \beta D} \boldsymbol{k} \cdot \nabla \times \boldsymbol{\tau}_T \end{aligned}$$

$$\Leftrightarrow \frac{\partial \psi}{\partial x} + \varepsilon \Delta \psi = \frac{\varepsilon}{r} \boldsymbol{k} \cdot \nabla \times \boldsymbol{\tau}_T \quad (21.13)$$

with

$$\varepsilon := \frac{r}{\rho_0 \beta D}. \quad (21.14)$$

Eq. (21.13) is the equation of motion of the Stommel model. It applies

$$\frac{\frac{\partial \psi}{\partial x}}{\varepsilon \Delta \psi} \sim \frac{L \rho_0 \beta D}{r} \quad (21.15)$$

with L as the horizontal length scale. For r you scale

$$fV \sim \frac{Vr}{D \rho_0} \Rightarrow r \sim D \rho_0 f. \quad (21.16)$$

Thus follows

$$\frac{\frac{\partial \psi}{\partial x}}{\varepsilon \Delta \psi} \sim \frac{L \beta}{f} \sim \frac{L}{a} \quad (21.17)$$

As a rough approximation, one can conceptually say for very large scales

$$\frac{\partial \psi}{\partial x} = \frac{\varepsilon}{r} \boldsymbol{k} \cdot \nabla \times \boldsymbol{\tau}_T \quad (21.18)$$

what is called *Sverdrup balance*. From this, the ocean current can be derived diagnostically for a given wind effect.

Now Eq. (21.13) solved on the set $[0, L] \times [0, L]$ with $L > 0$, i.e. for a square basin. This is only possible analytically approximately. For this one starts from a wind stress of the form

$$\tau_T^{(x)} = -\rho_o U^2 \cos\left(\pi \frac{y}{L}\right), \quad (21.19)$$

$$\tau_T^{(y)} = 0 \quad (21.20)$$

out of. From this it follows

$$\frac{\varepsilon}{r} \mathbf{k} \cdot \nabla \times \boldsymbol{\tau}_T = -\frac{\varepsilon\pi}{rL} \rho_o U^2 \sin\left(\pi \frac{y}{L}\right) \quad (21.21)$$

You make the approach

$$\psi = \psi_I + \varphi, \quad (21.22)$$

where ψ_I should approximate the solution inside the basin and φ should add the edge effects. Inside the basin, the larger scales are relevant, so the Sverdrup balance is used for ψ_I :

$$\frac{\partial \psi_I}{\partial x} = \frac{\varepsilon}{r} \mathbf{k} \cdot \nabla \times \boldsymbol{\tau}_T = -\frac{\varepsilon\pi}{rL} \rho_o U^2 \sin\left(\pi \frac{y}{L}\right) \quad (21.23)$$

to. This is solved by

$$\psi_I = (C - x) \frac{\varepsilon\pi}{rL} \rho_o U^2 \sin\left(\pi \frac{y}{L}\right). \quad (21.24)$$

with a constant C . The remaining part of the differential equation should be solved by φ :

$$\varepsilon \Delta \varphi = 0 \quad (21.25)$$

This is solved by

$$\varphi = -B \frac{\varepsilon\pi}{rL} \rho_o U^2 \sin\left(\pi \frac{y}{L}\right) \exp\left(\pm \pi \frac{x}{L}\right) \quad (21.26)$$

with a constant B . The overall solution is therefore

$$\psi = \psi_I + \varphi = \left(C - x - B \exp\left(\pm \pi \frac{x}{L}\right)\right) \frac{\varepsilon\pi}{rL} \rho_o U^2 \sin\left(\pi \frac{y}{L}\right). \quad (21.27)$$

This follows for the vertically averaged velocities

$$\bar{u} = -\frac{\partial \psi}{\partial y} = -\frac{\pi}{L} \left(C - x - B \exp\left(\pm \pi \frac{x}{L}\right)\right) \frac{\varepsilon\pi}{rL} \rho_o U^2 \cos\left(\pi \frac{y}{L}\right), \quad (21.28)$$

$$\bar{v} = \frac{\partial \psi}{\partial x} = \left(-1 \mp B \frac{\pi}{L} \exp\left(\pm \pi \frac{x}{L}\right)\right) \frac{\varepsilon\pi}{rL} \rho_o U^2 \sin\left(\pi \frac{y}{L}\right). \quad (21.29)$$

B und C werden aus den Randbedingungen abgeleitet. Diese lauten

$$\bar{u}(x = 0, L) = 0, \quad \bar{v}(y = 0, L) = 0. \quad (21.30)$$

The boundary conditions for $\bar{v}$ are automatically fulfilled. From which it follows for $\bar{u}$

$$C = B, \quad B - L - B \exp\left(-\pi \frac{L}{L}\right) = 0 \Rightarrow B = \frac{L}{1 - \exp(-\pi)}, \quad (21.31)$$

whereby the negative sign in the exponential function was arbitrarily determined. This follows

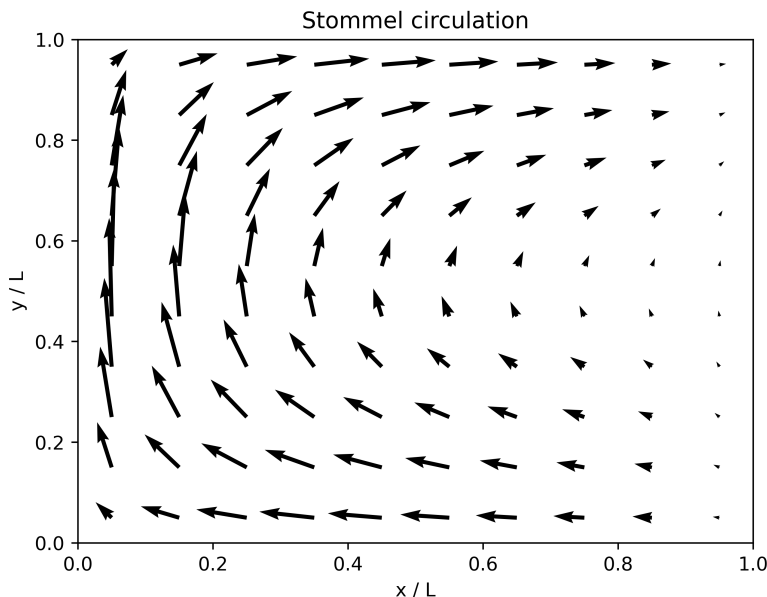


Figure 21.1: Visualization of the equations (21.28) - (21.29).

$$\psi = \left(\frac{L}{1 - \exp(-\pi)} - x - \frac{L}{1 - \exp(-\pi)} \exp\left(-\pi \frac{x}{L}\right) \right) \frac{\varepsilon \pi}{r L \rho_0} U^2 \sin\left(\pi \frac{y}{L}\right). \quad (21.32)$$

21.2 Thermohaline circulation

21.3 Ocean models

21.4 Sea state forecast

21.4.1 Prognostic variables

Sea state is another word for water surface waves. The prognostic variable targeted is the deflection of the water surface

$$h = h(x, y, t) \quad (21.33)$$

from the mean position of the water surface.¹ In many situations h is not a function of the horizontal coordinates, such as in the case of surf or turbulent seas, since in these cases the position of the water surface is no longer clearly defined. Such effects are taken into account later in the form of energy dissipating source terms.

The shallow water equations derived in Section 13.8.1 could now be used as a set of prognostic equations, possibly with some semi-empirical additional terms. However, this has several disadvantages:

- In order to capture a significant portion of the energy of the wave field, a very small time step and a very fine spatial resolution would be required.
- In most cases the phases of the waves are not known and are not very relevant. Rather, variables such as the direction and height of the waves are crucial.

Therefore, to describe water surface waves, a radiation transfer equation (radiative transfer equation (RTE)) is usually used. The spectral radiance is therefore used as a prognostic variable.

$$N = N(\mathbf{k}, \mathbf{r}, t) \quad (21.34)$$

¹ h cannot simply be defined as a deviation from the geoid, since the dynamic topography would still be superimposed here. This does not count towards the deflection associated with the waves. The length of the averaging interval must be chosen accordingly.

used. Here $\mathbf{r}$ is a two-dimensional position vector and $\mathbf{k}$ is a two-dimensional wave vector. Usually $\mathbf{k}$ is not given in Cartesian coordinates, but in polar coordinates (k, θ) . The dispersion relation $\omega = \omega(k, \theta)$ is that of the water surface waves

$$\omega^2 = gk \tanh(kD) \Rightarrow \omega = \sqrt{gk \tanh(kD)}, \quad (21.35)$$

used, where D is the average water depth (water depth without waves). Follow from this

$$c_{\text{ph}} = \frac{\omega}{k} = \sqrt{\frac{g \tanh(kD)}{k}}, \quad (21.36)$$

$$\begin{aligned} c_{\text{gr}} &= \frac{1}{2\omega} \frac{\partial \omega^2}{\partial k} = \frac{1}{2\omega} \left[g \tanh(kD) + \frac{gkD}{\cosh^2(kD)} \right] = \frac{g \tanh(kD)}{2\omega} \left[1 + \frac{kD}{\sinh(kD) \cosh(kD)} \right] \\ &= \frac{c_{\text{ph}}}{2} \left[1 + \frac{2kD}{\sinh(kD) \cosh(kD)} \right] = \frac{c_{\text{ph}}}{2} \left[1 + \frac{2kD}{\sinh(2kD)} \right]. \end{aligned} \quad (21.37)$$

So the group velocity is isotropic but not homogeneous,

$$c_{\text{gr}} = c_{\text{gr}}(k, \mathbf{r}, t). \quad (21.38)$$

The location and time dependence arises via the location and time dependence of D .

21.4.2 Wave action equation

From this one can derive a spectral radiation flux density

$$N(k, \theta, \mathbf{r}, t) (c_{\text{gr}}(k, \mathbf{r}, t) + \mathbf{v}(\mathbf{r}, t)) \quad (21.39)$$

derive, here $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$ is the current velocity. The radiation transfer equation is a kind of continuity equation for N , which is conceptually related to the conservation of energy:

$$\begin{aligned} \frac{\partial N(k, \theta)}{\partial t} + \nabla \cdot (N(k, \theta) c_{\text{gr}}(k)) &= S_{\text{nl}}(k, \theta) + S_{\text{ws}}(k, \theta) + S_{\text{wc}}(k, \theta) \\ &+ S_{\text{diss}}(k, \theta) + S_{\text{bd}}(k, \theta) \end{aligned} \quad (21.40)$$

The location and time dependency was no longer noted. Furthermore, five additional source terms were included:

- $S_{\text{nl}}(k, \theta)$ is the energy source resulting from nonlinear effects. This term is particularly relevant for the interaction of scales. An example is the creation of long waves (so-called *swell*) from the *wind sea* (waves arising directly from the action of wind), which consists of shorter waves, via upscaling.
- $S_{\text{ws}}(k, \theta)$ is the energy source resulting from the interaction with the wind field. This is the main source of energy in the wave field.
- $S_{\text{wc}}(k, \theta)$ is the energy source that results from the *spray* (the so-called *whitecapping*), this is a dissipative and therefore usually negative term.
- $S_{\text{diss}}(k, \theta)$ is the energy source related to the internal friction (viscosity). Since the viscosity has a stronger square effect on the smaller scales, this effect leads to wind sea being dissipated faster than swell.
- $S_{\text{bd}}(k, \theta)$ is the energy source that is related to the interaction with the bathymetry (*bottom drag*), this is also a dissipative and therefore usually negative term.

Depending on the specific situation, additional source terms can be included. Eq. (21.40) is also called *wave action equation*.

The total energy of the wave spectrum E at a certain location at a certain time is the integral over the entire spectrum:

$$E = \int_0^{2\pi} \int_0^\infty N(k, \theta) dk d\theta. \quad (21.41)$$

The energy-weighted spectral mean of a quantity ψ is therefore calculated via

$$\bar{\psi} := \frac{1}{E} \int_0^{2\pi} \int_0^\infty \psi(k, \theta) N(k, \theta) dk d\theta. \quad (21.42)$$

21.4.3 Diagnostic variables

21.4.3.1 Significant wave height

The *significant wave height* is a kind of representative wave height for which the following applies

$$H_s = 4\sqrt{E}. \quad (21.43)$$

21.4.3.2 Medium wave direction

The *mean wave direction* θ_m is calculated according to Eq. (21.42) as

$$\theta_m = \arctan_2(b, a) \quad (21.44)$$

with

$$\begin{aligned} a &:= \frac{1}{E} \int_0^{2\pi} \int_0^\infty \cos(\theta) N(k, \theta) dk d\theta, \\ b &:= \frac{1}{E} \int_0^{2\pi} \int_0^\infty \sin(\theta) N(k, \theta) dk d\theta. \end{aligned} \quad (21.45)$$

21.4.3.3 Medium wavelength

For the *mean wavelength* L_m applies

$$L_m = \overline{\left(\frac{2\pi}{k}\right)} = 2\pi \overline{k}^{-1}. \quad (21.46)$$

21.4.3.4 Mean wave period

There are different ways to calculate the *mean wave period*:

$$T_{m,1} = \frac{2\pi}{\bar{\sigma}}, \quad (21.47)$$

$$T_{m,2} = \frac{2\pi}{\sqrt{\overline{\sigma^2}}}, \quad (21.48)$$

$$T_{m,-1} = \overline{\left(\frac{2\pi}{\sigma}\right)} = 2\pi \overline{\sigma}^{-1}. \quad (21.49)$$

Here σ is the angular frequency measured relative to the seabed.

21.4.4 Sea state forecast models

The most common sea state forecast model is WAVEWATCH III. Models that follow Eq. (21.40) are so-called third generation sea state prediction models. They solve this equation on a grid and are therefore grid point models, although they are sometimes referred to as spectral models because their prognostic variable has spectral significance. You solve Eq. (21.40), where at each grid point a spectral direction-dependent grid is spanned in (k, θ) space. In most cases, a fairly large variety of semi-empirical source terms Q_i are also included.

Part V

Radiation and cloud microphysics

The central quantity in radiation transport is the spectral radiance $L_z(\mathbf{r}, \mathbf{n}, t)$, here z is the wave number and $\mathbf{n}$ is a direction vector. From it you can, among other things: Thermal power densities can be derived.

22.1 Simple models

22.1.1 Planet without an atmosphere

The solar constant S_o is the radiant flux density of the solar radiation that hits the Earth. Since the ratio of the surface to the cross-sectional area of a sphere is $\frac{1}{4}$, on average the radiation flux density $\frac{S_o}{4}$ occurs at the upper edge of the atmosphere. Assuming that the Earth is a black body, in the equilibrium case with the Stefan-Boltzmann law Eq. (5.320)

$$\frac{S_o}{4} = \sigma T_{\text{rad}}^4, \quad (22.1)$$

here T_{rad} is the so-called *radiation temperature*. This can be extended by assuming a wavelength-independent emissivity ε and an albedo $a := 1 - \varepsilon$:

$$\frac{S_o}{4} (1 - a) = \varepsilon \sigma T_{\text{rad}}^4 \quad (22.2)$$

Under the simplifying assumption that the long-wave (LW) and short-wave (SW) spectral ranges are separated from each other, one can use sizes $\varepsilon_{\text{SW}}, a_{\text{SW}}, \varepsilon_{\text{LW}}, a_{\text{LW}}$:

$$\begin{aligned} \frac{S_o}{4} (1 - a_{\text{SW}}) &= \varepsilon_{\text{LW}} \sigma T_{\text{rad}}^4 \\ T_{\text{rad}} &= \left[\frac{S_o}{4 \varepsilon_{\text{LW}} \sigma} (1 - a_{\text{SW}}) \right]^{1/4} \end{aligned} \quad (22.3)$$

This is referred to as:

$$a_p := a_{\text{SW}} \quad (22.4)$$

as *planetary albedo*.

22.1.2 One-layer atmosphere

Now a homogeneous atmosphere, which consists of only a single layer, is included in the model. Atmospheric properties are denoted by the index A , while surface properties are denoted by the index S . Every subcomponent of the system (atmosphere, surface) is in thermal equilibrium. The applicable system of equations is therefore:

$$S_A^{(\text{in})} = S_A^{(\text{out})} \Leftrightarrow S_{A,\text{SW}}^{(\text{in})} + S_{A,\text{LW}}^{(\text{in})} = S_{A,\text{SW}}^{(\text{out})} + S_{A,\text{LW}}^{(\text{out})}, \quad (22.5)$$

$$S_S^{(\text{in})} = S_S^{(\text{out})} \Leftrightarrow S_{S,\text{SW}}^{(\text{in})} + S_{S,\text{LW}}^{(\text{in})} = S_{S,\text{SW}}^{(\text{out})} + S_{S,\text{LW}}^{(\text{out})}. \quad (22.6)$$

Now make the following assumptions:

- The atmosphere does not interact with short-wave radiation, so it transmits 100 % of it.
- The earth's surface reflects a portion $a_{S,\text{SW}}$ of the short-wave radiation, the rest is absorbed. Since the reflected portion does not interact with the atmosphere, this energy propagates back into space.
- The atmosphere is imagined as a single bar of homogeneous temperature that has a lower and an upper surface. In this model, the atmosphere has two surfaces from which it can emit long-wave radiation.
- Within the short-wave or long-wave radiation range, the radiation properties are assumed to be independent of temperature and wavelength.

This results in the radiation flux densities

$$S_{A,SW}^{(in)} = 0, \quad S_{A,LW}^{(in)} = \varepsilon_{A,LW} \varepsilon_{S,LW} \sigma T_S^4, \quad (22.7)$$

$$S_{A,SW}^{(out)} = 0, \quad S_{A,LW}^{(out)} = 2\varepsilon_{A,LW} \sigma T_A^4, \quad (22.8)$$

$$S_{S,SW}^{(in)} = (1 - a_{S,SW}) \frac{S_o}{4}, \quad S_{S,LW}^{(in)} = \varepsilon_{A,LW} \sigma T_A^4, \quad (22.9)$$

$$S_{S,SW}^{(out)} = 0, \quad S_{S,LW}^{(out)} = \varepsilon_{S,LW} \sigma T_S^4. \quad (22.10)$$

If you insert this into the equations (22.5) - (22.6), you get

$$0 + \varepsilon_{A,LW} \varepsilon_{S,LW} \sigma T_S^4 = 0 + 2\varepsilon_{A,LW} \sigma T_A^4, \quad (22.11)$$

$$(1 - a_{S,SW}) \frac{S_o}{4} + \varepsilon_{A,LW} \sigma T_A^4 = 0 + \varepsilon_{S,LW} \sigma T_S^4. \quad (22.12)$$

Equivalence transformations result

$$T_A^4 = \frac{\varepsilon_{S,LW}}{2} T_S^4, \quad (22.13)$$

$$\varepsilon_{S,LW} \sigma T_S^4 - \varepsilon_{A,LW} \sigma T_A^4 = (1 - a_{S,SW}) \frac{S_o}{4}. \quad (22.14)$$

If you put Eq. (22.13) in Eq. (22.14), you get

$$\begin{aligned} \varepsilon_{S,LW} \sigma T_S^4 - \varepsilon_{A,LW} \sigma \frac{\varepsilon_{S,LW}}{2} T_S^4 &= (1 - a_{S,SW}) \frac{S_o}{4} \\ \Leftrightarrow \left(1 - \frac{\varepsilon_{A,LW}}{2}\right) \varepsilon_{S,LW} \sigma T_S^4 &= (1 - a_{S,SW}) \frac{S_o}{4} \\ \Leftrightarrow \left(1 - \frac{\varepsilon_{A,LW}}{2}\right) T_S^4 &= \frac{S_o}{4\sigma\varepsilon_{S,LW}} (1 - a_{S,SW}) \\ \Leftrightarrow T_S &= \left[\frac{S_o}{4\sigma\varepsilon_{S,LW} \left(1 - \frac{\varepsilon_{A,LW}}{2}\right)} (1 - a_{S,SW}) \right]^{1/4} = T_{\text{rad}} \left(1 - \frac{\varepsilon_{A,LW}}{2}\right)^{-1/4}. \end{aligned} \quad (22.15)$$

The inequality

$$T_S > T_{\text{rad}} \quad (22.16)$$

is called *greenhouse effect*. This is based on the assumptions $\varepsilon_{A,LW} > 0$ and $a_{A,SW} = 0$. The simplest clear justification for the greenhouse effect is that long-wave radiation is not emitted according to the temperature T_S , but rather according to the temperature $T_A < T_S$.

22.2 feedbacks

Interactions between subsets of the Earth system are referred to as *feedback*. A distinction is made between *positive feedback*, which reinforces itself, and *negative feedback*, which dampens itself.

22.2.1 Temperature-radiation feedback

According to the Stefan-Boltzmann law, the radiation from a body is proportional to the fourth power of the temperature. From this you get the following negative feedback:

Temperature increases $\rightarrow$ Radiation increases $\rightarrow$ Temperature decreases $\rightarrow$ Radiation decreases $\rightarrow$ Temperature increases

Ultimately, this process describes the leveling off at a temperature at which the body under consideration is in equilibrium with the radiation field. Such considerations are always to be understood conceptually, which means that the oscillation suggested here does not necessarily have to take place.

22.2.2 Temperature-ice-albedo feedback

The planetary albedo a_p depends on the Earth's ice coverage: the higher the ice-covered portion, the more solar radiation is reflected. The feedback can be conceptualized in the form

Temperature increases $\rightarrow$ Ice melts $\rightarrow$ Planetary albedo decreases $\rightarrow$ more solar radiation is absorbed $\rightarrow$
Temperature increases

or

Temperature drops $\rightarrow$ Water freezes $\rightarrow$ Planetary albedo increases $\rightarrow$ Less solar radiation is absorbed $\rightarrow$
Temperature drops

formulate. So it is a positive feedback.

To quantify this, two temperatures $T_o < T_i$ are introduced and the temperature-dependent planetary albedo is set

$$a_p(T) = \begin{cases} a_{\max}, & T < T_o \\ a_{\max} + (T - T_o) \frac{a_{\min} - a_{\max}}{T_i - T_o}, & T_o \leq T \leq T_i \\ a_{\min}, & T > T_i \end{cases} \quad (22.17)$$

with $0 \leq a_{\min} < a_{\max} \leq 1$. For the temperature-dependent radiation $S = S(T)$ of the planet we continue

$$S(T) = a + b(T - \bar{T}) \quad (22.18)$$

This corresponds to a linear development of the Stefan-Boltzmann law, so it applies

$$a = \sigma T_{\text{rad}}^4, \quad (22.19)$$

$$b = 4\sigma T_{\text{rad}}^3. \quad (22.20)$$

Here are

$$\bar{T} := \frac{T_o + T_i}{2} \quad (22.21)$$

the approximate temperature of the earth as well

$$T_{\text{rad}} := 0,9\bar{T} \quad (22.22)$$

a radiation temperature. In equilibrium now applies

$$\frac{S_o}{4} (1 - a_p(T)) = a + b(T - \bar{T}). \quad (22.23)$$

with the solar constant S_o . This equation has between one and three solutions depending on T_o , T_i , $a_{\min}$ and $a_{\max}$, as shown in Fig. 22.1. The equilibria in cases 2 and 3 are stable, while in case 1 the middle equilibrium is unstable and the outer two are stable.

22.3 Calculation of scattering and absorption coefficients

22.3.1 Effective radius

The *effective radius* is a size measure for condensates that well represents the properties they have in relation to their interaction with radiation. Assuming that all condensates are spherical and have radius r_{eff} ,

$$\frac{V}{A} = \frac{N \frac{4}{3} \pi r_{\text{eff}}^3}{N \pi r_{\text{eff}}^2} = \frac{4}{3} r_{\text{eff}}. \quad (22.24)$$

Here V is the total volume of the condensates, A is their summed cross-sectional area (ignoring overlap) and N is the number of condensates in the volume under consideration. From this it follows

$$r_{\text{eff}} = \frac{3V}{4A}. \quad (22.25)$$

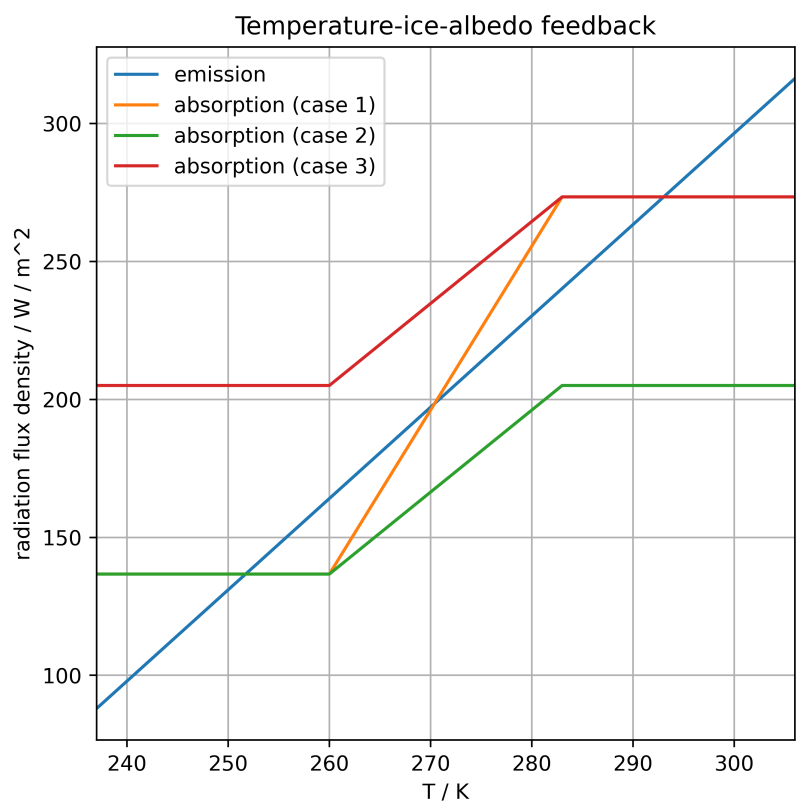


Figure 22.1: Possibilities for equilibria in the temperature-ice-albedo feedback. All curves were calculated with $T_o = 260$ K and $T_i = 283$ K. The parameters for the cases are $(a_{min}, a_{max}) = (0.2; 0.6)$ (case 1), $(a_{min}, a_{max}) = (0.4; 0.6)$ (case 2), $(a_{min}, a_{max}) = (0.2; 0.4)$ (case 3).

The effective radius therefore links the size V (bulk size) that can be derived from the average density with the size of the cross-sectional area, which is important for alternating working with radiation.

22.4 Approximations

The spectral radiance depends on six real numbers in addition to the time. Common fields depend on three coordinates. A first problem is the amount of storage space that is necessary to store even a very roughly discretized radiation state of an atmosphere. However, solving the radiation transfer equation is much more problematic. Therefore, rigorous approximations are necessary.

22.4.1 Plan-parallel atmosphere

This approximation assumes that the atmosphere within a certain area is horizontally homogeneous, so the properties only vary vertically. This is motivated by the fact that in the atmosphere on large scales, horizontal gradients are at least two orders of magnitude smaller than vertical ones.

22.4.2 Horizontal decoupling

This approximation divides the atmosphere into independent columns and thereby greatly limits the horizontal interaction. However, such a column can consist of different sub-columns or horizontal interactions can be parameterized in another way within the columns. As computing capacity increases, the areas with horizontal interaction can be enlarged until, in the limit, the entire atmosphere is viewed as a single column.

22.5 Radiation balance

The radiation state of the atmosphere is completely described by the spectral radiance

$$L = L(\mathbf{r}, \varphi, \lambda, \omega, t). \quad (22.26)$$

Many factors go into the evolution of this size. The aim of this section is to quantify the importance of subcomponents of the climate system for the radiation field. This is called *radiation balance* or also *radiation balance*.

22.6 Atmospheric optics

The so-called *cloud microphysics* is about answering the following questions:

- How do clouds and precipitation form?
- What size spectra do clouds and precipitation have?
- What is the falling speed of clouds and precipitation?
- What interactions exist between the condensates?

23.1 Köhler equation

The vapor pressure over a solution is given by equation (5.268):

$$\ln \left(\frac{p_S(n_s)}{p_S^{(o)}} \right) = -\frac{n_s}{n_w}. \quad (23.1)$$

The notation was adapted to that common in cloud physics.

The vapor pressure over a curved surface is given by equation (5.301):

$$\ln \left(\frac{p_S(R)}{p_S^{(o)}} \right) = \frac{2\gamma}{R_s T R \rho_w}. \quad (23.2)$$

If both effects occur at the same time, you get

$$\ln \left(\frac{p_S(R, n_s)}{p_S^{(o)}} \right) = \frac{2\gamma}{R_s T R \rho_w} - \frac{n_s}{n_w} \quad (23.3)$$

as an equation for the vapor pressure over a curved surface within which a solution is located. For n_w holds

$$n_w = \frac{m_w}{M_w} = \frac{4\pi R^3 \rho_w}{3M_w}. \quad (23.4)$$

From this it follows

$$\ln \left(\frac{p_S(R, n_s)}{p_S^{(o)}} \right) = \frac{2\gamma}{R_s T R \rho_w} - \frac{3M_w n_s}{4\pi R^3 \rho_w}. \quad (23.5)$$

If you use the diameter D instead of the radius R , it follows

$$\ln \left(\frac{p_S(D, n_s)}{p_S^{(o)}} \right) = \frac{4\gamma}{R_s T D \rho_w} - \frac{6M_w n_s}{\pi D^3 \rho_w}. \quad (23.6)$$

This equation is called *Köhler equation*.

If you derive this equation in terms of D and set the derivative equal to zero, you get

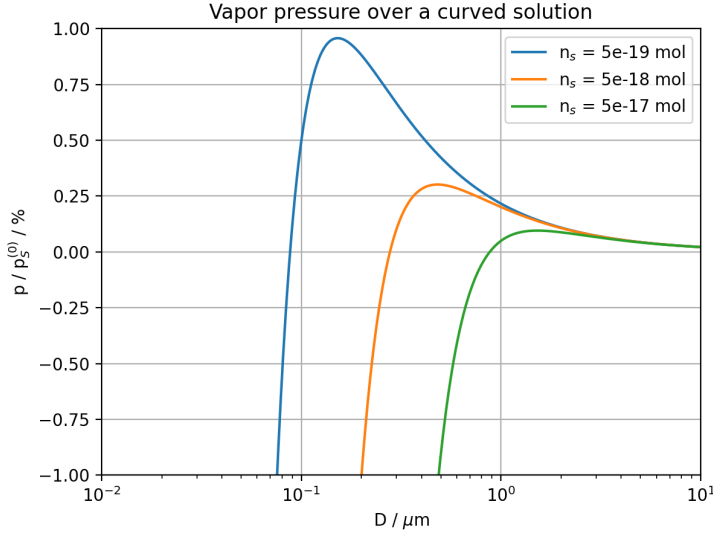


Figure 23.1: Köhler curves of water droplets.

$$\begin{aligned}
 0 &= -\frac{4\gamma}{R_s T D_c^2 \rho_w} + \frac{18 M_w n_s}{\pi D_c^4 \rho_w} \\
 \Leftrightarrow \frac{4\gamma}{R_s T D_c^2} &= \frac{18 M_w n_s}{\pi D_c^4} \\
 \Leftrightarrow \frac{4\gamma D_c^2}{R_s T} &= \frac{18 M_w n_s}{\pi} \\
 \Leftrightarrow D_c^2 &= \frac{9 R_s T M_w n_s}{2 \gamma \pi} = \frac{9 R T n_s}{2 \gamma \pi}.
 \end{aligned} \tag{23.7}$$

D_c is called *critical diameter*. The saturation vapor pressure is maximum at the critical diameter. Only drops with $D > D_c$ can continue to grow and become cloud and rain drops. Such drops only form in the free atmosphere for $p_v > p_s(D_c)$.

As can be seen from Fig. 23.1, the critical diameter increases with n_s , whereas the maximum saturation vapor pressure decreases.

23.2 Circulation around condensates

From the flow field around a condensate you can derive the force that acts on the condensate, which results in the falling speed by equating it with the weight.

23.2.1 Laminar flow

Imagine a sphere with radius a centered at the origin of a Cartesian coordinate system. One now looks for solutions to the incompressible system of equations without momentum advection

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{v}, \tag{23.8}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{23.9}$$

with the boundary conditions

$$\lim_{|\mathbf{r}| \rightarrow \infty} \mathbf{v} = U \mathbf{e}_z, \quad (23.10)$$

$$\mathbf{v}(|\mathbf{r}| = a) = \mathbf{o}. \quad (23.11)$$

One limits oneself to stationary, i.e. especially laminar solutions. This results in the momentum equation Eq. (23.8)

$$\nabla p = \eta \Delta \mathbf{v}. \quad (23.12)$$

The notation of $\mathbf{v}$ in spherical coordinates is

$$\mathbf{v} = v_r \mathbf{e}_r + v_\theta \mathbf{e}_\theta + v_\varphi \mathbf{e}_\varphi. \quad (23.13)$$

Here θ is the angle relative to the z-axis and φ is the angle relative to the xz-plane. Stationary solutions are rotationally symmetrical about the z-axis, and the following also applies

$$v_\varphi = \mathbf{o}. \quad (23.14)$$

The following applies to the friction force created by the flow, which acts on the ball

$$F = -2\pi a^2 \int_0^\pi \left[p \cos(\theta) + \eta \sin(\theta) \frac{\partial v_\theta}{\partial r} \right] \sin(\theta) d\theta. \quad (23.15)$$

Such a friction force is called *Stokes friction*. This is divided into a force F_p , which arises from the pressure p , and a force F_v , which arises from the shear of the velocity field, i.e

$$F_p := -2\pi a^2 \int_0^\pi p \cos(\theta) \sin(\theta) d\theta, \quad (23.16)$$

$$F_v := -2\pi \eta a^2 \int_0^\pi \frac{\partial v_\theta}{\partial r} \sin(\theta)^2 d\theta. \quad (23.17)$$

This applies

$$F = F_p + F_v. \quad (23.18)$$

According to the statements at the beginning of Chap. 15 and Eq. (23.9) can be $\mathbf{v}$ in the form

$$\mathbf{v} = \nabla \times \mathbf{A} \quad (23.19)$$

represented by a velocity potential $\mathbf{A}$. According to Eq. (B.98) applies

$$\begin{aligned} \nabla \times \mathbf{A} &= \frac{A_\theta}{r} \mathbf{e}_\varphi + \frac{A_\varphi}{r \tan(\theta)} \mathbf{e}_r - \frac{A_\varphi}{r} \mathbf{e}_\theta + \mathbf{e}_r \left(\frac{1}{r} \frac{\partial A_\varphi}{\partial \theta} - \frac{1}{r \sin(\theta)} \frac{\partial A_\theta}{\partial \varphi} \right) \\ &+ \mathbf{e}_\theta \left(\frac{1}{r \sin(\theta)} \frac{\partial A_r}{\partial \varphi} - \frac{\partial A_\varphi}{\partial r} \right) + \mathbf{e}_\varphi \left(\frac{\partial A_\theta}{\partial r} - \frac{1}{r} \frac{\partial A_r}{\partial \theta} \right). \end{aligned} \quad (23.20)$$

Due to rotational symmetry about the z-axis, $\mathbf{v}$ does not depend on φ . This implies

$$\nabla \times \mathbf{A} = \frac{A_\theta}{r} \mathbf{e}_\varphi + \frac{A_\varphi}{r \tan(\theta)} \mathbf{e}_r - \frac{A_\varphi}{r} \mathbf{e}_\theta + \mathbf{e}_r \frac{1}{r} \frac{\partial A_\varphi}{\partial \theta} - \mathbf{e}_\theta \frac{\partial A_\varphi}{\partial r} + \mathbf{e}_\varphi \left(\frac{\partial A_\theta}{\partial r} - \frac{1}{r} \frac{\partial A_r}{\partial \theta} \right). \quad (23.21)$$

By projections onto the location-dependent basis elements of the spherical coordinates one obtains

$$v_r = \frac{A_\varphi}{r \tan(\theta)} + \frac{\mathbf{i}}{r} \frac{\partial A_\varphi}{\partial \theta}, \quad (23.22)$$

$$v_\theta = -\frac{A_\varphi}{r} - \frac{\partial A_\varphi}{\partial r}, \quad (23.23)$$

$$v_\varphi = \frac{A_\theta}{r} + \frac{\partial A_\theta}{\partial r} - \frac{\mathbf{i}}{r} \frac{\partial A_r}{\partial \theta}. \quad (23.24)$$

The condition $v_\varphi = 0$ can therefore be fulfilled by $A_\theta = A_r = 0$ without affecting the other components. Define

$$\psi = \psi(r, \theta) := -r A_\varphi \sin(\theta), \quad (23.25)$$

then applies

$$v_r = -\frac{\mathbf{i}}{r^2 \sin(\theta)} \frac{\partial \psi}{\partial \theta}, \quad (23.26)$$

$$v_\theta = \frac{\mathbf{i}}{r \sin(\theta)} \frac{\partial \psi}{\partial r}. \quad (23.27)$$

The rotation of the wind field is:

$$\nabla \times \mathbf{v} = \frac{v_\theta}{r} \mathbf{e}_\varphi + \frac{v_\varphi}{r \tan(\theta)} \mathbf{e}_r - \frac{v_\varphi}{r} \mathbf{e}_\theta + \mathbf{e}_r \frac{\mathbf{i}}{r} \frac{\partial v_\varphi}{\partial \theta} - \mathbf{e}_\theta \frac{\partial v_\varphi}{\partial r} + \mathbf{e}_\varphi \left(\frac{\partial v_\theta}{\partial r} - \frac{\mathbf{i}}{r} \frac{\partial v_r}{\partial \theta} \right). \quad (23.28)$$

With $v_\varphi = 0$ it follows from this

$$\boldsymbol{\xi} = \nabla \times \mathbf{v} = \frac{v_\theta}{r} \mathbf{e}_\varphi + \mathbf{e}_\varphi \left(\frac{\partial v_\theta}{\partial r} - \frac{\mathbf{i}}{r} \frac{\partial v_r}{\partial \theta} \right) = \mathbf{e}_\varphi \left(\frac{\partial v_\theta}{\partial r} - \frac{\mathbf{i}}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_\theta}{r} \right). \quad (23.29)$$

If you insert the equations (23.26) - (23.27) here, you get

$$\begin{aligned} \boldsymbol{\xi} &= \nabla \times \mathbf{v} = \mathbf{e}_\varphi \left(\frac{\mathbf{i}}{r \sin(\theta)} \frac{\partial^2 \psi}{\partial r^2} - \frac{\mathbf{i}}{r^2 \sin(\theta)} \frac{\partial \psi}{\partial r} - \frac{\cos(\theta)}{r^3 \sin^2(\theta)} \frac{\partial \psi}{\partial \theta} + \frac{\mathbf{i}}{r^3 \sin(\theta)} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{\mathbf{i}}{r^2 \sin(\theta)} \frac{\partial \psi}{\partial r} \right) \\ &= \mathbf{e}_\varphi \left(\frac{\mathbf{i}}{r \sin(\theta)} \frac{\partial^2 \psi}{\partial r^2} - \frac{\cos(\theta)}{r^3 \sin^2(\theta)} \frac{\partial \psi}{\partial \theta} + \frac{\mathbf{i}}{r^3 \sin(\theta)} \frac{\partial^2 \psi}{\partial \theta^2} \right) \\ &= \frac{\mathbf{e}_\varphi}{r \sin(\theta)} \left(\frac{\partial^2 \psi}{\partial r^2} - \frac{\cos(\theta)}{r^2 \sin(\theta)} \frac{\partial \psi}{\partial \theta} + \frac{\mathbf{i}}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} \right) \\ &= \frac{\mathbf{e}_\varphi}{r \sin(\theta)} \left[\frac{\partial^2}{\partial r^2} + \frac{\sin(\theta)}{r^2} \frac{\partial}{\partial \theta} \left(\frac{\mathbf{i}}{\sin(\theta)} \frac{\partial}{\partial \theta} \right) \right] \psi \equiv \frac{\mathbf{e}_\varphi}{r \sin(\theta)} E^2 \psi \end{aligned} \quad (23.30)$$

with a differential operator

$$E^2 := \frac{\partial^2}{\partial r^2} - \frac{\mathbf{i}}{r^2 \tan(\theta)} \frac{\partial}{\partial \theta} + \frac{\mathbf{i}}{r^2} \frac{\partial^2}{\partial \theta^2} = \frac{\partial^2}{\partial r^2} + \frac{\sin(\theta)}{r^2} \frac{\partial}{\partial \theta} \left(\frac{\mathbf{i}}{\sin(\theta)} \frac{\partial}{\partial \theta} \right). \quad (23.31)$$

From this it follows that:

$$\boldsymbol{\xi} = \nabla \times (\nabla \times \mathbf{A}) = \nabla \times [\nabla \times (A_\varphi \mathbf{e}_\varphi)] = -\nabla \times \left[\nabla \times \left(\frac{\psi}{r \sin(\theta)} \mathbf{e}_\varphi \right) \right]. \quad (23.32)$$

For doubly continuously differentiable scalar fields ψ therefore holds

$$-\nabla \times \left[\nabla \times \left(\frac{\mathcal{X}}{r \sin(\theta)} \mathbf{e}_\varphi \right) \right] = \frac{\mathbf{e}_\varphi}{r \sin(\theta)} E^2 \mathcal{X}. \quad (23.33)$$

Eq. (B.54) is

$$\Delta \mathbf{v} = \nabla (\nabla \cdot \mathbf{v}) - \nabla \times (\nabla \times \mathbf{v}) \stackrel{\text{Glg. (23.9)}}{=} -\nabla \times (\nabla \times \mathbf{v}) = -\nabla \times \boldsymbol{\xi}. \quad (23.34)$$

This allows the momentum equation Eq. (23.12) in the form

$$\nabla p = -\eta \nabla \times \boldsymbol{\xi} \quad (23.35)$$

note down. If you apply the rotation again, it follows

$$\circ = -\eta \nabla \times (\nabla \times \boldsymbol{\xi}) = -\eta \nabla \times \left[\nabla \times \left(\frac{\mathbf{e}_\varphi}{r \sin(\theta)} E^2 \psi \right) \right] = \eta \frac{\mathbf{e}_\varphi}{r \sin(\theta)} E^4 \psi. \quad (23.36)$$

So you can

$$E^4 \psi = \circ \quad (23.37)$$

use as the differential equation for ψ . From the boundary condition Eq. (23.11) follow

$$\frac{\partial \psi}{\partial r} (r = a) = \circ, \quad (23.38)$$

$$\frac{\partial \psi}{\partial \theta} (r = a) = \circ. \quad (23.39)$$

So ψ is constant along the surface of the sphere, $\circ$. B. d. A. can be used as a boundary condition

$$\psi (r = a) = \circ \quad (23.40)$$

demand. The boundary condition Eq. (23.10) is in spherical coordinates

$$\lim_{|r| \rightarrow \infty} v_r = U \cos(\theta), \quad (23.41)$$

$$\lim_{|r| \rightarrow \infty} v_\theta = -U \sin(\theta). \quad (23.42)$$

The pressure is said to converge at infinity to a homogeneous background pressure $p_\circ$:

$$\lim_{|r| \rightarrow \infty} p = p_\circ \quad (23.43)$$

It applies

$$E^4 \psi = \left(\frac{\partial^2}{\partial r^2} - \frac{\mathbf{1}}{r^2 \tan(\theta)} \frac{\partial}{\partial \theta} + \frac{\mathbf{1}}{r^2} \frac{\partial^2}{\partial \theta^2} \right) \left(\frac{\partial^2 \psi}{\partial r^2} - \frac{\mathbf{1}}{r^2 \tan(\theta)} \frac{\partial \psi}{\partial \theta} + \frac{\mathbf{1}}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} \right). \quad (23.44)$$

Now you do the approach for ψ

$$\psi(r, \theta) = -\frac{U \sin(\theta)^2}{2} \left(Ar + Br^2 + \frac{C}{r} \right). \quad (23.45)$$

From Eq. (23.41) follows

$$\begin{aligned}
\lim_{|r| \rightarrow \infty} v_r &= - \lim_{|r| \rightarrow \infty} \frac{\mathbf{I}}{r^2 \sin(\theta)} \frac{\partial \psi}{\partial \theta} = \lim_{|r| \rightarrow \infty} \frac{\mathbf{I}}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \frac{U \sin(\theta)^2}{\mathbf{2}} \left(Ar + Br^2 + \frac{C}{r} \right) \\
&= \lim_{|r| \rightarrow \infty} \frac{\mathbf{I}}{r^2 \sin(\theta)} U \sin(\theta) \cos(\theta) \left(Ar + Br^2 + \frac{C}{r} \right) \\
&= \lim_{|r| \rightarrow \infty} U \cos(\theta) \left(\frac{A}{r} + B + \frac{C}{r^3} \right) \\
&= \lim_{|r| \rightarrow \infty} BU \cos(\theta) = BU \cos(\theta).
\end{aligned} \tag{23.46}$$

Comparison with Eq. (23.41) implied

$$B = \mathbf{I}. \tag{23.47}$$

From Eq. (23.42) follows

$$\begin{aligned}
\lim_{|r| \rightarrow \infty} v_\theta &= \lim_{|r| \rightarrow \infty} \frac{\mathbf{I}}{r \sin(\theta)} \frac{\partial \psi}{\partial r} = - \lim_{|r| \rightarrow \infty} \frac{\mathbf{I}}{r \sin(\theta)} \frac{\partial}{\partial r} \frac{U \sin(\theta)^2}{\mathbf{2}} \left(Ar + Br^2 + \frac{C}{r} \right) \\
&= - \lim_{|r| \rightarrow \infty} \frac{\mathbf{I}}{r \sin(\theta)} \frac{U \sin(\theta)^2}{\mathbf{2}} \left(A + \mathbf{2}Br - \frac{C}{r^2} \right) \\
&= - \lim_{|r| \rightarrow \infty} U \sin(\theta) \left(\frac{A}{\mathbf{2}r} + B - \frac{C}{\mathbf{2}r^3} \right) \\
&= - \lim_{|r| \rightarrow \infty} U \sin(\theta) B = -BU \sin(\theta).
\end{aligned} \tag{23.48}$$

Comparison with Eq. (23.42) again implies $B = \mathbf{I}$, so

$$\psi(r, \theta) = - \frac{U \sin(\theta)^2}{\mathbf{2}} \left(Ar + r^2 + \frac{C}{r} \right). \tag{23.49}$$

From Eq. (23.40) is further obtained

$$\psi(a, \theta) = - \frac{U \sin(\theta)^2}{\mathbf{2}} \left(Aa + a^2 + \frac{C}{a} \right) \stackrel{!}{=} \mathbf{o} \tag{23.50}$$

$$\Leftrightarrow Aa + a^2 + \frac{C}{a} = \mathbf{o} \tag{23.51}$$

$$\Leftrightarrow Aa^2 + a^3 + C = \mathbf{o} \tag{23.52}$$

$$\Leftrightarrow C = -Aa^2 - a^3, \tag{23.53}$$

so

$$\psi(r, \theta) = - \frac{U \sin(\theta)^2}{\mathbf{2}} \left(Ar + r^2 - \frac{Aa^2 + a^3}{r} \right). \tag{23.54}$$

From this it follows

$$\frac{\psi(r, \theta)}{\partial r} = - \frac{U \sin(\theta)^2}{\mathbf{2}} \left(A + \mathbf{2}r + \frac{Aa^2 + a^3}{r^2} \right). \tag{23.55}$$

From Eq. (23.38) follows

$$\begin{aligned}
A + \mathbf{2}a + \frac{Aa^2 + a^3}{a^2} &= A + \mathbf{2}a + A + a = \mathbf{2}A + \mathbf{3}a \stackrel{!}{=} \mathbf{o} \\
&\Leftrightarrow A = - \frac{\mathbf{3}a}{\mathbf{2}}.
\end{aligned} \tag{23.56}$$

So the approach is:

$$\begin{aligned}\psi(r, \theta) &= -\frac{U \sin(\theta)^2}{2} \left(-\frac{3a}{2}r + r^2 + \frac{3a^3}{2r} - \frac{a^3}{r} \right) \\ &= -\frac{U \sin(\theta)^2}{2} \left(-\frac{3a}{2}r + r^2 + \frac{a^3}{2r} \right).\end{aligned}\quad (23.57)$$

Now this is shown in Eq. (23.44) is used. Preparatory calculations are made

$$\frac{\partial^2 \psi}{\partial r^2} = -\frac{U \sin(\theta)^2}{2} \left(2 + \frac{a^3}{r^3} \right), \quad (23.58)$$

$$-\frac{1}{r^2 \tan(\theta)} \frac{\partial \psi}{\partial \theta} = U \cos(\theta)^2 \left(-\frac{3a}{2r} + 1 + \frac{a^3}{2r^3} \right), \quad (23.59)$$

$$\frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} = -U (\cos(\theta)^2 - \sin(\theta)^2) \left(-\frac{3a}{2r} + 1 + \frac{a^3}{2r^3} \right). \quad (23.60)$$

Adding these three terms together gives

$$E^2 \psi = \frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r^2 \tan(\theta)} \frac{\partial \psi}{\partial \theta} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} = -\frac{U \sin(\theta)^2}{2} \left(2 + \frac{a^3}{r^3} \right) + U \sin(\theta)^2 \left(-\frac{3a}{2r} + 1 + \frac{a^3}{2r^3} \right) \quad (23.61)$$

$$= -\frac{U \sin(\theta)^2}{2} \left(2 + \frac{a^3}{r^3} + \frac{3a}{r} - 2 - \frac{a^3}{r^3} \right) \quad (23.62)$$

$$= -\frac{3a U \sin(\theta)^2}{2r}. \quad (23.63)$$

From this it follows

$$\frac{\partial^2 E^2 \psi}{\partial r^2} = -\frac{6a U \sin(\theta)^2}{2r^3} = -\frac{3a U \sin(\theta)^2}{r^3}, \quad (23.64)$$

$$-\frac{1}{r^2 \tan(\theta)} \frac{\partial E^2 \psi}{\partial \theta} = \frac{3a U \cos(\theta)^2}{r^3}, \quad (23.65)$$

$$\frac{1}{r^2} \frac{\partial^2 E^2 \psi}{\partial \theta^2} = -\frac{3a U (\cos(\theta)^2 - \sin(\theta)^2)}{r^3}. \quad (23.66)$$

Adding these three equations together, it follows

$$E^4 \psi = 0. \quad (23.67)$$

Eq. (23.37) actually solves Eq. (23.37).

Now it remains to be shown that Eq. (23.35) from the approach Eq. (23.37) is solved. You first calculate this

$$\nabla \times \xi = \nabla \times \left[\mathbf{e}_\varphi \frac{E^2 \psi}{r \sin(\theta)} \right] \stackrel{\text{Glg. (B.51)}}{=} -\mathbf{e}_\varphi \times \nabla \frac{E^2 \psi}{r \sin(\theta)} + \frac{E^2 \psi}{r \sin(\theta)} \nabla \times \mathbf{e}_\varphi. \quad (23.68)$$

With

$$\nabla \times \mathbf{e}_\varphi \stackrel{\text{Glg. (B.98)}}{=} \frac{1}{r \tan(\theta)} \mathbf{e}_r - \frac{1}{r} \mathbf{e}_\theta \quad (23.69)$$

follows

$$\begin{aligned}\nabla \times \xi &= -\mathbf{e}_\varphi \times \nabla \frac{E^2 \psi}{r \sin(\theta)} + \frac{E^2 \psi}{r \sin(\theta)} \left(\frac{1}{r \tan(\theta)} \mathbf{e}_r - \frac{1}{r} \mathbf{e}_\theta \right) \\ &= -\mathbf{e}_\varphi \times \nabla \frac{E^2 \psi}{r \sin(\theta)} + \frac{\cos(\theta) E^2 \psi}{r^2 \sin(\theta)^2} \mathbf{e}_r - \frac{E^2 \psi}{r^2 \sin(\theta)} \mathbf{e}_\theta.\end{aligned}\quad (23.70)$$

If you put Eq. (23.63), you get

$$\nabla \times \boldsymbol{\xi} = -\frac{3aU}{2} \left(-\mathbf{e}_\varphi \times \nabla \frac{\sin(\theta)}{r^2} + \frac{\cos(\theta)}{r^3} \mathbf{e}_r - \frac{\sin(\theta)}{r^3} \mathbf{e}_\theta \right). \quad (23.71)$$

With Eq. (B.88) follows

$$\nabla \frac{\sin(\theta)}{r^2} = -\frac{2\sin(\theta)}{r^3} \mathbf{e}_r + \frac{\cos(\theta)}{r^3} \mathbf{e}_\theta. \quad (23.72)$$

Therefore applies

$$-\mathbf{e}_\varphi \times \nabla \frac{\sin(\theta)}{r^2} = \frac{2\sin(\theta)}{r^3} \mathbf{e}_\theta + \frac{\cos(\theta)}{r^3} \mathbf{e}_r. \quad (23.73)$$

Putting this into Eq. (23.71), you get

$$\begin{aligned} \nabla \times \boldsymbol{\xi} &= -\frac{3aU}{2} \left(\frac{2\sin(\theta)}{r^3} \mathbf{e}_\theta + \frac{\cos(\theta)}{r^3} \mathbf{e}_r + \frac{\cos(\theta)}{r^3} \mathbf{e}_r - \frac{\sin(\theta)}{r^3} \mathbf{e}_\theta \right) \\ &= -\frac{3aU}{2} \left(\frac{\sin(\theta)}{r^3} \mathbf{e}_\theta + \frac{2\cos(\theta)}{r^3} \mathbf{e}_r \right). \end{aligned} \quad (23.74)$$

Putting this into Eq. (23.35), you get

$$\nabla p = \frac{3aU}{2} \frac{\eta \sin(\theta)}{r^3} \mathbf{e}_\theta + \frac{3aU}{2} \frac{2\eta \cos(\theta)}{r^2} \mathbf{e}_r, \quad (23.75)$$

so

$$\begin{aligned} \frac{\partial p}{\partial r} &= \frac{3aU}{2} \frac{2\eta \cos(\theta)}{r^3}, \\ \frac{\partial p}{\partial \theta} &= \frac{3aU}{2} \frac{\eta \sin(\theta)}{r^2}. \end{aligned} \quad (23.76)$$

This is solved by

$$p = p_0 - \frac{3aU}{2} \frac{\eta \cos(\theta)}{r^2}. \quad (23.77)$$

This implies for the friction force created by the pressure according to Eq. (23.16)

$$\begin{aligned} F_p &= -2\pi a^2 \int_0^\pi -\frac{3\eta a U \cos(\theta)}{2a^2} \cos(\theta) \sin(\theta) d\theta = \pi \int_0^\pi 3\eta a U \cos(\theta) \cos(\theta) \sin(\theta) d\theta \\ &= 3\eta a U \pi \int_0^\pi \cos^2(\theta) \sin(\theta) d\theta = -3\eta a U \pi \left[\frac{1}{3} \cos^3(\theta) \right]_0^\pi = 2\eta a U \pi. \end{aligned} \quad (23.78)$$

For v_θ one obtains using Eq. (23.27) and the approach Eq. (23.57)

$$\begin{aligned} v_\theta &= \frac{1}{r \sin(\theta)} \frac{\partial \mathcal{V}}{\partial r} = \frac{1}{r \sin(\theta)} \frac{\partial}{\partial r} \left[-\frac{U \sin^2(\theta)}{2} \left(-\frac{3a}{2} r + r^2 + \frac{a^3}{2r} \right) \right] \\ &= \frac{1}{r} \frac{\partial}{\partial r} \left[\frac{U \sin(\theta)}{2} \left(\frac{3a}{2} r - r^2 - \frac{a^3}{2r} \right) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left[\frac{U a^2 \sin(\theta)}{2} \left(\frac{3}{2a} r - \frac{r^2}{a^2} - \frac{a}{2r} \right) \right] \\ &= \frac{1}{r} \left[\frac{U a^2 \sin(\theta)}{4} \left(-\frac{4r}{a^2} + \frac{3}{a} + \frac{a}{r^2} \right) \right] = \frac{U a^2 \sin(\theta)}{4} \left(-\frac{4}{a^2} + \frac{3}{ar} + \frac{a}{r^3} \right). \end{aligned} \quad (23.79)$$

From this it follows

$$\frac{\partial v_\theta}{\partial r} = -\frac{Ua^2 \sin(\theta)}{4} \left(\frac{3}{ar^2} + \frac{3a}{r^4} \right). \quad (23.80)$$

If you evaluate this at $r = a$, it follows

$$\frac{\partial v_\theta}{\partial r}(r = a) = -\frac{Ua^2 \sin(\theta)}{4} \left(\frac{3}{a^3} + \frac{3}{a^3} \right) = -\frac{6U \sin(\theta)}{4a} = -\frac{3U \sin(\theta)}{2a}. \quad (23.81)$$

Putting this into Eq. (23.17), you get

$$F_v = -2\pi\eta a^2 \int_0^\pi -\frac{3U \sin(\theta)}{2a} \sin(\theta)^2 d\theta = 3U\pi\eta a \int_0^\pi \sin(\theta)^3 d\theta. \quad (23.82)$$

You now integrate

$$\begin{aligned} \int_0^\pi \sin(\theta)^3 d\theta &= [-\cos(\theta) \sin(\theta)^2]_0^\pi + 2 \int_0^\pi \cos(\theta)^2 \sin(\theta) d\theta \\ &= 2 \int_0^\pi \cos(\theta)^2 \sin(\theta) d\theta = \frac{2}{3} [-\cos(\theta)^3]_0^\pi = \frac{2}{3} [\cos(\theta)^3]_\pi^0 = \frac{4}{3}. \end{aligned} \quad (23.83)$$

This implies

$$F_v = 3U\pi\eta a \frac{4}{3} = 4U\pi\eta a. \quad (23.84)$$

Therefore, according to Eq. (23.18) for the friction force

$$F = 6\pi a \eta U. \quad (23.85)$$

If you put this with the weight

$$F_g = mg = \frac{4}{3}\pi a^3 (\rho'_l - \rho'_h) g \quad (23.86)$$

equal, you get

$$v_F = \frac{F}{6\pi a \eta} = \frac{4\pi a^3 (\rho'_l - \rho'_h) g}{18\pi a \rho'_h r} = \frac{2a^2 (\rho'_l - \rho'_h) g}{9\rho'_h r} \quad (23.87)$$

as a formula for the equilibrium falling speed v_F . In Eq. (23.86) the static buoyancy of the condensate is subtracted.

23.2.2 Turbulent flow around

In the case of turbulent flow, the circulation surrounding the condensate is time-dependent in an aperiodic manner. Here the friction force F is proportional to the square of the speed U ,

$$F = \frac{1}{2} c_w \pi a^2 \rho'_h U^2, \quad (23.88)$$

where $c_w \geq 0$ is a constant dependent on the shape of the object flowed around, the so-called c_w -value. In English this quantity is called *drag coefficient* c_d . If you compare this with the weight force according to Eq. (23.86) is equal, you get

$$\frac{1}{2} c_w \pi a^2 \rho'_h v_F^2 = \frac{4}{3} \pi a^3 \rho'_l g \Leftrightarrow v_F^2 = \frac{8a\rho'_l g}{3\rho'_h c_w} \quad (23.89)$$

$$\Leftrightarrow v_F = \sqrt{\frac{8a\varrho'_l g}{3\varrho'_h c_w}} \quad (23.90)$$

as a formula for the equilibrium falling speed v_F .

23.2.3 Compound formula for falling speed

Small condensates flow around laminarly, larger ones flow turbulently. The parameter $a \in [0, 1]$ describes the proportion of turbulence in the friction force F , i.e

$$F = aF_{\text{turbulent}} + (1 - a)F_{\text{laminar}}. \quad (23.91)$$

If you insert the equations (23.85) and (23.88) here, you get

$$F = a \frac{1}{2} c_w \pi a^2 \varrho'_h U^2 + (1 - a) 6\pi a \varrho'_h r U. \quad (23.92)$$

Here $c_w \approx 0.8$ is a realistic value. If you compare this with the weight force according to Eq. (23.86) is the same, assuming $a \neq 0$

$$\begin{aligned} (1 - a) 6\pi a \varrho'_h r v_F + a \frac{1}{2} c_w \pi a^2 \varrho'_h v_F^2 &= \frac{4}{3} \pi a^3 \varrho'_l g \\ \Leftrightarrow a \frac{1}{2} c_w \pi a \varrho'_h v_F^2 + (1 - a) 6\pi \varrho'_h r v_F - \frac{4}{3} \pi a^2 \varrho'_l g &= 0 \\ \Leftrightarrow a c_w \pi a \varrho'_h v_F^2 + (1 - a) 12\pi \varrho'_h r v_F - \frac{8\pi a^2 \varrho'_l g}{3} &= 0 \\ \Leftrightarrow a c_w \pi a v_F^2 + (1 - a) 12\pi r v_F - \frac{8\pi a^2 \varrho'_l g}{3\varrho'_h} &= 0 \\ \Leftrightarrow \pi a v_F^2 + \frac{(1 - a)}{a c_w} 12\pi r v_F - \frac{8\pi a^2 \varrho'_l g}{3a\varrho'_h c_w} &= 0 \\ \Leftrightarrow v_F^2 + \frac{(1 - a)}{a a c_w} 12r v_F - \frac{8a\varrho'_l g}{3a\varrho'_h c_w} &= 0. \end{aligned} \quad (23.93)$$

It is expected that the transition from laminar to turbulent friction depends critically on the Reynolds number

$$R := \frac{U^2 a^2}{r U a} = \frac{U a}{r} \quad (23.94)$$

depends. It is now assumed that the transition from laminar to turbulent friction occurs at a critical Reynolds number R_k . To determine the equilibrium rate of descent, one can proceed as follows:

1. Calculate v_F from Eq. (23.87).
2. Calculate the Reynolds number R from this.
3. If the result is not greater than R_k , $R \leq R_k$, $a = 0$ and the result is already available. For balls it can be assumed that $R_k = 10$.
4. Otherwise $a = 1$, then use (23.90) to determine the equilibrium falling speed. For spheres, $c_w = 1$ can be assumed.

23.3 Growth of condensates

23.3.1 Size distribution of raindrops

The most commonly used size distribution for raindrops is the *Marshall-Palmer distribution* [26], which has the form

$$n(D) = n_o \exp(-\lambda D) \quad (23.95)$$

has. Here D is the diameter of the raindrops, λ is a parameter and $n(D)$ is the number of drops with a diameter between D and $D + dD$, divided by dD . $n_o = 8 \cdot 10^6 \text{ m}^{-4}$ is taken as a constant. This emerges empirically. The parameter λ can be linked to the density of liquid water ρ_l . To do this, you integrate

$$\rho_l = \int_0^\infty n(D) dD = \int_0^\infty n(D) \frac{4}{3} \pi \left(\frac{D}{2}\right)^3 \rho_l' dD = \frac{\pi}{6} \int_0^\infty n(D) D^3 \rho_l' dD = \frac{\pi}{6} \rho_l' n_o \int_0^\infty \exp(-\lambda D) D^3 dD, \quad (23.96)$$

here ρ_l' is the microscopic density of water. For the integral one obtains with Eq. (A.96)

$$\int_0^\infty \exp(-\lambda D) D^3 dD = \frac{6}{\lambda^4}. \quad (23.97)$$

Putting this into Eq. (23.96), you get

$$\rho_r = \frac{\pi}{6} \rho_l' n_o \int_0^\infty \exp(-\lambda D) D^3 dD = \frac{\pi \rho_l' n_o}{\lambda^4}, \quad (23.98)$$

it follows from this

$$\lambda = \left(\frac{\pi \rho_l' n_o}{\rho_r} \right)^{1/4}. \quad (23.99)$$

For the mean diameter D_o it follows, again with Eq. (A.96),

$$D_o = \frac{\int_0^\infty \exp(-\lambda D) D dD}{\int_0^\infty \exp(-\lambda D) dD} = \frac{1}{\lambda}, \quad (23.100)$$

so

$$D_o = \left(\frac{\rho_r}{\pi \rho_l' n_o} \right)^{1/4}. \quad (23.101)$$

This formula can be used to diagnostically derive an average diameter of raindrops from the density of the rainwater.

From Eq. (23.100) is obtained using the substitution rule Eq. (A.86) also

$$D_o = \frac{\int_0^\infty n_D(D) D dD}{\int_0^\infty n_D(D) dD} = \frac{\int_0^\infty n_D(2D) 2D \cdot 2 \cdot dD}{\int_0^\infty n_D(2D) \cdot 2 \cdot dD} = 2 \frac{\int_0^\infty 2 n_D(2r) r dr}{\int_0^\infty 2 n_D(2r) dr} = 2 \frac{\int_0^\infty n_r(r) r dr}{\int_0^\infty n_r(r) dr} = 2 r_o. \quad (23.102)$$

The mean diameter is therefore twice the mean radius, regardless of the size distribution. Here, the spectrum as a function of the radius $n_r(r)$ was deliberately distinguished from the spectrum as a function of the diameter $n_D(D)$ and $n_r(r) = 2 n_D(2r)$ was used. The same applies

$$\overline{D^n} = 2^n \overline{r^n}. \quad (23.103)$$

23.3.1.1 Application on snow

Empirically it has been shown that Marshall-Palmer distributions also approximate the size spectra of snowflakes well [21].¹ Here is

¹Ice crystals below a certain diameter are no longer referred to as snow, but as cloud ice, but across the entire size spectrum the Marshall-Palmer distribution is among the distributions that can be described by a parameter (here λ). most suitable.

$$n_o = 4,6 \cdot 10^6 \text{ m}^{-4}. \quad (23.104)$$

23.3.1.2 Application to sleet and hail

Empirically it is shown that Marshall-Palmer distributions also approximate the size spectra of graupel and hailstones well [21].² The approach is usually used here

$$n_o = A \mathcal{L}^b \quad (23.105)$$

with $b = 3.63$ and $A = 115 \frac{1}{1000^{b-1}} = 1.481 \cdot 10^{-6}$. Putting this into Eq. (23.98), you get

$$\rho_g = \frac{\pi \rho'_i n_o}{\mathcal{L}^4} = \frac{\pi \rho'_i A \mathcal{L}^b}{\mathcal{L}^4} = \frac{\pi \rho'_i A}{\mathcal{L}^{4-b}}, \quad (23.106)$$

here ρ_g is the density of sleet or hail and ρ'_i is the microscopic density of ice. If you convert this to $D_o = 1/\mathcal{L}$, you get

$$D_o = \left(\frac{\rho_g}{\pi \rho'_i A} \right)^{\frac{1}{4-b}}. \quad (23.107)$$

23.3.2 Auto conversion

The so-called *autoconversion* refers to the formation of precipitation through the growth of cloud particles. So several cloud particles combine to form one precipitation particle. This is the first step of precipitation formation.

23.3.2.1 Bergeron-Findeisen process

23.3.3 diffusion

Condensates can grow or shrink through diffusion. The diffusive flow arises because the vapor pressure on the surface of the condensate, which corresponds to the saturation vapor pressure above water or ice at the respective temperature, is different from the ambient vapor pressure. To do this, one starts from the diffusion equation Eq. (5.212) and from a stationary state:

$$0 = \psi \Delta \rho_v. \quad (23.108)$$

This assumes that the diffusion coefficient of water vapor in moist air ψ and the density of dry air ρ_d are homogeneous near the drop, which are justified assumptions due to the small size of tropics.

Since this is a radially symmetric problem, one can make the approach $\rho_v = \rho_v(r)$. Using the Laplace operator in spherical coordinates Eq. (B.91) is thus obtained

$$\psi \Delta \rho_v = \psi \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \rho_v}{\partial r} \right) = \psi \left(\frac{2}{r} \frac{\partial \rho_v}{\partial r} + \frac{\partial^2 \rho_v}{\partial r^2} \right) = 0. \quad (23.109)$$

This equation is with the boundary conditions

$$\rho_v(a) = \rho_{v,a}, \quad (23.110)$$

$$\rho_v(r \rightarrow \infty) = \rho_{v,\infty} \quad (23.111)$$

to solve, where a is the radius of the drop. The solution is

$$\rho_v(a) = \rho_{v,\infty} + \left(\rho_{v,a} - \rho_{v,\infty} \right) \frac{a}{r}, \quad (23.112)$$

how easily it can be verified:

²See the previous footnote.

$$\frac{2}{r} \frac{\partial \varrho_v}{\partial r} + \frac{\partial^2 \varrho_v}{\partial r^2} = (\varrho_{v,a} - \varrho_{v,\infty}) \left(-\frac{2a}{r^3} + \frac{2a}{r^3} \right) = 0, \quad (23.113)$$

$$\varrho_v(a) = \varrho_{v,\infty} + (\varrho_{v,a} - \varrho_{v,\infty}) \frac{a}{a} = \varrho_{v,a}, \quad (23.114)$$

$$\varrho_v(r \rightarrow \infty) = \varrho_{v,\infty} + (\varrho_{v,a} - \varrho_{v,\infty}) \frac{a}{\infty} = \varrho_{v,\infty}. \quad (23.115)$$

The corresponding mass flow density into the drop at the surface is therefore according to Eq. (5.208)

$$j = \psi \frac{\partial \varrho_v}{\partial r} = -\psi (\varrho_{v,a} - \varrho_{v,\infty}) \frac{a}{a^2} = -\psi (\varrho_{v,a} - \varrho_{v,\infty}) \frac{1}{a}. \quad (23.116)$$

If you integrate this over the entire surface, you get the growth rate of the mass of a drop:

$$\frac{dm}{dt} = 4\pi a^2 j = -4\pi a \psi (\varrho_{v,a} - \varrho_{v,\infty}) \frac{1}{a} = 4\pi a \psi (\varrho_{v,\infty} - \varrho_{v,a}) \quad (23.117)$$

Here $\varrho_{v,a}$ is the absolute saturation humidity $\varrho_S(T)$ at temperature T and $\varrho_{v,\infty}$ is the ambient vapor pressure, for which from now on ϱ_v is noted:

$$\frac{dm}{dt} = 4\pi a \psi (\varrho_v - \varrho_S(T)). \quad (23.118)$$

Due to the permanent phase transition taking place on the surface of the drop, it does not have the ambient temperature T , but the temperature T_s :

$$\frac{dm}{dt} = 4\pi a \psi (\varrho_v - \varrho_S(T_s)). \quad (23.119)$$

For $\varrho_S(T_s)$ you now do a first order Taylor expansion and use the Clausius-Clapeyron equation Eq. (5.231)

$$\begin{aligned} \varrho_S(T_s) &\approx \varrho_S(T) + \frac{\partial \varrho_S}{\partial T} (T_s - T) \approx \varrho_S(T) + \frac{1}{R_v T} \frac{dp_S}{dT} (T_s - T) \approx \varrho_S(T) + \frac{p_S}{R_v T} \frac{L_v}{R_v T^2} (T_s - T) \\ &= \varrho_S(T) + \varrho_S(T) \frac{L_v}{R_v T^2} (T_s - T). \end{aligned} \quad (23.120)$$

Now an expression for the surface temperature T_s must be derived. The basic approach for this is the assumption that the heat caused by the phase transition is compensated for by heat transfer on the surface of the drop. The heat transfer on the surface of the drop is also a diffusive process, so in generalization of Eq. (23.119)

$$\frac{dT_s}{dt} = \frac{4\pi a k_h}{m c_l^{(p)}} (T - T_s). \quad (23.121)$$

Here, $c_l^{(p)}$ is the specific heat capacity of water and $k_h = c_h^{(p)} \varrho_h \alpha_h$ is the thermal conductivity of moist air with α_h as the thermal conductivity. The temperature tendency due to the phase transition is:

$$\frac{dT_s}{dt} = \frac{L_v}{m c_l^{(p)}} \frac{dm}{dt}. \quad (23.122)$$

The sum of these two temperature tendencies is zero, so you get

$$\frac{4\pi a k_h}{m c_l^{(p)}} (T - T_s) = -\frac{L_v}{m c_l^{(p)}} \frac{dm}{dt} \Leftrightarrow T_s - T = \frac{L_v}{4\pi a k_h} \frac{dm}{dt}. \quad (23.123)$$

Putting this into Eq. (23.120), you get

$$\varrho_S(T_s) \approx \varrho_S(T) + \varrho_S(T) \frac{L_v^*}{R_v T^2} \frac{dm}{dt}. \quad (23.124)$$

Putting this into Eq. (23.119), follows

$$\begin{aligned} \frac{dm}{dt} &= 4\pi a \psi \left(\varrho_v - \varrho_S(T) - \varrho_S(T) \frac{L_v^*}{R_v T^2} \frac{dm}{dt} \right) \\ \Leftrightarrow \frac{dm}{dt} \left(1 + \varrho_S(T) \frac{L_v^* \psi}{R_v T^2 k_h} \right) &= 4\pi a D (\varrho_v - \varrho_S(T)) \\ \Leftrightarrow \frac{dm}{dt} &= \frac{4\pi a \psi}{1 + \varrho_S(T) \frac{L_v^* \psi}{R_v T^2 k_h}} (\varrho_v - \varrho_S(T)) = \frac{4\pi a}{\frac{1}{\psi} + \varrho_S(T) \frac{L_v^*}{R_v T^2 k_h}} (\varrho_v - \varrho_S(T)) \end{aligned}$$

$$\Leftrightarrow \frac{dm}{dt} = \frac{4\pi a}{\frac{1}{\psi \varrho_S(T)} + \frac{L_v^*}{R_v T^2 k_h}} \left(\frac{\varrho_v}{\varrho_S(T)} - 1 \right). \quad (23.125)$$

23.3.3.1 Ventilation coefficient

The previous derivations in this section refer to drops that do not move relative to the air surrounding them. However, if they fall through the air, the growth rate increases by a factor

$$f_v := \frac{dm/dt}{(dm/dt)_o}, \quad (23.126)$$

where $(dm/dt)_o$ denotes the growth rate of the non-moving drop. f_v is the *ventilation coefficient*. For f_v , experimental data became the formula

$$f_v = 0,78 + 0,308 \cdot S_c^{1/3} N_{\text{Re}}^{1/2} \quad (23.127)$$

derived [5]. Here $S_c := \frac{r}{\psi}$ is the *Schmidt number* ($\approx 0,71$ for air [21]) and $N_{\text{Re}} = \frac{U_2 r}{\nu}$ is the Reynolds number.

Assuming that the ventilation effect for heat and mass is the same, multiply Eq. (23.125) with Eq. (23.127) to get the diffusive growth rate of a falling drop:

$$\frac{dm}{dt} = \frac{4\pi a}{\frac{1}{\psi \varrho_S(T)} + \frac{L_v^*}{R_v T^2 k_h}} \left(\frac{\varrho_v}{\varrho_S(T)} - 1 \right) (0,78 + 0,308 \cdot S_c^{1/3} N_{\text{Re}}^{1/2}). \quad (23.128)$$

23.3.3.2 Integration across the spectrum

In order to use Eq. (23.128) to derive a source term per volume must be integrated over the size spectrum of the drops:

$$\begin{aligned}
Q_{d,p} &= \int_0^\infty \frac{dm}{dt} n(r) dr = \int_0^\infty \frac{dm}{dt} n(D) dD \\
&= \frac{2\pi}{\frac{1}{\psi \ell_S(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_S(T)} - 1 \right) \int_0^\infty \left(\circ, 78 D + \circ, 308 D S_c^{1/3} N_{\text{Re}}^{1/2} \right) n(D) dD \\
&= \frac{2\pi}{\frac{1}{\psi \ell_S(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_S(T)} - 1 \right) \left(\circ, 78 \int_0^\infty D n(D) dD + \circ, 308 S_c^{1/3} \int_0^\infty D N_{\text{Re}}^{1/2} n(D) dD \right) \\
&= \frac{2\pi}{\frac{1}{\psi \ell_S(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_S(T)} - 1 \right) n_{o,p} \left(\circ, 78 \int_0^\infty D \exp(-\lambda_p D) dD + \circ, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} v_F^{1/2} \exp(-\lambda_p D) dD \right)
\end{aligned} \tag{23.129}$$

From this it follows with Eq. (A.96)

$$Q_{d,p} = \frac{2\pi}{\frac{1}{\psi \ell_S(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_S(T)} - 1 \right) n_{o,p} \left(\circ, 78 \lambda_p^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} v_F^{1/2} \exp(-\lambda_p D) dD \right). \tag{23.130}$$

23.3.3.3 Application to rain

If you put in Eq. (23.130) Eq. (23.90) for the falling speed, you get

$$\begin{aligned}
Q_{d,r} &= \frac{2\pi}{\frac{1}{\psi \ell_{S,l}(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,l}(T)} - 1 \right) n_{o,r} \left(\circ, 78 \lambda_r^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} \left(\frac{4D \rho_l' g}{3 \rho_h' c_w} \right)^{1/4} \exp(-\lambda_r D) dD \right) \\
&= \frac{2\pi}{\frac{1}{\psi \ell_{S,l}(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,l}(T)} - 1 \right) n_{o,r} \left(\circ, 78 \lambda_r^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} \left(\frac{4 \rho_l' g}{3 \rho_h' c_w} \right)^{1/4} \int_0^\infty D^{7/4} \exp(-\lambda_r D) dD \right) \\
&= \frac{2\pi}{\frac{1}{\psi \ell_{S,l}(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,l}(T)} - 1 \right) n_{o,r} \left(\circ, 78 \lambda_r^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} \left(\frac{4 \rho_l' g}{3 \rho_h' c_w} \right)^{1/4} \lambda_r^{-11/4} \Gamma\left(\frac{11}{4}\right) \right). \tag{23.131}
\end{aligned}$$

Since $Q_{d,r}$ is a phase transition from gaseous to liquid ($\rho_v > \rho_{S,l}$, supersaturation) or from liquid to gaseous ($\rho_v < \rho_{S,l}$, undersaturation), a phase transition heat flux density is associated with this.

23.3.3.4 Application on snow

If you put in Eq. (23.130) Eq. (36.47) for the falling speed, you get

$$\begin{aligned}
Q_{d,s} &= \frac{2\pi}{\frac{1}{\psi \ell_{S,i}(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,i}(T)} - 1 \right) n_{o,i} \left(\circ, 78 \lambda_s^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} (aD^b)^{1/2} \exp(-\lambda_s D) dD \right) \\
&= \frac{2\pi}{\frac{1}{\psi \ell_{S,i}(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,i}(T)} - 1 \right) n_{o,i} \left(\circ, 78 \lambda_s^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} a^{1/2} \int_0^\infty D^{(3+b)/2} \exp(-\lambda_s D) dD \right) \\
&= \frac{2\pi}{\frac{1}{\psi \ell_{S,i}(T)} + \frac{L_v^2}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,i}(T)} - 1 \right) n_{o,i} \left(\circ, 78 \lambda_s^{-2} + \circ, 308 S_c^{1/3} r^{-1/2} a^{1/2} \lambda_s^{-(5+b)/2} \Gamma\left(\frac{5+b}{2}\right) \right). \tag{23.132}
\end{aligned}$$

Since $Q_{d,s}$ is a phase transition from gaseous to solid ($\rho_v > \rho_{S,i}$, supersaturation) or from solid to gaseous ($\rho_v < \rho_{S,i}$, undersaturation), a phase transition heat flux density is associated with this.

23.3.3.5 Application to sleet

For the diffusive growth or sublimation of graupel one obtains analogously to Eq. (23.131)

$$Q_{d,g} = \frac{2\pi}{\frac{1}{\psi_{S,i}(T)} + \frac{L_i}{R_v T^2 k_h}} \left(\frac{\rho_v}{\rho_{S,i}(T)} - 1 \right) n_{o,g} \left(0,78 \mathcal{A}_g^{-2} + 0,308 S_c^{1/3} r^{-1/2} \left(\frac{4\rho'_i g}{3\rho'_h c_w} \right)^{1/4} \mathcal{A}_g^{-11/4} \Gamma\left(\frac{11}{4}\right) \right). \quad (23.133)$$

Since $Q_{d,g}$ is a phase transition from gaseous to solid ($\rho_v > \rho_{S,i}$, supersaturation) or from solid to gaseous ($\rho_v < \rho_{S,i}$, undersaturation), a phase transition heat flux density is associated with this.

23.3.4 Accretion

The so-called *Accretion* refers to the growth of precipitation particles p due to collisions with cloud droplets or cloud ice particles. The terms *coalescence* and *coagulation* are sometimes used for this purpose, although the meaning is not always entirely uniform. Coalescence is usually used synonymously with accretion, often in reference to raindrops (Sect. 23.3.4.1). Coagulation is basically synonymous with accretion and coalescence, but usually refers to the growth of snow at the expense of other condensate classes (Sect. 23.3.4.2). In this text we will therefore only speak of accretion.

To determine the corresponding source density $Q_{a,p}$, one assumes that cloud particles have no falling speed and precipitation particles have a falling speed $v_p = v_p(r) > 0$. First, the simplifying assumption is made that all precipitation particles have radius r :

$$Q_{a,p} = E_{p,c} n_p \pi r^2 v_p(r) \rho_c. \quad (23.134)$$

Here ρ_c and n_p are the particle densities of the cloud and precipitation particles and $E_{p,c}$ is the probability that two particles merge into one particle after a collision. From now on it will be neglected, i.e. h. it is set at one:

$$Q_{a,p} = n_p \pi r^2 v_p(r) \rho_c. \quad (23.135)$$

If, on the other hand, you assume a size distribution of the raindrops $n_p(r)$, you get

$$Q_{a,p} = \int_0^\infty n_p(r) \pi r^2 v_p(r) \rho_c dr = \pi \rho_c \int_0^\infty n_p(r) r^2 v_p(r) dr = \pi \rho_c \int_0^\infty n_p(r) r^2 v_p(r) dr. \quad (23.136)$$

If you put Eq. (23.95), you get

$$Q_{a,p} = \pi \rho_c \int_0^\infty n_{o,p} \exp(-\lambda_p D) \frac{D^2}{4} v_p\left(\frac{D}{2}\right) dD = \frac{n_{o,p} \pi \rho_c}{4} \int_0^\infty \exp(-\lambda_p D) D^2 v_p\left(\frac{D}{2}\right) dD. \quad (23.137)$$

23.3.4.1 Application to rain

If you put in Eq. (23.137) Eq. (23.90) for the falling speed as well as $n_{o,p} = n_{o,r}$ and $E_{r,c} = 1$, you get

$$\begin{aligned} Q_{a,r,l} &= \frac{n_{o,r} \pi \rho_l}{4} \int_0^\infty \exp(-\lambda_r D) D^2 \sqrt{\frac{4D \rho'_l g}{3\rho'_h c_w}} dD = \frac{n_{o,r} \pi \rho_l}{4} \sqrt{\frac{4\rho'_l g}{3\rho'_h c_w}} \int_0^\infty \exp(-\lambda_r D) D^{5/2} dD \\ &= \frac{n_{o,r} \pi \rho_c}{4 \mathcal{A}_r^{7/2}} \sqrt{\frac{4\rho'_l g}{3\rho'_h c_w}} \Gamma\left(\frac{7}{2}\right) = \frac{n_{o,r} \pi \rho_l}{\mathcal{A}_r^{7/2}} \sqrt{\frac{\rho'_l g}{12\rho'_h c_w}} \Gamma\left(\frac{7}{2}\right). \end{aligned} \quad (23.138)$$

Analogously you get

$$Q_{a,r,i} = \frac{n_{o,r} \pi \rho_i}{\mathcal{A}_r^{7/2}} \sqrt{\frac{\rho'_i g}{12\rho'_h c_w}} \Gamma\left(\frac{7}{2}\right). \quad (23.139)$$

Since the ice particles at $T < T_o$ cause them to freeze when they collide with supercooled raindrops, this is a swelling density for snow. $Q_{a,r,i}$ is not accompanied by phase transition heat because the ice crystals are already frozen when they hit. The accretion of ice by rain is a *three-component process*, since the collision of particles of two condensate classes leads to the formation of a third.

For the accretion of rain through ice crystals (mass of rain per volume and time that collides with ice crystals) is given

$$Q_{a,i,r} = \frac{n_{o,r}\pi\mathcal{G}_i}{4M_i} \sqrt{\frac{4\mathcal{G}_i'g}{3\mathcal{G}_h'c_w}} \int_0^\infty \exp(-\mathcal{L}_r D) D^{5/2} \frac{D^3}{6} \pi \mathcal{G}_i' dD = \frac{n_{o,r}\pi^2 \mathcal{G}_i' \mathcal{G}_i}{6M_i \mathcal{L}_r^{13/2}} \sqrt{\frac{\mathcal{G}_i'g}{12\mathcal{G}_h'c_w}} \Gamma\left(\frac{13}{2}\right). \quad (23.140)$$

Here M_i is an assumed mass of all ice crystals. Since supercooled rain freezes when colliding with ice crystals, $Q_{a,i,r}$ is a source density for snow. This is accompanied by a phase transition heat flux density, as a phase transition from liquid to solid takes place.

For the accretion of snow by rain, Eq. is first modified. (23.134) as follows:

$$\begin{aligned} Q_{a,r,s} &= E_{r,s} n_r \pi (r_r + r_s)^2 |v_r - v_s| \mathcal{G}_s = E_{r,s} n_r n_s \pi (r_r + r_s)^2 |v_r - v_s| \frac{4}{3} \pi r_s^3 \mathcal{G}_i' \\ &= E_{r,s} n_r n_s \pi \frac{1}{24} (D_r + D_s)^2 |v_r - v_s| \pi D_s^3 \mathcal{G}_i' \\ &= E_{r,s} \mathcal{G}_i' n_r n_s \pi^2 |v_r - v_s| \frac{1}{24} (r_s^3 r_r^2 + 2r_s^4 r_r + r_s^5). \end{aligned} \quad (23.141)$$

It was assumed that all raindrops have radius r_r and all snowflakes have radius r_s . Now one sets Marshall-Palmer distributions Eq. (23.95), and integrates over the entire size spectrum. The mass-weighted falling speed is used for the relative speed:

$$\begin{aligned} Q_{a,r,s} &= E_{r,s} \mathcal{G}_i' \pi^2 |v_r - v_s| \frac{1}{24} \int_{D_s=0}^\infty \int_{r_r=0}^\infty n_{o,r} n_{o,s} \exp(-\mathcal{L}_r D_g - \mathcal{L}_s D_s) (D_s^3 D_g^2 + 2D_s^4 D_g + D_s^5) dr_r dD_s \\ &= E_{r,s} \mathcal{G}_i' \pi^2 n_{o,r} n_{o,s} |v_r - v_s| \frac{1}{24} \int_{D_s=0}^\infty \int_{r_r=0}^\infty \exp(-\mathcal{L}_r r_r - \mathcal{L}_s D_s) (D_s^3 r_r^2 + 2D_s^4 r_r + D_s^5) dr_r dD_s \end{aligned} \quad (23.142)$$

$$= E_{r,s} \mathcal{G}_i' \pi^2 n_{o,r} n_{o,s} |v_r - v_s| \frac{1}{24} \int_{D_s=0}^\infty \exp(-\mathcal{L}_s D_s) \int_{D_g=0}^\infty \exp(-\mathcal{L}_r r_r) (D_s^3 r_r^2 + 2D_s^4 D_g + D_s^5) dr_r dD_s. \quad (23.143)$$

From this it follows with Eq. (A.96)

$$\begin{aligned} Q_{a,r,s} &= E_{r,s} \mathcal{G}_i' \pi^2 n_{o,r} n_{o,s} |v_r - v_s| \frac{1}{24} \int_{D_s=0}^\infty \exp(-\mathcal{L}_s D_s) \left(\frac{2D_s^3}{\mathcal{L}_r^3} + \frac{D_s^4}{\mathcal{L}_r^2} + \frac{D_s^5}{\mathcal{L}_r} \right) dD_s \\ &= E_{r,s} \mathcal{G}_i' \pi^2 n_{o,r} n_{o,s} |v_r - v_s| \frac{1}{24} \left(\frac{2 \cdot 3!}{\mathcal{L}_r^3 \mathcal{L}_s^4} + \frac{2 \cdot 4!}{\mathcal{L}_r^2 \mathcal{L}_s^5} + \frac{5!}{\mathcal{L}_r \mathcal{L}_s^6} \right) \\ &= E_{r,s} \mathcal{G}_i' \pi^2 n_{o,r} n_{o,s} |v_r - v_s| \left(\frac{1}{2\mathcal{L}_r^3 \mathcal{L}_s^4} + \frac{2}{\mathcal{L}_r^2 \mathcal{L}_s^5} + \frac{5}{\mathcal{L}_r \mathcal{L}_s^6} \right). \end{aligned} \quad (23.144)$$

For the collision efficiency $E_{r,s}$ one assumes $E_{r,s} = 1$ [24]. A phase transition heat flux density is associated with $Q_{a,r,s}$, as a phase transition from solid to liquid occurs.

23.3.4.2 Application on snow

If you put in Eq. (23.137) Eq. (36.47) and $n_{o,p} = n_{o,s}$ and takes for the collision efficiency

$$E_{s,i} = \exp[0,025 \cdot (T - T_o)] \quad (23.145)$$

[24], you get

$$\begin{aligned} Q_{a,s,i} &= \frac{E_{s,i} n_{o,s} \pi \mathcal{G}_i}{4} \int_0^\infty \exp(-\mathcal{L}_s D) D^2 \frac{a}{2^b} D^b dD = \frac{E_{s,i} n_{o,s} \pi \mathcal{G}_i a}{4 \cdot 2^b} \int_0^\infty \exp(-\mathcal{L}_s D) D^{2+b} dD \\ &= E_{s,i} \frac{n_{o,s} \pi \mathcal{G}_i a \Gamma(3+b)}{4 \cdot 2^b \mathcal{L}_s^{3+b}}. \end{aligned} \quad (23.146)$$

Analogously, one obtains for the accretion of cloud water through snow

$$Q_{a,s,l} = E_{s,l} \frac{n_{o,s} \pi \rho_l a \Gamma (3 + b)}{4 \cdot 2^b \lambda_s^{3+b}}. \quad (23.147)$$

This will

$$E_{s,l} = 1 \quad (23.148)$$

[24] adopted. A phase transition heat flux density is associated with $Q_{a,s,l}$, since a phase transition from liquid to solid occurs.

Analogous to Eq. (23.144) is obtained for the accretion of rain by snow

$$Q_{a,s,r} = E_{s,r} \rho_l' \pi^2 n_{o,r} n_{o,s} |v_r - v_s| \left(\frac{1}{2 \lambda_s^3 \lambda_r^4} + \frac{2}{\lambda_s^2 \lambda_r^5} + \frac{5}{\lambda_s \lambda_r^6} \right). \quad (23.149)$$

For the collision efficiency $E_{s,r}$ one assumes $E_{s,r} = 1$ [24]. A phase transition heat flux density is associated with $Q_{a,s,r}$ because a phase transition from liquid to solid occurs.

23.3.4.3 Application to sleet

For the accretion of snow by hail, analogous to Eq. (23.144)

$$Q_{a,g,s} = E_{g,s} \rho_l' \pi^2 n_{o,g} n_{o,s} |v_g - v_s| \left(\frac{1}{2 \lambda_g^3 \lambda_s^4} + \frac{2}{\lambda_g^2 \lambda_s^5} + \frac{5}{\lambda_g \lambda_s^6} \right). \quad (23.150)$$

The following approach is chosen for collision efficiency [24]:

$$E_{g,s} = \begin{cases} \exp [0, 0.1 (T - T_o)], & T < T_o, \\ 1, & \text{sonst.} \end{cases} \quad (23.151)$$

For the accretion of snow by rain, analogous to Eq. (23.144)

$$Q_{a,g,r} = E_{g,r} \rho_l' \pi^2 n_{o,g} n_{o,r} |v_g - v_r| \left(\frac{1}{2 \lambda_g^3 \lambda_r^4} + \frac{2}{\lambda_g^2 \lambda_r^5} + \frac{5}{\lambda_g \lambda_r^6} \right). \quad (23.152)$$

The collision efficiency $E_{g,r}$ is set at 1 [24]. $Q_{a,g,r}$ is accompanied by a phase transition heat flux density at $T < T_o$, since a phase transition from liquid to solid then takes place.

For the accretion of liquid cloud water through sleet, analogous to Eq. (23.138)

$$Q_{a,g,l} = E_{g,l} \frac{n_{o,g} \pi \rho_l}{\lambda_g^{7/2}} \sqrt{\frac{\rho_l' g}{12 \rho_h' c_w}} \Gamma \left(\frac{7}{2} \right). \quad (23.153)$$

The collision efficiency $E_{g,l}$ is set at 1 [24]. $Q_{a,g,l}$ is accompanied by a phase transition heat flux density at $T < T_o$, since a phase transition from liquid to solid then takes place.

Analogous to Eq. (23.139) is obtained for the accretion of cloud ice by sleet

$$Q_{a,g,i} = E_{g,i} \frac{n_{o,g} \pi \rho_i}{\lambda_g^{7/2}} \sqrt{\frac{\rho_i' g}{12 \rho_h' c_w}} \Gamma \left(\frac{7}{2} \right). \quad (23.154)$$

For the collision efficiency $E_{g,i}$ the following approach is made [24]:

$$E_{g,i} = \begin{cases} 0, 1, & T < T_o, \\ 1, & \text{sonst.} \end{cases} \quad (23.155)$$

23.4 Phase transitions of precipitation

In this section, equations for the mass source densities resulting from phase transitions of precipitation particles are derived.

23.4.1 Freezing of raindrops

For the probability that a drop with volume V' in air at temperature T freezes and melts within a time t , one chooses the stochastic approach [40]

$$P = 1 - \exp \{ -B' V' t [\exp (A' (T_o - T)) - 1] \}. \quad (23.156)$$

From this, $A' = 0.66 \text{ K}^{-1}$ and $B' = 100 \frac{1}{\text{m}^3 \text{s}}$ are empirical coefficients. From this it follows

$$\begin{aligned} 1 - P &= \exp \{ -B' V' t [\exp (A' (T_o - T)) - 1] \} \\ \Leftrightarrow \ln (1 - P) &= -B' V' t [\exp (A' (T_o - T)) - 1] \\ \Leftrightarrow P &\approx B' V' t [\exp (A' (T_o - T)) - 1]. \end{aligned} \quad (23.157)$$

From this you can easily derive the rate of change in the number of raindrops:

$$\frac{dN_r}{dt} = -NB' V' [\exp (A' (T_o - T)) - 1] \quad (23.158)$$

If these drops have a diameter D , it follows

$$\frac{dN_r}{dt} = -NB' \frac{\pi D^3}{6} [\exp (A' (T_o - T)) - 1]. \quad (23.159)$$

For the swelling density of hail or snow $Q_{f,g,r}$, which follows from this process, one obtains using Eq. (A.96)

$$\begin{aligned} Q_{f,g,r} &= B' \frac{\pi}{6} [\exp (A' (T_o - T)) - 1] \int_0^D \rho'_l \pi \frac{D^3}{6} D^3 N(D) dD \\ &= \rho'_l B' \frac{\pi^2}{6^2} [\exp (A' (T_o - T)) - 1] n_{o,r} \int_0^D \exp (-\mathcal{A}_r D) D^6 dD \\ &= \rho'_l B' \frac{\pi^2}{6^2} [\exp (A' (T_o - T)) - 1] n_{o,r} \frac{6!}{\mathcal{A}_r^7} \\ &= \rho'_l B' \frac{\pi^2}{6} [\exp (A' (T_o - T)) - 1] n_{o,r} \frac{5!}{\mathcal{A}_r^7} \end{aligned}$$

$$\Leftrightarrow Q_{f,g,r} = \rho'_l B' 20 \pi^2 [\exp (A' (T_o - T)) - 1] \frac{n_{o,r}}{\mathcal{A}_r^7}. \quad (23.160)$$

Since this process involves a phase transition from liquid to solid, a phase transition heat flux density is associated with this.

23.4.2 Melting of solid precipitate

Melting of snow or sleet occurs at $T > T_o$ if and only if the sum of the other heat fluxes is positive:

$$\begin{aligned} L_s Q_{s,r,p} &= c_l^{(p)} (T - T_o) (Q_{a,g,l} + Q_{a,g,r}) + c_v^{(p)} (T - T_o) Q_{\text{conduction}} - L_v Q_{\text{sublimation}} \\ \Leftrightarrow Q_{s,r,p} &= \frac{c_l^{(p)}}{L_s} (T - T_o) (Q_{a,g,l} + Q_{a,g,r}) + \frac{1}{L_s} [c_v^{(p)} (T - T_o) Q_{\text{conduction}} - L_v Q_{\text{sublimation}}]. \end{aligned} \quad (23.161)$$

$Q_{a,g,l}$ and $Q_{a,g,r}$ are from Eq. (23.153) or Eq. (23.152) is known. $Q_{\text{sublimation}}$ arises from sublimation on the surface of the precipitation particle, this term can be found from Eq. (23.130), whereby the second term in the denominator is omitted, since the heat flux density here is not compensated by the phase transition of sublimation,

but by that of melting:

$$\begin{aligned}
Q_{s,r,p} &= \frac{c_l^{(p)}}{L_s} (T - T_o) (Q_{a,g,l} + Q_{a,g,r}) \\
&\quad + \frac{1}{L_s} \left[L_v \frac{2\pi}{\psi_{\ell_S(T)}} \left(\frac{\rho_v}{\rho_S(T)} - 1 \right) n_{o,p} \left(o, 78 \lambda_p^{-2} + o, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} v_F^{1/2} \exp(-\lambda_p D) dD \right) \right. \\
&\quad \left. + c_v^{(p)} (T - T_o) Q_{\text{conduction}} \right] \\
&= \frac{c_l^{(p)}}{L_s} (T - T_o) (Q_{a,g,l} + Q_{a,g,r}) \\
&\quad + \frac{1}{L_s} \left[L_v 2\pi \psi(\rho_v - \rho_S(T)) n_{o,p} \left(o, 78 \lambda_p^{-2} + o, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} v_F^{1/2} \exp(-\lambda_p D) dD \right) \right. \\
&\quad \left. + c_v^{(p)} (T - T_o) Q_{\text{conduction}} \right]. \tag{23.162}
\end{aligned}$$

To determine $c_v^{(p)} (T - T_o) Q_{\text{conduction}}$, use Eq. (23.121):

$$m c_l^{(p)} \frac{dT_s}{dt} = 2\pi D k_h (T - T_o). \tag{23.163}$$

This results in a term analogous to Eq. (23.130) with the replacement

$$L_v \psi(\rho_v - \rho_S(T)) \rightarrow k_h (T - T_o). \tag{23.164}$$

From this it follows

$$\begin{aligned}
Q_{s,r,p} &= \frac{c_l^{(p)}}{L_s} (T - T_o) (Q_{a,g,l} + Q_{a,g,r}) \\
&\quad + \frac{2\pi}{L_s} \left[L_v \psi[\rho_v - \rho_S(T) + k_h (T - T_o)] n_{o,p} \left(o, 78 \lambda_p^{-2} + o, 308 S_c^{1/3} r^{-1/2} \int_0^\infty D^{3/2} v_F^{1/2} \exp(-\lambda_p D) dD \right) \right]. \tag{23.165}
\end{aligned}$$

Since $Q_{s,r,p}$ is associated with a phase transition from solid to liquid, a phase transition heat flux density is associated with this.

23.4.2.1 Application on snow

If you apply Eq. (23.165) on snow, follows

$$\begin{aligned}
Q_{s,r,s} &= \frac{c_l^{(p)}}{L_s} (T - T_o) (Q_{a,s,l} + Q_{a,s,r}) \\
&\quad + \frac{2\pi}{L_s} \left[L_v \psi[\rho_v - \rho_{S,i}(T) + k_h (T - T_o)] n_{o,s} \left(o, 78 \lambda_s^{-2} + o, 308 S_c^{1/3} r^{-1/2} a^{1/2} \lambda_s^{-(5+b)/2} \Gamma\left(\frac{5+b}{2}\right) \right) \right]. \tag{23.166}
\end{aligned}$$

23.4.2.2 Application to sleet

If you apply Eq. (23.165) on sleet, follows

$$\begin{aligned} Q_{s,r,g} &= \frac{c_l^{(p)}}{L_s} (T - T_o) (Q_{a,g,l} + Q_{a,g,r}) \\ &+ \frac{2\pi}{L_s} \left[L_v \mathcal{Y} \left[\rho_v - \rho_{S,i}(T) + k_h (T - T_o) \right] n_{o,g} \left(\mathfrak{o}, 78 \mathcal{A}_g^{-2} + \mathfrak{o}, 3 \mathfrak{o} 8 S_c^{1/3} r^{-1/2} \left(\frac{4 \rho'_i g}{3 \rho'_h c_w} \right)^{1/4} \mathcal{A}_g^{-11/4} \Gamma \left(\frac{11}{4} \right) \right) \right]. \end{aligned} \tag{23.167}$$

Part VI
Numerics

24 BASIC CONCEPTS OF NUMERICS

A weather model is a copy of the atmosphere. In it, all fields and differential operators are replaced by discretized versions, since you can only store a finite amount of information. One writes a substitution for a differential operator D

$$D \rightarrow D', \quad (24.1)$$

analogous for atmospheric conditions

$$Z \rightarrow Z'. \quad (24.2)$$

Then you define a dynamic, i.e. a procedure

$$Z'(t) \xrightarrow{D'} Z'(t + \Delta t) \quad (24.3)$$

to determine the time evolution of the model atmosphere with the aim of bringing the state trajectory of the model as close as possible to that of the real atmosphere. To do this, you define a distance

$$|Z - Z'| \geq \mathfrak{o}. \quad (24.4)$$

Weather forecast has the following workflow:

1. Observation of the state of the atmosphere.
2. Determination of the initial state of the model.
3. Integration of the model.

Errors arise for the following reasons:

1. The initial state was not fully observed.
2. The initial state was incorrectly observed.
3. The governing equations are equations of statistical physics and therefore do not apply exactly.
4. The model can store less information than the real atmosphere.
5. The dynamics of the model are different from those of the real atmosphere.
6. There are rounding errors due to the finite computer precision.
7. The computer is making errors.

24.1 Basic concepts of discretizations

Let the solution of a differential equation be denoted by F and the solution of a discretized version of the equation by F_d . A numerical procedure is called *consistent* if and only if the solution of the scheme converges to the solution of the differential equation as Δx and Δt become smaller, i.e. $\lim_{\Delta \rightarrow \mathfrak{o}} F_d = F$ in the above terms. A discretization is called *self-consistent* if all conserved quantities of the continuous system are also conserved quantities of the discretized system. This can also be transferred to approximations. A scheme is called *stable* if and only if the calculated solution is bounded for all times, i.e. if a $C > \mathfrak{o}$ exists with $|F_d| < C$ for all $t \geq t_0$ with t_0 as the starting time. *Linear instability* already arises with linear differential equations, whereas *nonlinear instability* can only arise with nonlinear differential equations.

24.2 Finite differences

Let an infinitely often differentiable function $f: \mathbb{R} \rightarrow \mathbb{R}$ be given. You can write using a Taylor series

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{f''(x)}{2!} \Delta x^2 + \frac{f'''(x)}{3!} \Delta x^3 + \dots \quad (24.5)$$

and

$$f(x - \Delta x) = f(x) - \Delta x f'(x) + \frac{f''(x)}{2!} \Delta x^2 - \frac{f'''(x)}{3!} \Delta x^3 + \dots \quad (24.6)$$

If you subtract both equations, you get

$$f(x + \Delta x) - f(x - \Delta x) = 2\Delta x f'(x) + R', \quad (24.7)$$

where the remainder R' represents the third and higher order terms. This results in a change

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + R, \quad (24.8)$$

where R is a polynomial in Δx with the lowest power 2, one says that (24.8) gives a second-order approximation of the derivative and instead of R writes the symbol $\mathcal{O}(\Delta x^2)$. This way of approximating derivatives is called central difference quotients. A one-sided difference quotient, for example

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x} \quad (24.9)$$

is also a suitable approximation, but this only converges to the first order, as can be easily done by rearranging Eq. (24.5) can be seen. The higher the order, the better, since the accuracy of a Taylor expansion increases with the order. For this reason, central spatial difference quotients are used wherever possible. You can also derive an approximation for the second derivative of a function from the equations (24.5) and (24.6):

$$\begin{aligned} f(x + \Delta x) + f(x - \Delta x) &= 2f(x) + f''(x) \Delta x^2 + \mathcal{O}(\Delta x^4) \\ \Leftrightarrow f''(\Delta x) &= \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \end{aligned} \quad (24.10)$$

For example, if you were given a function $f(x) = A \sin(kx)$, then $f' = Ak \cos(kx)$, Eq. However, (24.8) gives

$$f' \approx \frac{A}{2\Delta x} (\sin(kx + k\Delta x) - \sin(kx - k\Delta x)) = \frac{A}{\Delta x} \cos(kx) \sin(k\Delta x) = \frac{\sin(k\Delta x)}{k\Delta x} f'. \quad (24.11)$$

This shows that the approximation, as expected, converges to the correct value of the derivative if Δx approaches zero (we have $\lim_{a \rightarrow 0} \frac{\sin(a)}{a} = 1$ according to L'Hospital's rule). If you write $k = \frac{2\pi}{\lambda}$ with λ as the wavelength and insert $\Delta x = \lambda/2$, the central difference quotient always results in $f' = 0$. However, sufficiently long waves ($\lambda \gg 2\Delta x$) are resolved well.

24.3 Plane spectral method

24.4 Spherical spectral method

Let $\psi = \psi(\varphi, \lambda, z)$ be a scalar field. Since the spherical surface functions presented in Sect. C.5 form a complete orthonormal basis on spherical shells, it is possible to express the horizontal dependence of ψ by this set of functions:

$$\psi(\varphi, \lambda, z) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \tilde{\psi}_{l,m}(z) Y_{l,m}(\varphi, \lambda) \quad (24.12)$$

The definition of the spherical area functions Eq. (C.155) is formulated here in geographical coordinates:

$$Y_{l,m}(\varphi, \lambda) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l,m}(\sin(\varphi)) \exp(im\lambda) \quad (24.13)$$

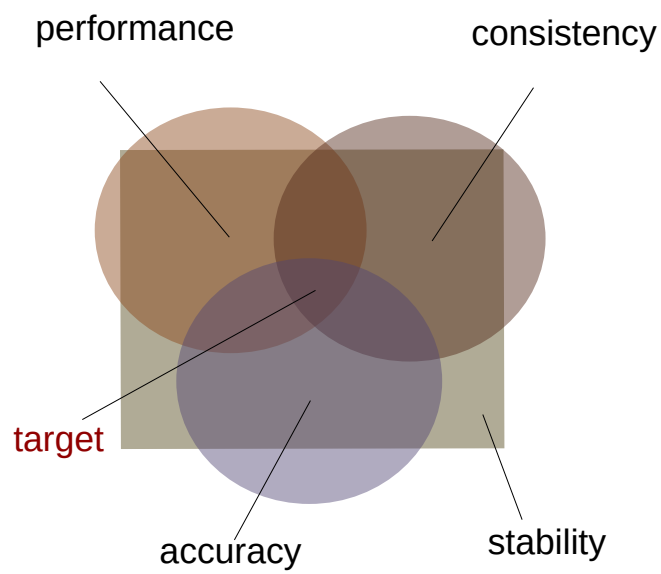


Figure 24.1: Sets of discretizations.

25 TIME STEP METHOD

Let $\mathcal{V} : A \subseteq \mathbb{R}^3 \times \mathbb{R} \rightarrow \mathbb{R}^n$ be the atmospheric state vector. All fundamental physical laws are first order in time, therefore one can write

$$\frac{d\mathcal{V}}{dt} = F(\mathcal{V}), \quad (25.1)$$

where F contains the physics. If you discretize this onto a temporal grid $n\Delta t$ with $n \in \mathbb{Z}$ and interpolate between two time steps $n, n+l$, you get

$$\mathcal{V}_{n+l} - \mathcal{V}_n = \int_{n\Delta t}^{(n+l)\Delta t} F(\mathcal{V}) dt. \quad (25.2)$$

The number of time steps involved is $l+1$. You can now discretize the integral on the right-hand side in a variety of ways. The explicit Euler method results from the approximation with $l=1$

$$\int_{n\Delta t}^{(n+1)\Delta t} F(\mathcal{V}) dt \approx F(\mathcal{V}_n) \Delta t \quad (25.3)$$

with $\mathcal{V}_n := \mathcal{V}(n\Delta t)$. The implicit Euler method, on the other hand, is obtained via

$$\int_{n\Delta t}^{(n+1)\Delta t} F(\mathcal{V}) dt \approx F(\mathcal{V}_{n+1}) \Delta t \quad (25.4)$$

This chapter aims to explain how the time discretization of a linear differential equation can affect the dispersion relation and the stability of a wave solution. It becomes the linear advection equation

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = 0 \quad (25.5)$$

considered with $U \neq 0$ as a homogeneous advection velocity and f as some particle property. The analytical solution is in the complex notation

$$f = \exp(i(kx - \omega t)), \quad (25.6)$$

If you insert this, $-i\omega + Uik = 0$, i.e. as a dispersion relation

$$\omega = Uk. \quad (25.7)$$

So phase and group speed are equal to U . Now place and time are discretized, you write $f_l^{(m)} = f(l\Delta x, m\Delta t)$ and start

$$f_l^{(m)} = e^{Cm\Delta t} e^{i(kl\Delta x - \omega m\Delta t)} \quad (25.8)$$

with $f_l^{(0)} = e^{ikl\Delta x}$ as the initial state. Here C, k and ω are real numbers. For reasons of symmetry, k cannot have an imaginary part. C and the dispersion $\omega(k)$ are to be determined.

25.1 Purely explicit procedures

25.1.1 Explicit Euler method

First, the following discretization is examined:

$$\frac{f_l^{(m+1)} - f_l^{(m)}}{\Delta t} + U \frac{f_{l+1}^{(m)} - f_{l-1}^{(m)}}{2\Delta x} = 0 \quad (25.9)$$

This is called *explicit Euler method*. insertion results in

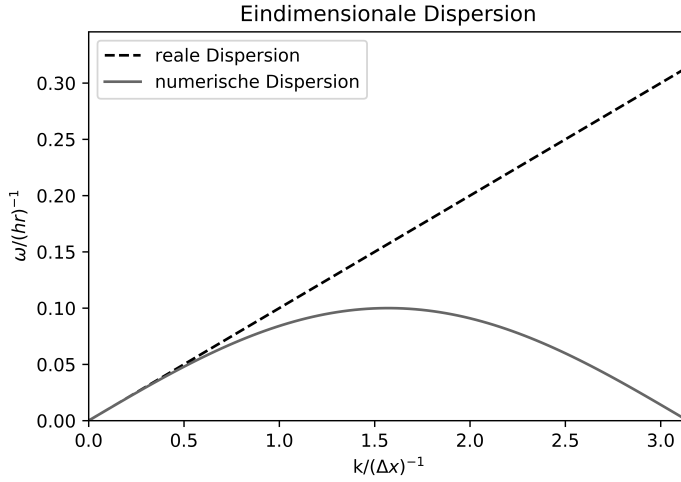


Figure 25.1: Numerical and actual dispersion in the 1D advection equation. $U = 10$ m/s was calculated; a very low value was used for Δt . Note the change in sign of the group velocity. Waves with the lowest resolved wavelength $2\Delta x$ are stationary. Waves with a wavelength $\geq 6\Delta x$ are well simulated.

$$\frac{e^{C\Delta t}e^{-i\omega\Delta t} - 1}{\Delta t} + U \frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} = \frac{e^{C\Delta t}\cos(\omega\Delta t) - ie^{C\Delta t}\sin(\omega\Delta t) - 1}{\Delta t} + \frac{iU\sin(k\Delta x)}{\Delta x} = 0. \quad (25.10)$$

The real part is

$$e^{C\Delta t}\cos(\omega\Delta t) = 1, \quad (25.11)$$

from this it follows i. A. $C > 0$, there is instability. This is *linear instability*, since Eq. (25.5) is linear in f . The imaginary part is

$$e^{C\Delta t}\sin(\omega\Delta t) = \frac{U\Delta t\sin(k\Delta x)}{\Delta x}. \quad (25.12)$$

From this it follows

$$\tan(\omega\Delta t) = \frac{U\Delta t\sin(k\Delta x)}{\Delta x}, \quad (25.13)$$

so the dispersion

$$\omega(k) = \frac{1}{\Delta t} \arctan\left(\frac{U\Delta t\sin(k\Delta x)}{\Delta x}\right). \quad (25.14)$$

Let λ be the wavelength, i.e. $k = \frac{2\pi}{\lambda}$. For $\lambda \gg \Delta x$ we have $\sin(k\Delta x) \approx k\Delta x$, i.e. $\omega \approx \frac{1}{\Delta t} \arctan(Uk\Delta t)$. In the case $U\Delta t \ll \lambda$, i.e. $Uk\Delta t \ll 1$, $\omega \approx \frac{1}{\Delta t} U\Delta tk = Uk$ as in the continuous case. Long waves are resolved well with a sufficiently small time step. However, for the shortest resolved wave $\lambda = 2\Delta x$ it follows $\omega = \frac{1}{\Delta t} \arctan\left(\frac{U\Delta t\sin\pi}{\Delta x}\right) = 0$, so the wave is stationary. Fig. 25.1 shows the dispersion relation for the case $U = 10$ m/s. You can see that waves with $k \leq \frac{1}{\Delta x}$, i.e. $\lambda \geq 2\pi\Delta x$, are simulated decently.

25.1.1.1 First-order upwind procedure

In the case $U > 0$ it is called discretization

$$\frac{f_l^{(m+1)} - f_l^{(m)}}{\Delta t} + U \frac{f_l^{(m)} - f_{l-1}^{(m)}}{\Delta x} = 0 \quad (25.15)$$

as *first-order-upwind method*. This leads to

$$\frac{e^{C\Delta t} e^{-i\omega\Delta t} - 1}{\Delta t} + U \frac{1 - e^{-ik\Delta x}}{\Delta x} = \frac{e^{C\Delta t} \cos(\omega\Delta t) - ie^{C\Delta t} \sin(\omega\Delta t) - 1}{\Delta t} + U \frac{1 - \cos(k\Delta x) + i \sin(k\Delta x)}{\Delta x} = 0. \quad (25.16)$$

The imaginary part of this is

$$\begin{aligned} \frac{e^{C\Delta t} \sin(\omega\Delta t)}{\Delta t} &= U \frac{\sin(k\Delta x)}{\Delta x} \\ \Leftrightarrow e^{C\Delta t} \sin(\omega\Delta t) &= U \frac{\Delta t \sin(k\Delta x)}{\Delta x} \\ \Leftrightarrow e^{C\Delta t} &= U \frac{\Delta t \sin(k\Delta x)}{\Delta x \sin(\omega\Delta t)}. \end{aligned} \quad (25.17)$$

The discretization is stable if and only if $C \leq 1$, i.e. for

$$U \frac{\Delta t \sin(k\Delta x)}{\Delta x \sin(\omega\Delta t)} \leq 1. \quad (25.18)$$

Because of

$$c = \frac{\omega}{k} \leq \frac{\Delta x}{\Delta t} \Leftrightarrow \omega\Delta t \leq k\Delta x \quad (25.19)$$

the estimate continues

$$U \frac{\Delta t}{\Delta x} \leq U \frac{\Delta t \sin(k\Delta x)}{\Delta x \sin(\omega\Delta t)} \leq 1. \quad (25.20)$$

This equation is called *Courant-Friedrichs-Lewy criterion (CFL criterion)*. One defines the *Courant number* or *CFL number* c by

$$c := \frac{U\Delta t}{\Delta x}. \quad (25.21)$$

The CFL criterion is linguistic

If the explicit Euler method for the 1D linear advection equation is stable, $c \leq 1$.

25.1.2 Leapfrog procedure

If you use a central temporal difference quotient, write:

$$\frac{f_l^{(m+2)} - f_l^{(m)}}{2\Delta t} + U \frac{f_{l+1}^{(m+1)} - f_{l-1}^{(m+1)}}{2\Delta x} = 0, \quad (25.22)$$

so this results in used

$$\begin{aligned} \frac{e^{2C\Delta t} e^{-2i\omega\Delta t} - 1}{2\Delta t} + U \frac{e^{ik\Delta x} e^{C\Delta t} e^{-i\omega\Delta t} - e^{-ik\Delta x} e^{C\Delta t} e^{-i\omega\Delta t}}{2\Delta x} &= 0 \\ \Leftrightarrow \frac{e^{C\Delta t} e^{-i\omega\Delta t} - e^{-C\Delta t} e^{i\omega\Delta t}}{2\Delta t} + U \frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} &= 0. \end{aligned} \quad (25.23)$$

The real part results

$$e^{C\Delta t} \cos(\omega\Delta t) = e^{-C\Delta t} \cos(\omega\Delta t). \quad (25.24)$$

This means $C = 0$, so the solution is stable. The imaginary part becomes

$$\frac{\sin(\omega\Delta t)}{2\Delta t} (e^{-C\Delta t} + e^{C\Delta t}) = \frac{\sin(\omega\Delta t)}{\Delta t} = U \frac{\sin(k\Delta x)}{\Delta x}. \quad (25.25)$$

It follows

$$\sin(\omega\Delta t) = U \frac{\Delta t}{\Delta x} \sin(k\Delta x) \Rightarrow \omega = \frac{1}{\Delta t} \arcsin \left[\frac{U\Delta t}{\Delta x} \sin(k\Delta x) \right], \quad (25.26)$$

i.e. a different dispersion relation than in the explicit case. In general, the stability of the solution seems to follow from the real part, while the dispersion seems to follow from the imaginary part. Schemes are still either stable ($C \leq 0$), labile ($C > 0$) or conditionally stable (stable for sufficiently small Δt). This is influenced by the time step method. The optimal case is $C = 0$, which results from the leapfrog method, so this method is the most suitable.

25.1.3 General multistep procedures

25.1.4 Runge-Kutta method

Let $f : \mathbb{R}^l \times \mathbb{R} \rightarrow \mathbb{R}^m$ with $l, m \geq 1$ be an infinitely often continuously differentiable function, which solves the initial value problem

$$\frac{df}{dt} = F[f(t)], \quad f_0 = f_0 \quad (25.27)$$

fulfilled. So-called *Runge-Kutta procedures* are based on calculating several values for df/dt and superimposing them in such a way that as many terms of the Taylor series as possible are covered.

25.1.4.1 Linear case

The Taylor expansion of f is

$$f(t) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} t^k. \quad (25.28)$$

The function F turns a function f into its time derivative, so it follows

$$f(t) = \sum_{k=0}^{\infty} \frac{F^k(0)}{k!} t^k \quad (25.29)$$

with $F^0 = f$. Assuming that F continues to be linear, this can be done

$$\begin{aligned} f(t) &= \sum_{k=0}^n \frac{F^k(0)}{k!} t^k + \sum_{k=n+1}^{\infty} \frac{F^k(0)}{k!} t^k \\ &= f_0 + tF \left\{ f_0 + \frac{t}{2} F \left[f_0 + \cdots + \frac{t}{n} F(f_0) \right] \right\} + O(t^{n+1}) \end{aligned} \quad (25.30)$$

rephrase. So the first n derivatives of f are approximated by this method, which is called *linear Runge-Kutta method of third order*.

25.1.4.2 Nonlinear case

You define it

$$f_1 := \frac{t}{2} F \left[f_0 + \dots + \frac{t}{n} F(f_0) \right], \quad (25.31)$$

one can use Eq. (25.30) in the form

$$f(t) = f_0 + tF(f_0 + f_1) + O(t^{n+1}) \quad (25.32)$$

note down. If the function F , which determines the time evolution of the system, is nonlinear, it no longer applies

$$tF(f_0 + f_1) = tF(f_0) + tF(f_1), \quad (25.33)$$

rather

$$tF(f_0 + f_1) = tF(f_0) + tF'(f_0)f_1 + tO(f_1^2). \quad (25.34)$$

modify. This therefore applies in this case

$$f(t) = f_0 + tF(f_0 + f_1) + O(t^3). \quad (25.35)$$

In the nonlinear case, a discretization in the form of Eq. (25.30) is always second order.

25.2 Method with implicit shares

25.2.1 Implicit Euler method

If you use a left-sided difference quotient for the time derivative (this is called *implicit Euler method*), then write

$$\frac{f_l^{(m+1)} - f_l^{(m)}}{\Delta t} + U \frac{f_{l+1}^{(m+1)} - f_{l-1}^{(m+1)}}{2\Delta x} = 0, \quad (25.36)$$

so this results in used

$$\begin{aligned} & \frac{e^{C\Delta t} e^{-i\omega\Delta t} - 1}{\Delta t} + U \frac{e^{ik\Delta x} e^{C\Delta t} e^{-i\omega\Delta t} - e^{-ik\Delta x} e^{C\Delta t} e^{-i\omega\Delta t}}{2\Delta x} = 0 \\ \Leftrightarrow & \frac{1 - e^{-C\Delta t} e^{i\omega\Delta t}}{\Delta t} + U \frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x} = 0. \end{aligned} \quad (25.37)$$

The real part results

$$1 = e^{-C\Delta t} \cos(\omega\Delta t). \quad (25.38)$$

This means $C < 0$, so the solution is always stable, but it converges to zero. The imaginary part becomes

$$\frac{e^{-C\Delta t} \sin(\omega\Delta t)}{\Delta t} = U \frac{\sin(k\Delta x)}{\Delta x}. \quad (25.39)$$

It follows

$$\tan(\omega\Delta t) = U \frac{\Delta t}{\Delta x} \sin(k\Delta x), \quad (25.40)$$

i.e. the same dispersion relation as in the explicit Euler method.

25.2.2 Crank-Nicolson method

The Crank-Nicolson method is a combination of explicit and implicit Euler methods:

$$\frac{f_l^{(m+1)} - f_l^{(m)}}{\Delta t} + U \frac{f_{l+1}^{(m)} - f_{l-1}^{(m)} + f_{l+1}^{(m+1)} - f_{l-1}^{(m+1)}}{4\Delta x} = 0 \quad (25.41)$$

If you put Eq. (25.8), you get

$$\begin{aligned} & \frac{e^{C\Delta t} e^{-i\omega\Delta t} - 1}{\Delta t} + U \frac{e^{ik\Delta x} - e^{-ik\Delta x} + e^{ik\Delta x} e^{C\Delta t} e^{-i\omega\Delta t} - e^{-ik\Delta x} e^{C\Delta t} e^{-i\omega\Delta t}}{4\Delta x} = 0 \\ \Leftrightarrow & \frac{e^{C\Delta t} \cos(\omega\Delta t) - ie^{C\Delta t} \sin(\omega\Delta t) - 1}{\Delta t} + U \frac{2i \sin(\omega\Delta t) + 2i \sin(k\Delta x) e^{C\Delta t} e^{-i\omega\Delta t}}{4\Delta x} = 0 \\ \Leftrightarrow & \frac{e^{C\Delta t} \cos(\omega\Delta t) - ie^{C\Delta t} \sin(\omega\Delta t) - 1}{\Delta t} + U \frac{2i \sin(\omega\Delta t) + 2ie^{C\Delta t} \sin(k\Delta x) \cos(\omega\Delta t) + 2e^{C\Delta t} \sin(k\Delta x) \sin(\omega\Delta t)}{4\Delta x} = 0. \end{aligned} \quad (25.42)$$

The real part results

$$\begin{aligned} \Leftrightarrow & \frac{e^{C\Delta t} \cos(\omega\Delta t) - 1}{\Delta t} + U \frac{2e^{C\Delta t} \sin(k\Delta x) \sin(\omega\Delta t)}{4\Delta x} = 0 \\ \Leftrightarrow & \frac{\cos(\omega\Delta t) - e^{-C\Delta t}}{\Delta t} + U \frac{\sin(k\Delta x) \sin(\omega\Delta t)}{2\Delta x} = 0. \end{aligned}$$

The imaginary part yields

$$\begin{aligned} \Leftrightarrow & -\frac{ie^{C\Delta t} \sin(\omega\Delta t)}{\Delta t} + U \frac{2i \sin(\omega\Delta t) + 2ie^{C\Delta t} \sin(k\Delta x) \cos(\omega\Delta t)}{4\Delta x} = 0 \\ \Leftrightarrow & -\frac{e^{C\Delta t}}{\Delta t} + U \frac{1 + e^{C\Delta t} \sin(k\Delta x) \cot(\omega\Delta t)}{2\Delta x} = 0. \end{aligned}$$

This means $C < 0$, so the solution is stable, but it disappears at some point. The imaginary part becomes

$$\frac{e^{-C\Delta t} \sin(\omega\Delta t)}{\Delta t} = U \frac{\sin(k\Delta x)}{\Delta x}. \quad (25.43)$$

It follows

$$\tan(\omega\Delta t) = U \frac{\Delta t}{\Delta x} \sin(k\Delta x), \quad (25.44)$$

i.e. the same dispersion relation as in the explicit Euler method.

25.3 Mixture of time step methods

One is not limited to solving a differential equation either explicitly or only implicitly. Let $\tilde{f}$ be the discretized analogue of a continuous field f and let $\mathbf{r}_i$ be the grid points. A two-step procedure for a first-order differential equation in time for f can be in the form

$$\tilde{f}(\mathbf{r}_i, (n+1)\Delta t) = \tilde{f}(\mathbf{r}_i, n\Delta t) + \Delta t \sum_{j=1}^N \tilde{F}_j \left[\tilde{f}((n+m_j)\Delta t) \right] \quad (25.45)$$

note down. Here $\tilde{F}_j$ for $j = 1, \dots, N$ are the discretized forcings acting on $\tilde{f}$. This should apply

$$m_j = \begin{cases} 0, & \text{Term } j \text{ wird explizit behandelt,} \\ 1, & \text{Term } j \text{ wird implizit behandelt.} \end{cases} \quad (25.46)$$

It was tacitly assumed that f was the only field appearing. In general, f can be viewed as a tuple of fields, i.e. as a state vector. Furthermore, you can allow $0 \leq m_j \leq 1$, here m_j is the implicit share. The Crank-Nicolson method means $m_j = \frac{1}{2}$.

25.4 Aspects of partial differential equations

25.4.1 Forward-backward method

25.5 Energetic self-consistency in the ideal gas

25.5.1 Advection of momentum

25.5.1.1 Advection of kinetic energy

Since $\mathbf{v} \cdot [(\nabla \times \mathbf{v}) \times \mathbf{v}] = 0$, the generalized Coriolis term is energetically insignificant. The system of equations is therefore used for a self-consistent temporal discretization of the advection of kinetic energy

$$\frac{\partial \mathbf{v}}{\partial t} = -\nabla \frac{\mathbf{v}^2}{2}, \quad \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}). \quad (25.47)$$

In the continuous case applies

$$\begin{aligned} \rho \mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} &= -\rho \mathbf{v} \cdot \nabla \frac{\mathbf{v}^2}{2} = -\nabla \cdot \left(\rho \mathbf{v} \frac{\mathbf{v}^2}{2} \right) + \frac{\mathbf{v}^2}{2} \nabla \cdot (\rho \mathbf{v}) = -\nabla \cdot \left(\rho \mathbf{v} \frac{\mathbf{v}^2}{2} \right) - \frac{\mathbf{v}^2}{2} \frac{\partial \rho}{\partial t} \\ \Rightarrow \rho \mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} + \frac{\mathbf{v}^2}{2} \frac{\partial \rho}{\partial t} &= \frac{\partial (\rho \mathbf{v}^2 / 2)}{\partial t} = -\nabla \cdot \left(\rho \mathbf{v} \frac{\mathbf{v}^2}{2} \right) \end{aligned} \quad (25.48)$$

for the effect of kinetic energy flux density on the local kinetic energy density. These transformation steps must be transferable to the discretization. One now defines $\delta_0, \delta_1, \delta_2, \delta_3, \delta_4, \delta_5 \in \{0, 1\}$ to determine the temporal discretization of the kinetic energy and the mass flux density in the form

$$\frac{\mathbf{v}^2}{2} = \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2}, \quad \rho \mathbf{v} = \frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \quad (25.49)$$

to note down. This initially results in a system of equations

$$\frac{\mathbf{v}_1 - \mathbf{v}_0}{\Delta t} = -\nabla \frac{\mathbf{v}^2}{2}, \quad \frac{\rho_1 - \rho_0}{\Delta t} = -\nabla \cdot (\rho \mathbf{v}). \quad (25.50)$$

From this it follows

$$\begin{aligned} \frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \cdot \frac{\mathbf{v}_1 - \mathbf{v}_0}{\Delta t} &= -\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \cdot \nabla \frac{\mathbf{v}^2}{2} = -\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \cdot \nabla \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \\ &= -\nabla \cdot \left(\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \right) + \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \nabla \cdot \frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \\ &= -\nabla \cdot \left(\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \right) - \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \frac{\rho_1 - \rho_0}{\Delta t} \\ \Leftrightarrow \frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \cdot \frac{\mathbf{v}_1 - \mathbf{v}_0}{\Delta t} + \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \frac{\rho_1 - \rho_0}{\Delta t} &= -\nabla \cdot \left(\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \right) \\ \Leftrightarrow \frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 - \rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 + \rho_1 \mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1} - \rho_0 \mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2 \Delta t} &= -\nabla \cdot \left(\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \right) \\ \Leftrightarrow \frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1} - \rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2 \Delta t} &= -\nabla \cdot \left(\frac{\rho_{\delta_2} \mathbf{v}_{\delta_3} + \rho_{\delta_4} \mathbf{v}_{\delta_5}}{2} \frac{\mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1}}{2} \right) \end{aligned} \quad (25.51)$$

It has to apply

$$\rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1} - \rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_{\delta_0} \cdot \mathbf{v}_{\delta_1} = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.52)$$

If you insert $\delta_0 = \delta_1 = \mathbf{o}$, it follows

$$\rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_0 \cdot \mathbf{v}_0 - \rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0 = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.53)$$

With $\delta_2 = \delta_3 = \mathbf{i}$ it follows

$$\rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_0 \cdot \mathbf{v}_0 - \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0 = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.54)$$

This in turn results in $\delta_4 = \mathbf{i}$, $\delta_5 = \mathbf{o}$. The pairs (δ_2, δ_3) , (δ_4, δ_5) are interchangeable, but this is not a new possibility since the mass flux density does not change.

If you insert $\delta_0 = \delta_1 = \mathbf{i}$, it follows

$$\rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_1 \cdot \mathbf{v}_1 = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.55)$$

With $\delta_2 = \mathbf{o}$, $\delta_3 = \mathbf{i}$ follows

$$\rho_0 \mathbf{v}_1 \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_1 \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_1 \cdot \mathbf{v}_1 = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.56)$$

This in turn follows $\delta_4 = \mathbf{o}$, $\delta_5 = \mathbf{o}$.

If you insert $\delta_0 = \mathbf{o}$, $\delta_1 = \mathbf{i}$, it follows

$$\rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_0 \cdot \mathbf{v}_1 - \rho_{\delta_2} \mathbf{v}_{\delta_3} \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_1 = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.57)$$

With $\delta_2 = \delta_3 = \mathbf{o}$ it follows

$$\rho_0 \mathbf{v}_0 \cdot \mathbf{v}_1 + \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_1 + \rho_1 \mathbf{v}_0 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0 - \rho_{\delta_4} \mathbf{v}_{\delta_5} \cdot \mathbf{v}_0 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_1 = \rho_1 \mathbf{v}_1 \cdot \mathbf{v}_1 - \rho_0 \mathbf{v}_0 \cdot \mathbf{v}_0. \quad (25.58)$$

This in turn results in $\delta_4 = \mathbf{i}$, $\delta_5 = \mathbf{i}$.

In summary, there are the following three options:

$$\frac{\mathbf{v}^2}{2} = \frac{\mathbf{v}_0 \cdot \mathbf{v}_0}{2}, \rho \mathbf{v} = \frac{\rho_1 \mathbf{v}_0 + \rho_1 \mathbf{v}_1}{2} \quad (25.59)$$

$$\frac{\mathbf{v}^2}{2} = \frac{\mathbf{v}_1 \cdot \mathbf{v}_1}{2}, \rho \mathbf{v} = \frac{\rho_0 \mathbf{v}_0 + \rho_0 \mathbf{v}_1}{2} \quad (25.60)$$

$$\frac{\mathbf{v}^2}{2} = \frac{\mathbf{v}_0 \cdot \mathbf{v}_1}{2}, \rho \mathbf{v} = \frac{\rho_0 \mathbf{v}_0 + \rho_1 \mathbf{v}_1}{2} \quad (25.61)$$

25.5.1.2 Generalized Coriolis terms

The following applies to the time development of kinetic energy

$$\frac{\mathbf{v}_1^2 - \mathbf{v}_0^2}{2\Delta t} = \frac{(\mathbf{v}_1 + \mathbf{v}_0) \cdot (\mathbf{v}_1 - \mathbf{v}_0)}{2\Delta t} = \mathbf{v}_{1/2} \cdot \frac{\mathbf{v}_1 - \mathbf{v}_0}{\Delta t} \quad (25.62)$$

with

$$\mathbf{v}_{1/2} := \frac{\mathbf{v}_0 + \mathbf{v}_1}{2}. \quad (25.63)$$

If the generalized Coriolis term is not to contribute to the evolution of kinetic energy, it must be calculated using the velocity field $\mathbf{v}_{1/2}$. The considerations in this section (25.5.1) were first put forward by Gassmann and Herzog in [14].

25.5.1.3 Time development of internal energy

You can note the time evolution of the internal energy density $\tilde{I}$

$$\frac{\Delta \tilde{I}}{\Delta t} = \frac{\tilde{I}_1 - \tilde{I}_0}{\Delta t} = c^{(v)} \rho_0 \frac{T_1 - T_0}{\Delta t} + c^{(v)} T_1 \frac{\rho_1 - \rho_0}{\Delta t} \quad (25.64)$$

$$= \frac{\tilde{I}_1 - \tilde{I}_0}{\Delta t} = c^{(v)} \rho_1 \frac{T_1 - T_0}{\Delta t} + c^{(v)} T_0 \frac{\rho_1 - \rho_0}{\Delta t}. \quad (25.65)$$

First, one starts from Eq. (25.64). Using the continuity equation one obtains

$$\frac{D\rho}{Dt} = -\rho_0 \nabla \cdot \mathbf{v}. \quad (25.66)$$

From Eq. (9.14) follows

$$\frac{T_1 - T_0}{\Delta t} = -\frac{R_d}{c^{(v)}} T_0 \nabla \cdot \mathbf{v}. \quad (25.67)$$

Both times it was assumed that the scalar variables from the old time step would be used, as e.g. B. is the case with a forward-backward procedure. Putting these two findings into Eq. (25.64), you get

$$\begin{aligned} \frac{\tilde{I}_1 - \tilde{I}_0}{\Delta t} &= -c^{(v)} \rho_0 \frac{R_d}{c^{(v)}} T_0 \nabla \cdot \mathbf{v} - c^{(v)} T_1 \rho_0 \nabla \cdot \mathbf{v} = -c^{(v)} \rho_0 \nabla \cdot \mathbf{v} \left(\frac{R_d}{c^{(v)}} T_0 + T_1 \right) \\ &= -c^{(p)} \rho_0 \nabla \cdot \mathbf{v} \left(\frac{R_d}{c^{(p)}} T_0 + \frac{c^{(v)}}{c^{(p)}} T_1 \right). \end{aligned} \quad (25.68)$$

From this it can be concluded that the temperature is in the weighting

$$T^* := \frac{R_d}{c^{(p)}} T_0 + \frac{c^{(v)}}{c^{(p)}} T_1 \quad (25.69)$$

enters into the discretized evolution of the internal energy density.

However, if one goes by Eq. (25.65) does this

$$\frac{D\rho}{Dt} = -\rho_1 \nabla \cdot \mathbf{v} \quad (25.70)$$

and

$$\frac{T_1 - T_0}{\Delta t} = -\frac{R_d}{c^{(v)}} T_1 \nabla \cdot \mathbf{v} \quad (25.71)$$

on

$$\frac{\tilde{I}_1 - \tilde{I}_0}{\Delta t} = -c^{(p)} \rho_1 \nabla \cdot \mathbf{v} \left(\frac{c^{(v)}}{c^{(p)}} T_0 + \frac{R_d}{c^{(p)}} T_1 \right), \quad (25.72)$$

$$T^* := \frac{c^{(v)}}{c^{(p)}} T_0 + \frac{R_d}{c^{(p)}} T_1. \quad (25.73)$$

These are the two possibilities for energetically self-consistent temporal discretizations of the internal energy.

The variety of numerical methods for the discretization of the governing equations is large, as is the effort involved in implementing such a discretization up to operational applicability. Therefore, it is important to make a good decision about the basic structure of the dynamic core to be formulated in part VII before proceeding with further development and programming.

26.1 Restrictions following from the CFL criterion

The CFL criterion is

$$\Delta t \leq \frac{\Delta r_{\min}}{c_{\max}}, \quad (26.1)$$

Here $\Delta r_{\min}$ is the minimum grid point spacing and $c_{\max}$ is the maximum phase velocity of the system of equations. Therefore, for the efficiency of the model as the resolution becomes finer, it is useful if the ratio

$$r := \frac{\Delta r_{\max}}{\Delta r_{\min}} \quad (26.2)$$

from maximum to minimum grid point spacing as the resolution becomes finer is limited to a value not much larger than one. Such a grid is called *quasi-uniform*. On the longitude-latitude grid with angular resolution φ applies

$$r = \frac{\varphi}{\varphi \sin(\varphi)} = \frac{1}{\sin(\varphi)}. \quad (26.3)$$

The length-width grid must therefore be excluded at this point.

26.1.1 Platonic solids

It is therefore necessary that the atmospheric model to be developed in part VII is formulated on a quasi-uniform grid. One speaks of actual *uniformity* when two surfaces are congruent in pairs. The bodies that are spanned by these grids are called *Platonic solids*. The number of corners of such a body is denoted by V , the number of edges by E and the number of faces by F . Now we assume that all surfaces v have vertices and therefore also edges. Then apply

$$V = \frac{Fv}{f}, \quad (26.4)$$

$$E = \frac{Fv}{2}, \quad (26.5)$$

$$2E = fV, \quad (26.6)$$

$$(26.7)$$

with f as the number of edges or faces that meet at a corner. Eq. (26.6) can also be obtained by dividing the equations (26.4) and (26.5) by each other, Eq. (26.6) therefore contains no new information. This still applies to all grids that are only made up of v -corners. Now you have to create an equation that determines the uniformity of the grid.

(tetrahedron, cube, octahedron, dodecahedron, icosahedron)

So there are only five uniform grids on the sphere. These are created from the Platonic solids by projecting their corners from the center onto the surface of the sphere. All of these grids are too coarse for an atmospheric model and therefore cannot be used directly. Furthermore, it follows from this fact that all usable grids have somewhere points, lines or areas where the local grid structure deviates from the general structure. At these locations, the discretization errors are also different, which can result in visibility of the grid in the solution or create waves that propagate through the solution as noise. This is called *grid imprinting*.

26.1.2 Grid imprinting

Quasi-uniform lattices can, for example, be created by starting from one of the Platonic solids and then dividing the surfaces by successive bisections. The starting point for this is usually the icosahedron, as it has the most corners and therefore generates the most homogeneous grid. Bisections of the triangular surfaces create further

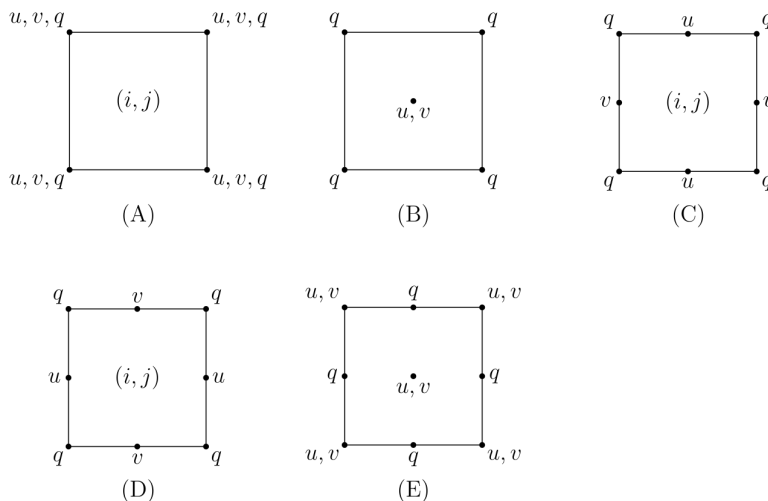


Figure 26.1: The five lattice structures according to Arakawa. The mass variable was denoted q [37].

triangles, which form a so-called *Voronoi lattice*. The *Voronoi centers* of these cells are obtained as intersection points of the perpendicular bisectors on the edges. If you connect these points, you get twelve pentagons (at the corners of the icosahedron) and a number of hexagons depending on the number of bisections.

26.2 Restrictions resulting from rotational symmetry

The governing equations are locally rotationally symmetric with respect to $\mathbf{k}$. This means that when rotating around this axis through any angle $\varphi \in \mathbb{R}$ the equations are converted back into themselves. It is therefore desirable to achieve this as well as possible for the grid. This means that after rotation through the smallest possible angle φ , the lattice should be converted back into itself. $2\pi/\varphi$ is the number of this axis of rotation. This should be as high as possible. This cannot be achieved for spherical non-uniform gratings. However, it makes sense to try to get as close as possible to isotropy (rotational symmetry). This implies, for example, that the standard deviation of the edge lengths of the cells should be small in relation to the mean length.

26.3 Exclusion of spectral formulations

If you develop horizontal fields according to spherical surface functions as described in section 24.4, it is necessary to carry out transformations between the spectral and real grids for two reasons:

1. Fields with steep gradients, such as humidity variables, must be left in real space, otherwise too many Gibbs phenomena would occur.
2. To write out the data, it must be transformed to a real grid.

The transformation between the spectral and real lattice is the Legendre transformation discussed in Sect. This scales $\propto N^2$, whereas the numerical effort of the horizontal numerics of a grid point model scales $\propto N$, here N is the number of horizontal grid points. As resolution increases, spectral models become increasingly inefficient and are therefore excluded at this point.

26.4 Arakawa grid

If you discretize a two-dimensional vector field onto a flat grid, all variables do not have to be evaluated at the same points. The different sizes can be defined at different locations on the polygons. Five ways to do this are the Arakawa lattices [3], shown in Fig. 26.1.

Here only the A-lattice and the C-lattice are examined one-dimensionally. For this purpose, one starts from the system of linearized shallow water equations equations (13.173) - (13.174) without Coriolis force:

$$\frac{\partial h}{\partial t} = -H \frac{\partial u}{\partial x} \quad (26.8)$$

$$\frac{\partial u}{\partial t} = -g \frac{\partial h}{\partial x} \quad (26.9)$$

The approach is here

$$h = \hat{h} \exp(ikx - i\omega t) \quad u = \hat{u} \exp(ikx - i\omega t) \quad (26.10)$$

with $\hat{h}, \hat{u} \in \mathbb{C}$. This leads to

$$-i\omega\hat{h} = -Hik\hat{u} \Leftrightarrow \omega\hat{h} - Hk\hat{u} = 0, \quad -i\omega\hat{u} = -gik\hat{h} \Leftrightarrow \omega\hat{u} - gk\hat{h} = 0. \quad (26.11)$$

In matrix notation this becomes

$$\begin{pmatrix} \omega & -Hk \\ -gk & \omega \end{pmatrix} \begin{pmatrix} \hat{h} \\ \hat{u} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (26.12)$$

Nontrivial solutions exist if the determinant of the matrix vanishes:

$$\omega^2 - gHk^2 = 0 \Rightarrow \omega = k\sqrt{gH} \quad (26.13)$$

This follows for the speeds

$$c_{\text{ph}} = \frac{\omega}{k} = \sqrt{gH}, \quad c_{\text{gr}} = \frac{\partial\omega}{\partial k} = \sqrt{gH} = c_{\text{ph}}. \quad (26.14)$$

This is already the case from Eq. (16.77) known dispersion relation of shallow water waves.

In the following derivation of the numerical versions of these equations, temporally continuous and spatially discretized equations are assumed in order not to influence the results through a chosen time step procedure.

26.4.1 A grid

For the A-grid, the surface deflection h and the wind speed u are defined at the same locations $j\Delta x$ with $j \in \mathbb{N}$. One notes here as a starting point

$$h_j = \hat{h} \exp(ikj\Delta x - i\omega t), \quad u_j = \hat{u} \exp(ikj\Delta x - i\omega t). \quad (26.15)$$

The equations (26.8) - (26.9) are discretized as follows:

$$\frac{\partial h_j}{\partial t} = -H \frac{u_{j+1} - u_{j-1}}{2\Delta x} \quad \frac{\partial u_j}{\partial t} = -g \frac{h_{j+1} - h_{j-1}}{2\Delta x} \quad (26.16)$$

If you use the approach here, you get

$$\begin{aligned} -i\omega\hat{h} &= -\frac{H\hat{u}}{2\Delta x} [\exp(ik\Delta x) - \exp(-ik\Delta x)] \\ \Leftrightarrow -i\omega\hat{h} &= -\frac{H\hat{u}}{2\Delta x} [i\sin(k\Delta x) + i\sin(k\Delta x)] \\ \Leftrightarrow -i\omega\hat{h} &= -\frac{H\hat{u}i}{\Delta x} \sin(k\Delta x) \\ \Leftrightarrow \omega\hat{h} - \frac{H\hat{u}}{\Delta x} \sin(k\Delta x) &= 0 \end{aligned} \quad (26.17)$$

as well as

$$\begin{aligned} -i\omega\hat{u} &= -\frac{g\hat{h}}{2\Delta x} [\exp(ik\Delta x) - \exp(-ik\Delta x)] \\ \Leftrightarrow -i\omega\hat{u} &= -\frac{g\hat{h}}{2\Delta x} 2i\sin(k\Delta x) = -\frac{g\hat{h}}{\Delta x} i\sin(k\Delta x) \\ \Leftrightarrow \omega\hat{u} - \frac{g\hat{h}}{\Delta x} \sin(k\Delta x) &= 0. \end{aligned} \quad (26.18)$$

If you write down equations (26.17) - (26.18) in matrix notation, you get

$$\begin{pmatrix} \omega & -\frac{H}{\Delta x} \sin(k\Delta x) \\ -\frac{g}{\Delta x} \sin(k\Delta x) & \omega \end{pmatrix} \begin{pmatrix} \hat{h} \\ \hat{u} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (26.19)$$

Nontrivial solutions exist if the determinant of the matrix vanishes, i.e. for

$$\omega^2 - gH \frac{\sin^2(k\Delta x)}{(\Delta x)^2} = 0, \quad \Rightarrow \omega = \sqrt{gH} \frac{\sin(k\Delta x)}{\Delta x}. \quad (26.20)$$

From this it follows that the phase velocity is

$$c_{\text{ph}} = c_{\text{ph}}^{(\text{real})} \frac{\sin(k\Delta x)}{k\Delta x} \quad (26.21)$$

and for the group speed

$$c_{\text{gr}} = \frac{\partial \omega}{\partial k} = c_{\text{gr}}^{(\text{real})} \cos(k\Delta x). \quad (26.22)$$

If one introduces the dimensionless velocity

$$\tilde{c} := \frac{c}{\sqrt{gH}} \quad (26.23)$$

as well as the dimensionless wave number

$$\kappa := k\Delta x \quad (26.24)$$

one, then the equations (26.21) - (26.22) can be written in the form

$$\tilde{c}_{\text{ph}} = \frac{\sin(\kappa)}{\kappa}, \quad (26.25)$$

$$\tilde{c}_{\text{gr}} = \cos(\kappa) \quad (26.26)$$

note down.

26.4.2 C grid

For the C-grid, the wind speed u at locations $j\Delta x$ and the surface deflection h at locations $(j + \frac{1}{2})\Delta x$ are defined by $j \in \mathbb{N}$. One notes here as a starting point

$$h_{j+\frac{1}{2}} = \hat{h} \exp(ikj\Delta x - i\omega t) \exp\left(\frac{ik\Delta x}{2}\right), \quad u_j = \hat{u} \exp(ikj\Delta x - i\omega t). \quad (26.27)$$

The equations (26.8) - (26.9) are discretized as follows:

$$\frac{\partial h_{j+\frac{1}{2}}}{\partial t} = -H \frac{u_{j+1} - u_j}{2\Delta x}, \quad \frac{\partial u_j}{\partial t} = -g \frac{h_{j+\frac{1}{2}} - h_{j-\frac{1}{2}}}{2\Delta x} \quad (26.28)$$

If you use the approach here, you get

$$\begin{aligned}
 & -i\omega\hat{h}\exp\left(\frac{ik\Delta x}{2}\right) = -\frac{H\hat{u}}{\Delta x} [\exp(ik\Delta x) - \mathbf{1}] \\
 \Leftrightarrow & i\omega\hat{h}\exp\left(\frac{ik\Delta x}{2}\right) - \frac{H\hat{u}}{\Delta x} [\exp(ik\Delta x) - \mathbf{1}] = \mathbf{0}
 \end{aligned} \tag{26.29}$$

as well as

$$\begin{aligned}
 & -i\omega\hat{u} = -\frac{g\hat{h}}{\Delta x}\exp\left(\frac{ik\Delta x}{2}\right) [\mathbf{1} - \exp(-ik\Delta x)] \\
 \Leftrightarrow & i\omega\hat{u} - \frac{g\hat{h}}{\Delta x}\exp\left(\frac{ik\Delta x}{2}\right) [\mathbf{1} - \exp(-ik\Delta x)] = \mathbf{0}.
 \end{aligned} \tag{26.30}$$

If you write down equations (26.29) - (26.30) in matrix notation, you get

$$\begin{pmatrix} i\omega\exp\left(\frac{ik\Delta x}{2}\right) & -\frac{H}{\Delta x} [\exp(ik\Delta x) - \mathbf{1}] \\ -\frac{g}{\Delta x} [\mathbf{1} - \exp(-ik\Delta x)] & i\omega \end{pmatrix} \begin{pmatrix} \hat{h} \\ \hat{u} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{26.31}$$

Nontrivial solutions exist if the determinant of the matrix vanishes, i.e. for

$$\begin{aligned}
 & -\omega^2 - gH \frac{[\exp(ik\Delta x) - \mathbf{1}] [\mathbf{1} - \exp(-ik\Delta x)]}{(\Delta x)^2} = \mathbf{0} \\
 \Rightarrow & \omega^2 = gH \frac{[\mathbf{1} - \exp(ik\Delta x)] [\mathbf{1} - \exp(-ik\Delta x)]}{(\Delta x)^2} \\
 \Rightarrow & \omega^2 = gH^2 \frac{2 - 2\cos(k\Delta x)}{(\Delta x)^2} = gH^2 \frac{1 - \cos(k\Delta x)}{(\Delta x)^2}.
 \end{aligned} \tag{26.32}$$

From this it follows that the phase velocity is

$$c_{\text{ph}} = c_{\text{ph}}^{(\text{real})} \sqrt{2 \frac{1 - \cos(k\Delta x)}{(k\Delta x)^2}} \tag{26.33}$$

and for the group speed

$$c_{\text{gr}} = \frac{\partial \omega}{\partial k} = \frac{1}{2\omega} \frac{\partial \omega^2}{\partial k} = gH^2 \frac{\sin(k\Delta x)}{2\omega\Delta x} = gH \frac{\sin(k\Delta x)}{\omega\Delta x} = c_{\text{gr}}^{(\text{real})} \frac{\sin(k\Delta x)}{\sqrt{2 - 2\cos(k\Delta x)}}. \tag{26.34}$$

In terms of the dimensionless quantities equations (26.23) - (26.24) one can use the equations (26.33) - (26.34) in the form

$$\tilde{c}_{\text{ph}} = \sqrt{2 \frac{1 - \cos(\kappa)}{\kappa^2}}, \quad \tilde{c}_{\text{gr}} = \frac{\sin(\kappa)}{\sqrt{2 - 2\cos(\kappa)}} \tag{26.35}$$

note down. Fig. 26.2 shows the dispersion relations of the A-lattice and the C-lattice.

26.5 Scalar conservation properties on the C-lattice

If q is a conserved quantity, i.e. a quantity for which $\frac{Dq}{Dt} = \mathbf{0}$, then one can derive a continuity equation for $\tilde{q} := \rho q$:

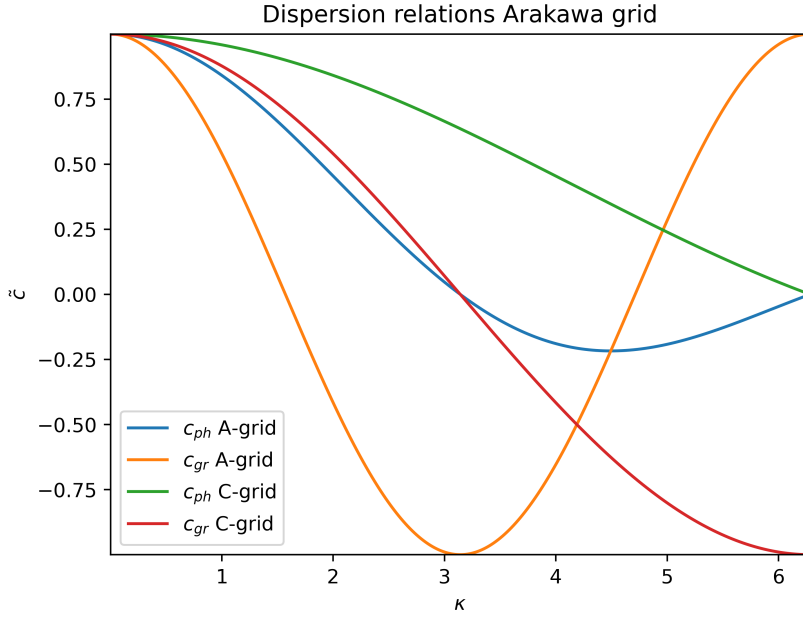


Figure 26.2: The dispersion relations of the A-lattice and the C-lattice.

$$\frac{Dq}{Dt} = \frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q = 0, \quad (26.36)$$

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} = 0, \quad (26.37)$$

$$\Rightarrow \frac{\partial \tilde{q}}{\partial t} + \nabla \cdot \mathbf{j}_{\tilde{q}} = 0, \quad (26.38)$$

where the size $\mathbf{j}_{\tilde{q}} := \tilde{q}\mathbf{v}$ denotes the flow of size q . You define it

$$Q := \int_A \tilde{q} d^3 r \quad (26.39)$$

as the global integral of the quantity q , then Q is obtained under kinematic boundary conditions:

$$\frac{dQ}{dt} = - \int_A \nabla \cdot \mathbf{j}_{\tilde{q}} d^3 r = - \int_{\partial A} \mathbf{j}_{\tilde{q}} \cdot d\mathbf{n} \quad (26.40)$$

If you now decompose A into $N \geq 1$ grid boxes $A = A_1 \cup A_2 \cup \dots \cup A_N$, the following applies

$$Q = \sum_{i=1}^N Q_i \quad (26.41)$$

with

$$Q_i := \int_{A_i} \tilde{q} d^3 r. \quad (26.42)$$

Therefore applies

$$\frac{dQ}{dt} = \sum_{i=1}^N \frac{dQ_i}{dt} = - \sum_{i=1}^N \int_{\partial A_i} \tilde{j}_{\tilde{q}} \cdot d\mathbf{n} = - \sum_{i=1}^N \sum_{F \in F_i} \tilde{j}_{\tilde{q}} \cdot \mathbf{n}_F, \quad (26.43)$$

where F_i is the set of all side surfaces of the grid box i , and $\mathbf{n}_F$ is the normal vector perpendicular to the surface F (pointing outwards). It is assumed that ∂A_i consists of a number of smooth surfaces, which have to be summed individually because they are separated by edges. Since each surface F occurs twice in the double sum, but the vector $\mathbf{n}$ points in two opposite directions, the sum results in zero, so that on a C-lattice even after discretization

$$Q = \text{const.} \quad (26.44)$$

applies. Surfaces that are part of ∂A trivially do not pose a problem because, by definition, no mass flow occurs through them at all under kinematic boundary conditions. This is still true even under the generalized assumption that $\tilde{j}_{\tilde{q}}$ consists not only of $\tilde{q}\mathbf{v}$, but of other, especially diffusive, flows. It should also be noted that even if lattice geometries are calculated incorrectly, Q remains a conserved quantity.

26.6 Gradient fields on the C-grid

Let ψ be a scalar field $\nabla\psi$ be the gradient of this scalar field, this is a vector field. On the C-grid, the rotation of a vector field $\mathbf{v}$ is determined by applying Stokes' theorem to a polygon with area A and edge lengths l_i . So it applies

$$\mathbf{k} \cdot \nabla \times \mathbf{v} = \frac{1}{A} \sum_i \gamma_i l_i v_i, \quad (26.45)$$

where v_i is the value of $\mathbf{v}$ at edge i and $\gamma_i = 1$ if the unit vector of the edge points in the mathematically positive direction of circulation around the polygon, otherwise $\gamma_i = -1$. For the sake of simplicity, one takes o. B. d. A. assume that $\gamma_i = 1$ for all i , so one

$$\mathbf{k} \cdot \nabla \times \mathbf{v} = \frac{1}{A} \sum_i l_i v_i \quad (26.46)$$

can note down. Now you bet

$$\mathbf{v} = \nabla\psi \quad (26.47)$$

on what on

$$\mathbf{k} \cdot \nabla \times \mathbf{v} = \frac{1}{A} \sum_i l_i (\nabla\psi)_i \quad (26.48)$$

leads. It applies

$$(\nabla\psi)_i = \frac{\psi_{\text{to}(i)} - \psi_{\text{from}(i)}}{l_i}. \quad (26.49)$$

Putting this into Eq. (26.48), you get

$$\mathbf{k} \cdot \nabla \times \psi = \frac{1}{A} \sum_i l_i \frac{\psi_{\text{to}(i)} - \psi_{\text{from}(i)}}{l_i} = \frac{1}{A} \sum_i \psi_{\text{to}(i)} - \psi_{\text{from}(i)}. \quad (26.50)$$

If you sort the edges in a mathematically positive direction of circulation around the polygon under consideration, the following applies

$$\psi_{\text{to}(i)} = \psi_{\text{from}(i+1)}. \quad (26.51)$$

Every value of ψ occurs in Eq. (26.50) appears twice, once with a positive sign and once with a negative sign. This applies regardless of the spatial direction being considered. This therefore applies on a C-lattice

$$\nabla \times \nabla \psi = \mathbf{0}. \quad (26.52)$$

26.7 Int product on the C-lattice

First of all, this section assumes a rectangular C-grid. While the discretizations of gradient and divergence are clear on such a grid, this is not the case with the dot product. As a requirement for the discretization of the scalar product one uses that the identity

$$\nabla \cdot (\psi \mathbf{v}) = \mathbf{v} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{v} \quad (26.53)$$

should be transferred to the discretization.

26.7.1 One-dimensional case

The notation is taken from section 26.4.2 with the replacement $h \rightarrow \psi$. Averaging cells on edges is simply the arithmetic mean

$$\tilde{\psi}_j = \frac{\psi_{j-1/2} + \psi_{j+1/2}}{2}, \quad (26.54)$$

since the edge j is located in the middle between the two cells $j - 1/2$ and $j + 1/2$. Now you do the math

$$\begin{aligned} \nabla \cdot (\psi u) &= \frac{\tilde{\psi}_{j+1} u_{j+1} - \tilde{\psi}_j u_j}{\Delta x} = \frac{(\psi_{j+3/2} + \psi_{j+1/2}) u_{j+1} - (\psi_{j+1/2} + \psi_{j-1/2}) u_j}{2 \Delta x} \\ &= \frac{\psi_{j+3/2} u_{j+1} - \psi_{j-1/2} u_j + \psi_{j+1/2} (u_{j+1} - u_j)}{2 \Delta x} \\ &= \frac{\psi_{j+3/2} u_{j+1} - \psi_{j-1/2} u_j - \psi_{j+1/2} (u_{j+1} - u_j) + 2 \psi_{j+1/2} (u_{j+1} - u_j)}{2 \Delta x} \\ &= \frac{(\psi_{j+3/2} - \psi_{j+1/2}) u_{j+1} - (\psi_{j-1/2} - \psi_{j+1/2}) u_j + 2 \psi_{j+1/2} (u_{j+1} - u_j)}{2 \Delta x} \\ &= \frac{1}{2} \left[\frac{\psi_{j+3/2} - \psi_{j+1/2}}{\Delta x} u_{j+1} + \frac{\psi_{j+1/2} - \psi_{j-1/2}}{\Delta x} u_j \right] + \psi_{j+1/2} \frac{u_{j+1} - u_j}{\Delta x} \\ &\stackrel{!}{=} \psi \nabla \cdot (u) + u \frac{\partial \psi}{\partial x}. \end{aligned} \quad (26.55)$$

The product rule is transferred if one passes the dot product uv of two vector fields u, v

$$(uv)_{j+1/2} = \frac{u_j v_j + u_{j+1} v_{j+1}}{2} \quad (26.56)$$

defined.

26.7.2 Three-dimensional rectangular case

If you sum the derivation in the previous section over all three spatial directions, you get the analogous statement for the three-dimensional case with a dot product

$$\mathbf{u} \cdot \mathbf{v} = \sum_{e \in c} \frac{u_e v_e}{2}, \quad (26.57)$$

where c is the set of all side surfaces e of the box under consideration.

26.7.3 Two-dimensional orthogonal grid

Let A_c be the area of the cell c , e an edge of the cell, $o(e)$ the neighboring cell of c bordering the edge e , d_e a dual edge length and l_e a primary edge length. First you take notes

$$\nabla \cdot (\psi \mathbf{v}) = \frac{1}{A_c} \sum_{e \in c} l_e \frac{\psi_{o(e)} + \psi_c}{2} u_e, \quad (26.58)$$

$$\psi \nabla \cdot \mathbf{v} = \frac{\psi_c}{A_c} \sum_{e \in c} l_e u_e. \quad (26.59)$$

People are now demanding

$$\begin{aligned} \mathbf{v} \cdot \nabla \psi &\stackrel{!}{=} \nabla \cdot (\psi \mathbf{v}) - \psi \nabla \cdot \mathbf{v} \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \frac{1}{A_c} \sum_{e \in c} l_e \frac{\psi_{o(e)} + \psi_c}{2} u_e - \frac{\psi_c}{A_c} \sum_{e \in c} l_e u_e = \frac{1}{A_c} \sum_{e \in c} l_e \frac{\psi_{o(e)} - \psi_c}{2} u_e = \frac{1}{A_c} \sum_{e \in c} \frac{\psi_{o(e)} - \psi_c}{d_e} u_e \frac{l_e d_e}{2} \\ &= \sum_{e \in c} \frac{l_e d_e}{2 A_c} \frac{\psi_{o(e)} - \psi_c}{d_e} u_e. \end{aligned} \quad (26.60)$$

This is where you derive from

$$(\mathbf{u} \cdot \mathbf{v})_c = \sum_{e \in c} \frac{l_e d_e}{2 A_c} u_e v_e \quad (26.61)$$

as a discretization for the dot product. In the flat case, this results in the sum of the weighting factors

$$\sum_{e \in c} \frac{l_e d_e}{2 A_c} = 2. \quad (26.62)$$

In a curved case, such as B. a spherical surface, however, this is generally no longer the case.

26.7.4 Three-dimensional orthogonal grid (shallow)

Now the derivation in the previous section is generalized to a three-dimensional grid whose layer thickness Δz_k depends only on the vertical index k . Vertical vector components are denoted by w , the index u denotes the vector or scalar grid point above the grid box under consideration, the index l denotes the respective grid point below. This leads to

$$\nabla \cdot (\psi \mathbf{v}) = \frac{1}{A_c \Delta z_k} \left(\sum_{e \in c} l_e \Delta z_k \frac{\psi_{o(e)} + \psi_c}{2} u_e + A_c \frac{\psi_u + \psi_c}{2} w_u - A_c \frac{\psi_l + \psi_c}{2} w_l \right), \quad (26.63)$$

$$\psi \nabla \cdot \mathbf{v} = \frac{\psi_c}{A_c \Delta z_k} \left(\sum_{e \in c} l_e \Delta z_k u_e + A_c w_u - A_c w_l \right). \quad (26.64)$$

They are now demanding again

$$\begin{aligned} \mathbf{v} \cdot \nabla \psi &\stackrel{!}{=} \nabla \cdot (\psi \mathbf{v}) - \psi \nabla \cdot \mathbf{v} \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \frac{1}{A_c \Delta z_k} \left(\sum_{e \in c} l_e \Delta z_k \frac{\psi_{o(e)} + \psi_c}{2} u_e + A_c \frac{\psi_u + \psi_c}{2} w_u - A_c \frac{\psi_l + \psi_c}{2} w_l - \psi_c \sum_{e \in c} l_e \Delta z_k u_e - \psi_c A_c w_u + \psi_c A_c w_l \right) \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \frac{1}{A_c \Delta z_k} \left(\sum_{e \in c} l_e \Delta z_k \frac{\psi_{o(e)} - \psi_c}{2} u_e + A_c \frac{\psi_u - \psi_c}{2} w_u + A_c \frac{\psi_c - \psi_l}{2} w_l \right) \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \sum_{e \in c} \frac{l_e d_e}{2 A_c} \frac{\psi_{o(e)} - \psi_c}{d_e} u_e + \frac{\Delta z_{k-1/2}}{2 \Delta z_k} \frac{\psi_u - \psi_c}{\Delta z_{k-1/2}} w_u + \frac{\Delta z_{k+1/2}}{2 \Delta z_k} \frac{\psi_c - \psi_l}{\Delta z_{k+1/2}} w_l. \end{aligned} \quad (26.65)$$

This is where you derive from

$$\mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)} = \sum_{e \in c} \frac{l_e d_e}{2A_c} u_e^{(1)} u_e^{(2)} + \frac{\Delta z_{k-1/2}}{2\Delta z_k} w_u^{(1)} w_u^{(2)} + \frac{\Delta z_{k+1/2}}{2\Delta z_k} w_l^{(1)} w_l^{(2)} \quad (26.66)$$

as a discretization for the dot product $\mathbf{ab}$ in the shallow atmosphere. In the flat case, this results in the sum of the weighting factors

$$\sum_{e \in c} \frac{l_e d_e}{2A_c} + \frac{\Delta z_{k-1/2} + \Delta z_{k+1/2}}{2\Delta z_k} = 3, \quad (26.67)$$

where

$$\begin{aligned} \Delta z_k &= z_{k-1/2} - z_{k+1/2} = \frac{z_{k-1} + z_k}{2} - \frac{z_k + z_{k+1}}{2} = \frac{z_{k-1} + z_k - z_k - z_{k+1}}{2} \\ &= \frac{z_{k-1} - z_k + z_k - z_{k+1}}{2} = \frac{\Delta z_{k-1/2} + \Delta z_{k+1/2}}{2} \end{aligned} \quad (26.68)$$

was used. In a curved case, such as B. a spherical surface, however, this is generally no longer the case.

26.7.5 Three-dimensional orthogonal grid (deep)

Now the derivation in the previous section is generalized to the deep atmosphere, i.e. h. the shallow atmosphere approximation is canceled. It is again assumed that the layer thickness Δz_k only depends on the vertical index k . Using the same index notation as in the previous section one obtains

$$\nabla \cdot (\psi \mathbf{v}) = \frac{1}{V_{c,k}} \left(\sum_{e \in c} A_{e,k} \frac{\psi_{o(e)} + \psi_c}{2} u_{e,k} + A_{c,k+1/2} \frac{\psi_{c,k} + \psi_{c,k-1}}{2} w_{c,k+1/2} - A_{c,k+1/2} \frac{\psi_{c,k-1} + \psi_{c,k}}{2} w_{c,k+1/2} \right), \quad (26.69)$$

$$\psi \nabla \cdot \mathbf{v} = \frac{\psi_c}{V_{c,k}} \left(\sum_{e \in c} A_{e,k} u_{e,k} + A_{c,k+1/2} w_{c,k+1/2} - A_{c,k+1/2} w_{c,k+1/2} \right). \quad (26.70)$$

The cell base area $A_{c,k+1/2}$ now also depends on the vertical index. $A_{e,k}$ is the vertical surface whose subset is the edge (e, k) . They are now demanding again

$$\begin{aligned} \mathbf{v} \cdot \nabla \psi &\stackrel{!}{=} \nabla \cdot (\psi \mathbf{v}) - \psi \nabla \cdot \mathbf{v} \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \frac{1}{V_{c,k}} \left(\sum_{e \in c} A_{e,k} \frac{\psi_{o(e),k} + \psi_{c,k}}{2} u_{e,k} + A_{c,k+1/2} \frac{\psi_{c,k} + \psi_{c,k-1}}{2} w_{c,k+1/2} - A_{c,k+1/2} \frac{\psi_{c,k-1} + \psi_{c,k}}{2} w_{c,k+1/2} \right. \\ &\quad \left. - \sum_{e \in c} A_{e,k} \psi_{c,k} u_{e,k} - A_{c,k+1/2} \psi_{c,k} w_{c,k+1/2} + A_{c,k+1/2} \psi_{c,k} w_{c,k+1/2} \right) \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \frac{1}{V_{c,k}} \left(\sum_{e \in c} A_{e,k} \frac{\psi_{o(e),k} - \psi_{c,k}}{2} u_{e,k} + A_{c,k+1/2} \frac{\psi_{c,k-1} - \psi_{c,k}}{2} w_{c,k+1/2} + A_{c,k+1/2} \frac{\psi_{c,k} - \psi_{c,k+1}}{2} w_{c,k+1/2} \right) \\ \Leftrightarrow \mathbf{v} \cdot \nabla \psi &= \sum_{e \in c} \frac{A_{e,k} d_{e,k}}{2V_{c,k}} \frac{\psi_{o(e),k} - \psi_{c,k}}{d_{e,k}} u_{e,k} + \frac{A_{c,k+1/2} \Delta z_{k-1/2}}{2V_{c,k}} \frac{\psi_{c,k-1} - \psi_{c,k}}{\Delta z_{k-1/2}} w_{c,k+1/2} \\ &\quad + \frac{A_{c,k+1/2} \Delta z_{k+1/2}}{2V_{c,k}} \frac{\psi_{c,k} - \psi_{c,k+1}}{\Delta z_{k+1/2}} w_{c,k+1/2}. \end{aligned} \quad (26.71)$$

This is where you derive from

$$\begin{aligned}
\mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)} = & \sum_{e \in c} \frac{A_{e,k} d_{e,k}}{2 V_{c,k}} u_{e,k}^{(1)} u_{e,k}^{(2)} + \frac{A_{c,k+1/2} \Delta z_{k-1/2}}{2 V_{c,k}} w_{c,k+1/2}^{(1)} w_{c,k+1/2}^{(2)} \\
& + \frac{A_{c,k+1/2} \Delta z_{k+1/2}}{2 V_{c,k}} w_{c,k+1/2}^{(1)} w_{c,k+1/2}^{(2)}
\end{aligned} \tag{26.72}$$

as a discretization for the dot product.

26.8 Fixing on the C-grid

The C-lattice has three advantages over the other lattices:

1. It has advantageous dispersion relations.
2. Conservation of scalar variables is easy to ensure.
3. Gradient fields are rotation-free.
4. The product rule $\nabla \cdot (\psi \mathbf{v}) = \mathbf{v} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{v}$ is reproduced with appropriate discretization of the scalar product.

Therefore, the decision is made at this point to use a C-grid for the dynamic core to be developed in part VII.

26.8.1 Conclusions

In a C-grid, the vectors are located on the edges and intersect them orthogonally. If you extend the vector arrows in both directions, you end up at the scalar data points. The lattice obtained in this way is the so-called *dual lattice*. Grids that have a dual lattice are called *orthogonal*. This is not always the case. In order to be able to use the positive properties of the C-grid, one decides at this point on an orthogonal lattice for the dynamic core to be formulated in part VII.

26.9 The problem of the ratio of degrees of freedom

In the continuous case, for $N \geq 1$ prognostic variables ψ_i with $1 \leq i \leq N$ there is a system of N prognostic equations. If you linearize these, a linear coupled partial differential equation system is created. If you don't include any external forcings, it is homogeneous. If one uses a plane wave $\psi_i = \hat{\psi}_i \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t)$ with $\hat{\psi}_i \in \mathbb{C}$ for each of the prognostic variables, a homogeneous linear system of equations for the complex amplitudes is created $\hat{\psi}_i$. This is an eigenvalue problem for frequency ω . The eigenvalues can be found by setting the characteristic polynomial (the determinant) of this system of equations to zero. According to the Law of Algebra, the characteristic polynomial has complex, but not necessarily different, zeros. Each of the different zeros corresponds to a branch of the dispersion relation.

When discretizing, this is particularly important when staggering vector fields. In the case of the linearized shallow water equations you have three equations for the three variables (u, v, h) , so you have „twice as many arrows as points“. If a grid has too few arrows, the dispersion relation can no longer contain the necessary number of modes. If you have too many arrows, the dispersion relation could contain additional, unphysical branches. However, this can be prevented by applying special averaging operators in the prognostic equations.

26.9.1 Conclusions

On the triangular grid you have 1.5 vector points per scalar grid point, whereas the correct ratio is 2. Such grids are therefore excluded. Square grids are optimal in this regard. For grids with more than four corners, one has to eliminate the overspecification by m algebraic conditions on vector fields (one could also say: diagnostic equations or equations of state) per scalar grid point. For N vertices applies

$$m = \frac{N - 4}{2}, \tag{26.73}$$

since two cells each share an edge. For odd N , m lies midway between two natural numbers, so in this case a diagnostic vector equation must apply to two cells, which destroys the isotropy of the lattice. Therefore it is

necessary that N is even. Furthermore, if possible, you only want to set up one additional algebraic condition on vector fields per cell, so the first choice for N is 4 and the second choice is 6.

The problem discussed in this section will be formulated in more detail in the next chapter for the hexagonal grid.

26.10 Exclusion of square grids

The simplest quadrangular grid is the length-width grid already excluded in Section 26.1. It is found that all known quadrangular grids have at least one of the following fundamental problems, which have already been identified as exclusion criteria:

- Orthogonality is violated (e.g. with the *cubed-sphere lattice*)
- Quasi-uniformity is violated (e.g. with the length-width grid).
- Isotropy is grossly violated (e.g. with the *kite grid*).
- The grid has edges or points where the structure deviates greatly from the grid structure in other regions (e.g. in the reduced length-width grid).

Therefore, square grids are excluded at this point.

26.11 Fixing on the hexagonal icosahedral lattice

The only lattice remaining after this elimination process is the hexagonal icosahedral lattice.

27.1 Differential operators

The two unit vectors of the plane are given by

$$\mathbf{i} := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (27.1)$$

$$\mathbf{j} := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (27.2)$$

$$(27.3)$$

designated. Now we further define a three-element generating system $(\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3)$ by

$$\mathbf{i}_1 := \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{i}, \quad (27.4)$$

$$\mathbf{i}_2 := \begin{pmatrix} -\sin(30^\circ) \\ \cos(30^\circ) \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} = -\frac{1}{2}\mathbf{i} + \frac{\sqrt{3}}{2}\mathbf{j}, \quad (27.5)$$

$$\mathbf{i}_3 := \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} = -\frac{1}{2}\mathbf{i} - \frac{\sqrt{3}}{2}\mathbf{j}, \quad (27.6)$$

whose elements are each rotated by 120° relative to each other. We further define a generating system $(\mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3)$ that is rotated by 90°

$$\mathbf{j}_1 := \mathbf{k} \times \mathbf{i}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad (27.7)$$

$$\mathbf{j}_2 := \mathbf{k} \times \mathbf{i}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ -\frac{1}{2} \\ 0 \end{pmatrix} = -\frac{\sqrt{3}}{2}\mathbf{i} - \frac{1}{2}\mathbf{j}, \quad (27.8)$$

$$\mathbf{j}_3 := \mathbf{k} \times \mathbf{i}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \\ 0 \end{pmatrix} = \frac{\sqrt{3}}{2}\mathbf{i} - \frac{1}{2}\mathbf{j}. \quad (27.9)$$

You observe

$$\mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3 = \mathbf{o}, \quad \mathbf{j}_1 + \mathbf{j}_2 + \mathbf{j}_3 = \mathbf{o}. \quad (27.10)$$

For a two-dimensional vector $\mathbf{v}$ one can

$$\mathbf{v} = u\mathbf{i} + v\mathbf{j} \quad (27.11)$$

write, apply here

$$u = \mathbf{i} \cdot \mathbf{v}, \quad v = \mathbf{j} \cdot \mathbf{v}. \quad (27.12)$$

Since the $\mathbf{i}_k, \mathbf{j}_l$ are each pairwise linearly independent, one can note down

$$\mathbf{v} = u'_k \mathbf{i}_k + u'_l \mathbf{i}_l = v'_k \mathbf{j}_k + v'_l \mathbf{j}_l. \quad (27.13)$$

Since the choice of k, l is not unique and one could also use all three unit vectors, one can introduce another linear condition. You use this freedom to change the spelling

$$\mathbf{v} = \frac{2}{3} (u_1 \mathbf{i}_1 + u_2 \mathbf{i}_2 + u_3 \mathbf{i}_3) = \frac{2}{3} (v_1 \mathbf{j}_1 + v_2 \mathbf{j}_2 + v_3 \mathbf{j}_3) \quad (27.14)$$

to demand. This is with

$$u_k = \mathbf{i}_k \cdot \mathbf{v}, \quad v_k = \mathbf{j}_k \cdot \mathbf{v} \quad (27.15)$$

fulfilled, because it follows from this

$$\begin{aligned}
 \mathbf{v} &= u\mathbf{i} + v\mathbf{j} = \frac{2}{3} \left(\frac{6}{4}u\mathbf{i} + \frac{6}{4}v\mathbf{j} \right) \\
 &= \frac{2}{3} \left(u\mathbf{i} + \frac{1}{4}u\mathbf{i} - \frac{\sqrt{3}}{4}u\mathbf{j} - \frac{\sqrt{3}}{4}v\mathbf{i} + \frac{3}{4}v\mathbf{j} + \frac{1}{4}u\mathbf{i} + \frac{\sqrt{3}}{4}u\mathbf{j} + \frac{\sqrt{3}}{4}v\mathbf{i} + \frac{3}{4}v\mathbf{j} \right) \\
 &= \frac{2}{3} \left(u\mathbf{i} + \left(-\frac{1}{2}u + \frac{\sqrt{3}}{2}v \right) \left(-\frac{1}{2}\mathbf{i} + \frac{\sqrt{3}}{2}\mathbf{j} \right) + \left(-\frac{1}{2}u - \frac{\sqrt{3}}{2}v \right) \left(-\frac{1}{2}\mathbf{i} - \frac{\sqrt{3}}{2}\mathbf{j} \right) \right) \\
 &= \frac{2}{3} (u_1\mathbf{i}_1 + u_2\mathbf{i}_2 + u_3\mathbf{i}_3),
 \end{aligned} \tag{27.16}$$

where

$$u_1 = u, \quad u_2 = -\frac{1}{2}u + \frac{\sqrt{3}}{2}v, \quad u_3 = -\frac{1}{2}u - \frac{\sqrt{3}}{2}v. \tag{27.17}$$

was used. This applies analogously to the v_k . From this it follows

$$\mathbf{o} = \mathbf{v} \cdot \mathbf{o} = \mathbf{v} \cdot (\mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) = u_1 + u_2 + u_3 \tag{27.18}$$

and analogously for the v_k . For the gradient ∇a of a scalar field we now get a

$$\nabla a = \frac{2}{3} [(\mathbf{i}_1 \cdot \nabla a) \mathbf{i}_1 + (\mathbf{i}_2 \cdot \nabla a) \mathbf{i}_2 + (\mathbf{i}_3 \cdot \nabla a) \mathbf{i}_3]. \tag{27.19}$$

Because of

$$\mathbf{i}_k \cdot \nabla a = \frac{\partial a}{\partial x_k} \tag{27.20}$$

follows

$$\nabla a = \frac{2}{3} \left(\frac{\partial a}{\partial x_1} \mathbf{i}_1 + \frac{\partial a}{\partial x_2} \mathbf{i}_2 + \frac{\partial a}{\partial x_3} \mathbf{i}_3 \right). \tag{27.21}$$

This also provides:

$$\frac{\partial a}{\partial x_1} + \frac{\partial a}{\partial x_2} + \frac{\partial a}{\partial x_3} = \mathbf{o} \tag{27.22}$$

firmly. It applies

$$\mathbf{i}_1 = \frac{1}{\sqrt{3}} (\mathbf{j}_3 - \mathbf{j}_2) \tag{27.23}$$

and cyclically:

$$\mathbf{i}_2 = \frac{1}{\sqrt{3}} (\mathbf{j}_1 - \mathbf{j}_3), \quad \mathbf{i}_3 = \frac{1}{\sqrt{3}} (\mathbf{j}_2 - \mathbf{j}_1) \tag{27.24}$$

From this it follows

$$\nabla a = \frac{2}{3\sqrt{3}} \left(\frac{\partial a}{\partial x_1} (\mathbf{j}_3 - \mathbf{j}_2) + \frac{\partial a}{\partial x_2} (\mathbf{j}_1 - \mathbf{j}_3) + \frac{\partial a}{\partial x_3} (\mathbf{j}_2 - \mathbf{j}_1) \right). \tag{27.25}$$

Rearrangement results

$$\nabla a = \frac{2}{3\sqrt{3}} \left(\left(\frac{\partial a}{\partial x_2} - \frac{\partial a}{\partial x_3} \right) j_1 + \left(\frac{\partial a}{\partial x_3} - \frac{\partial a}{\partial x_1} \right) j_2 + \left(\frac{\partial a}{\partial x_1} - \frac{\partial a}{\partial x_2} \right) j_3 \right). \quad (27.26)$$

It applies

$$\begin{aligned} \mathbf{v} &= \frac{2}{3} (u_1 \mathbf{i}_1 + u_2 \mathbf{i}_2 + u_3 \mathbf{i}_3) = \frac{2}{3} \left[u_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + u_2 \begin{pmatrix} -\frac{1}{\sqrt{3}} \\ \frac{2}{3} \\ 0 \end{pmatrix} + u_3 \begin{pmatrix} -\frac{1}{\sqrt{3}} \\ 0 \\ \frac{2}{3} \end{pmatrix} \right] = \frac{2}{3} \begin{pmatrix} u_1 - \frac{u_2}{\sqrt{3}} - \frac{u_3}{\sqrt{3}} \\ \frac{2}{3} u_2 \\ \frac{2}{3} u_3 \end{pmatrix} \\ &= \begin{pmatrix} \frac{2}{3} u_1 - \frac{u_2}{\sqrt{3}} - \frac{u_3}{\sqrt{3}} \\ \frac{2}{3} u_2 \\ \frac{2}{3} u_3 \end{pmatrix}. \end{aligned} \quad (27.27)$$

From this it follows that the divergence

$$D := \nabla \cdot \mathbf{v} = \frac{2}{3} \frac{u_1}{\partial x} - \frac{1}{3} \frac{u_2}{\partial x} - \frac{1}{3} \frac{u_3}{\partial x} + \frac{1}{\sqrt{3}} \frac{u_2}{\partial y} - \frac{1}{\sqrt{3}} \frac{u_3}{\partial y}. \quad (27.28)$$

It applies

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x_1}, \quad (27.29)$$

because of

$$\mathbf{j} = \frac{1}{\sqrt{3}} (\mathbf{i}_2 - \mathbf{i}_3) \quad (27.30)$$

is also

$$\frac{\partial}{\partial y} = \frac{1}{\sqrt{3}} \left(\frac{\partial}{\partial x_2} - \frac{\partial}{\partial x_3} \right). \quad (27.31)$$

From this it follows

$$\begin{aligned} D &= \frac{2}{3} \frac{\partial u_1}{\partial x} - \frac{1}{3} \frac{\partial u_2}{\partial x} - \frac{1}{3} \frac{\partial u_3}{\partial x} + \frac{1}{3} \left(\frac{\partial u_2}{\partial x_2} - \frac{\partial u_2}{\partial x_3} \right) - \frac{1}{3} \left(\frac{\partial u_3}{\partial x_2} - \frac{\partial u_3}{\partial x_3} \right) \\ &= \frac{2}{3} \frac{\partial u_1}{\partial x_1} + \frac{1}{3} \frac{u_2}{\partial x_2} + \frac{1}{3} \frac{u_3}{\partial x_3} - \frac{1}{3} \frac{u_2}{\partial x_1} - \frac{1}{3} \frac{\partial u_3}{\partial x_1} - \frac{1}{3} \frac{\partial u_2}{\partial x_3} - \frac{1}{3} \frac{\partial u_3}{\partial x_2} \\ &= \frac{2}{3} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) - \frac{1}{3} \left(\frac{\partial u_2}{\partial x_1} + \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_1} + \frac{\partial u_3}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right). \end{aligned} \quad (27.32)$$

With Eq. (27.22) follows

$$D = \frac{2}{3} \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right). \quad (27.33)$$

By combining with Eq. (27.21) is still obtained

$$\Delta a = \frac{2}{3} \left(\frac{\partial^2 a}{\partial x_1^2} + \frac{\partial^2 a}{\partial x_2^2} + \frac{\partial^2 a}{\partial x_3^2} \right). \quad (27.34)$$

It applies

$$\begin{aligned} u_1 &= \mathbf{v} \cdot \mathbf{i}_1 = \frac{2}{3} (v_1 \mathbf{j}_1 \cdot \mathbf{i}_1 + v_2 \mathbf{j}_2 \cdot \mathbf{i}_1 + v_3 \mathbf{j}_3 \cdot \mathbf{i}_1) = \frac{2}{3} \left(0 \cdot v_1 - \frac{\sqrt{3}}{2} v_2 + \frac{\sqrt{3}}{2} v_3 \right) \\ &= \frac{1}{\sqrt{3}} (v_3 - v_2). \end{aligned} \quad (27.35)$$

By cyclically moving the indices you get

$$u_2 = \frac{1}{\sqrt{3}} (v_1 - v_3), \quad u_3 = \frac{1}{\sqrt{3}} (v_2 - v_1). \quad (27.36)$$

This gives another representation of the divergence:

$$D = \frac{2}{3\sqrt{3}} \left[\left(\frac{\partial v_2}{\partial x_3} - \frac{\partial v_3}{\partial x_2} \right) + \left(\frac{\partial v_3}{\partial x_1} - \frac{\partial v_1}{\partial x_3} \right) + \left(\frac{\partial v_1}{\partial x_2} - \frac{\partial v_2}{\partial x_1} \right) \right] \quad (27.37)$$

It applies

$$\begin{aligned} \frac{\partial v_2}{\partial x_3} - \frac{\partial v_3}{\partial x_2} &= \frac{\partial v_2}{\partial x_3} + \frac{\partial v_2}{\partial x_2} - \frac{\partial v_2}{\partial x_2} - \frac{\partial v_3}{\partial x_2} = \left(\frac{\partial}{\partial x_3} + \frac{\partial}{\partial x_2} \right) v_2 - \frac{\partial}{\partial x_2} (v_2 + v_3) \\ &= -\frac{\partial v_2}{\partial x_1} + \frac{\partial v_1}{\partial x_2} = \frac{\partial v_1}{\partial x_2} - \frac{\partial v_2}{\partial x_1}. \end{aligned} \quad (27.38)$$

By cyclically exchanging this equation, one can see that all three summands in brackets in Eq. (27.37) are the same. Follow from this

$$D = \frac{2}{\sqrt{3}} \left(\frac{\partial v_2}{\partial x_3} - \frac{\partial v_3}{\partial x_2} \right), \quad (27.39)$$

$$D = \frac{2}{\sqrt{3}} \left(\frac{\partial v_3}{\partial x_1} - \frac{\partial v_1}{\partial x_3} \right), \quad (27.40)$$

$$D = \frac{2}{\sqrt{3}} \left(\frac{\partial v_1}{\partial x_2} - \frac{\partial v_2}{\partial x_1} \right). \quad (27.41)$$

It applies

$$\begin{aligned} \mathbf{v} &= \frac{2}{3} (v_1 \mathbf{j}_1 + v_2 \mathbf{j}_2 + v_3 \mathbf{j}_3) = \frac{2}{3} \left[v_1 \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} + v_2 \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix} + v_3 \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix} \right] \\ &= \begin{pmatrix} \frac{1}{\sqrt{3}} v_3 - \frac{1}{\sqrt{3}} v_2 \\ \frac{2}{3} v_1 - \frac{v_2}{3} - \frac{v_3}{3} \end{pmatrix}. \end{aligned} \quad (27.42)$$

For the vorticity one obtains

$$\begin{aligned} \zeta &= \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = \frac{\partial}{\partial x} \left(\frac{2}{3} v_1 - \frac{v_2}{3} - \frac{v_3}{3} \right) - \frac{\partial}{\partial y} \left(\frac{1}{\sqrt{3}} v_3 - \frac{1}{\sqrt{3}} v_2 \right) \\ &= \frac{\partial}{\partial x_1} \left(\frac{2}{3} v_1 - \frac{v_2}{3} - \frac{v_3}{3} \right) - \frac{1}{\sqrt{3}} \left(\frac{\partial}{\partial x_2} - \frac{\partial}{\partial x_3} \right) \left(\frac{1}{\sqrt{3}} v_3 - \frac{1}{\sqrt{3}} v_2 \right) \\ &= \frac{2}{3} \frac{\partial v_1}{\partial x_1} + \frac{1}{3} \frac{\partial v_2}{\partial x_2} + \frac{1}{3} \frac{\partial v_3}{\partial x_3} - \frac{1}{3} \frac{\partial v_2}{\partial x_1} - \frac{1}{3} \frac{\partial v_3}{\partial x_1} - \frac{1}{3} \frac{\partial v_3}{\partial x_2} - \frac{1}{3} \frac{\partial v_2}{\partial x_3} \\ &= \frac{2}{3} \left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} \right) - \frac{1}{3} \left(\frac{\partial v_2}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_1} + \frac{\partial v_3}{\partial x_2} + \frac{\partial v_3}{\partial x_3} \right). \end{aligned} \quad (27.43)$$

With Eq. (27.22) follows

$$\zeta = \frac{2}{3} \left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} \right). \quad (27.44)$$

It applies

$$\begin{aligned} v_1 &= \mathbf{v} \cdot \mathbf{j}_1 = \frac{2}{3} (u_1 \mathbf{i}_1 + u_2 \mathbf{i}_2 + u_3 \mathbf{i}_3) \cdot \mathbf{j}_1 = \frac{2}{3} (u_1 \mathbf{i}_1 + u_2 \mathbf{i}_2 + u_3 \mathbf{i}_3) \cdot \mathbf{j} \\ &= \frac{2}{3} \left(\frac{\sqrt{3}}{2} u_2 - \frac{\sqrt{3}}{2} u_3 \right) = \frac{1}{\sqrt{3}} (u_2 - u_3). \end{aligned} \quad (27.45)$$

By cyclically moving the indices you get

$$v_2 = \frac{1}{\sqrt{3}} (u_3 - u_1), \quad v_3 = \frac{1}{\sqrt{3}} (u_1 - u_2). \quad (27.46)$$

From this follows another representation of the vorticity:

$$\zeta = \frac{2}{3\sqrt{3}} \left(\frac{\partial u_2}{\partial x_1} - \frac{\partial u_3}{\partial x_1} + \frac{\partial u_3}{\partial x_2} - \frac{\partial u_1}{\partial x_2} + \frac{\partial u_1}{\partial x_3} - \frac{\partial u_2}{\partial x_3} \right) \quad (27.47)$$

By rearranging you get

$$\zeta = \frac{2}{3\sqrt{3}} \left[\left(\frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_3} \right) + \left(\frac{\partial u_1}{\partial x_3} - \frac{\partial u_3}{\partial x_1} \right) + \left(\frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2} \right) \right]. \quad (27.48)$$

Analogous to the case of Eq. (27.37) also apply here

$$\zeta = \frac{2}{\sqrt{3}} \left(\frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_3} \right), \quad (27.49)$$

$$\zeta = \frac{2}{\sqrt{3}} \left(\frac{\partial u_1}{\partial x_3} - \frac{\partial u_3}{\partial x_1} \right), \quad (27.50)$$

$$\zeta = \frac{2}{\sqrt{3}} \left(\frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2} \right). \quad (27.51)$$

27.2 Main theorem of vector analysis

With the main theorem of vector analysis one can get the vector field $\mathbf{v}$ in the form

$$\mathbf{v} = \mathbf{k} \times \nabla \psi + \nabla \chi \quad (27.52)$$

note down. This applies

$$\mathbf{k} \times \nabla \psi = \frac{2}{3} \left(\frac{\partial \psi}{\partial x_1} \mathbf{j}_1 + \frac{\partial \psi}{\partial x_2} \mathbf{j}_2 + \frac{\partial \psi}{\partial x_3} \mathbf{j}_3 \right), \quad (27.53)$$

$$\nabla \chi = \frac{2}{3} \left(\frac{\partial \chi}{\partial x_1} \mathbf{i}_1 + \frac{\partial \chi}{\partial x_2} \mathbf{i}_2 + \frac{\partial \chi}{\partial x_3} \mathbf{i}_3 \right). \quad (27.54)$$

Follow from this

$$u_1 = \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \psi}{\partial x_3} - \frac{\partial \psi}{\partial x_2} \right) + \frac{\partial \chi}{\partial x_1} = -\frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \psi}{\partial x_2} - \frac{\partial \psi}{\partial x_3} \right) + \frac{\partial \chi}{\partial x_1}, \quad (27.55)$$

$$u_2 = -\frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \psi}{\partial x_3} - \frac{\partial \psi}{\partial x_1} \right) + \frac{\partial \chi}{\partial x_2}, \quad (27.56)$$

$$u_3 = -\frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \psi}{\partial x_1} - \frac{\partial \psi}{\partial x_2} \right) + \frac{\partial \chi}{\partial x_3}. \quad (27.57)$$

and

$$v_1 = \frac{\partial \psi}{\partial x_1} + \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \chi}{\partial x_2} - \frac{\partial \chi}{\partial x_3} \right), \quad (27.58)$$

$$v_2 = \frac{\partial \psi}{\partial x_2} + \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \chi}{\partial x_3} - \frac{\partial \chi}{\partial x_1} \right), \quad (27.59)$$

$$v_3 = \frac{\partial \psi}{\partial x_3} + \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \chi}{\partial x_1} - \frac{\partial \chi}{\partial x_2} \right). \quad (27.60)$$

Because of

$$D = \Delta \chi, \quad \zeta = \Delta \psi \quad (27.61)$$

continue to apply

$$\Delta u_1 = -\frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \zeta}{\partial x_2} - \frac{\partial \zeta}{\partial x_3} \right) + \frac{\partial D}{\partial x_1}, \quad (27.62)$$

$$\Delta u_2 = -\frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \zeta}{\partial x_3} - \frac{\partial \zeta}{\partial x_1} \right) + \frac{\partial D}{\partial x_2}, \quad (27.63)$$

$$\Delta u_3 = -\frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial \zeta}{\partial x_1} - \frac{\partial \zeta}{\partial x_2} \right) + \frac{\partial D}{\partial x_3}, \quad (27.64)$$

$$\Delta v_1 = \frac{\partial \zeta}{\partial x_1} + \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial D}{\partial x_2} - \frac{\partial D}{\partial x_3} \right), \quad (27.65)$$

$$\Delta v_2 = \frac{\partial \zeta}{\partial x_2} + \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial D}{\partial x_3} - \frac{\partial D}{\partial x_1} \right), \quad (27.66)$$

$$\Delta v_3 = \frac{\partial \zeta}{\partial x_3} + \frac{\mathbf{i}}{\sqrt{3}} \left(\frac{\partial D}{\partial x_1} - \frac{\partial D}{\partial x_2} \right). \quad (27.67)$$

27.3 Dispersion relation

Let a be a field of the form

$$a(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}). \quad (27.68)$$

The distance between the centers of two hexagons is called d (from now on this quantity is called the lattice constant). Now define the central difference quotient in the j direction for $1 \leq j \leq 3$

$$\delta_j a = \frac{a(\mathbf{r} + i_j \frac{d}{2}) - a(\mathbf{r} - i_j \frac{d}{2})}{d}. \quad (27.69)$$

This applies to this

$$\begin{aligned}
\delta_j a &= \frac{\exp[i\mathbf{k} \cdot (\mathbf{r} + \mathbf{i}_{j\frac{d}{2}})] - \exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{i}_{j\frac{d}{2}})]}{d} \\
&= \exp(i\mathbf{k} \cdot \mathbf{r}) \frac{\exp(i\mathbf{k} \cdot \mathbf{i}_{j\frac{d}{2}}) - \exp(-i\mathbf{k} \cdot \mathbf{i}_{j\frac{d}{2}})}{d} = a(\mathbf{r}) \frac{\exp(i\mathbf{k} \cdot \mathbf{i}_{j\frac{d}{2}}) - \exp(-i\mathbf{k} \cdot \mathbf{i}_{j\frac{d}{2}})}{d} \\
&= a(\mathbf{r}) \frac{\exp(ik_{j\frac{d}{2}}) - \exp(-ik_{j\frac{d}{2}})}{d} = a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_j d}{2}\right). \tag{27.70}
\end{aligned}$$

You define it

$$s_j := \sin\left(\frac{k_j d}{2}\right), \tag{27.71}$$

you can do this in the form

$$\delta_j a = \frac{2i}{d} s_j a \tag{27.72}$$

note down. We now continue to define a simple averaging operator in the j direction

$$\begin{aligned}
\bar{a}^{(j)} &:= \frac{a(\mathbf{r} + \mathbf{i}_{j\frac{d}{2}}) + a(\mathbf{r} - \mathbf{i}_{j\frac{d}{2}})}{2} = \frac{\exp[i\mathbf{k} \cdot (\mathbf{r} + \mathbf{i}_{j\frac{d}{2}})] + \exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{i}_{j\frac{d}{2}})]}{2} \\
&= \exp(i\mathbf{k} \cdot \mathbf{r}) \frac{\exp(i\mathbf{k} \cdot \mathbf{i}_{j\frac{d}{2}}) + \exp(-i\mathbf{k} \cdot \mathbf{i}_{j\frac{d}{2}})}{2} \\
&= a(\mathbf{r}) \frac{\exp(ik_{j\frac{d}{2}}) + \exp(-ik_{j\frac{d}{2}})}{2} = a(\mathbf{r}) \cos\left(\frac{k_j d}{2}\right). \tag{27.73}
\end{aligned}$$

You define it

$$c_j := \cos\left(\frac{k_j d}{2}\right), \tag{27.74}$$

you can do this in the form

$$\bar{a}^{(j)} = c_j a \tag{27.75}$$

note down.

The linearized shallow water equations (13.173) - (13.174) on the f-plane can be written with the geopotential $\Phi := gh$ in the form

$$\frac{\partial \Phi}{\partial t} + \Phi_o \nabla \cdot \mathbf{v} = 0, \quad \frac{\partial \mathbf{v}}{\partial t} + f_o \mathbf{k} \times \mathbf{v} - \nabla \Phi = 0 \tag{27.76}$$

note down. Here $\Phi_o := gD$. With the equations (27.33) and (27.45) this leads to the evolution equations for the components regarding the three-element generating system:

$$\frac{\partial \Phi}{\partial t} + \frac{2}{3} \Phi_o \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) = 0, \tag{27.77}$$

$$\frac{\partial u_1}{\partial t} - \frac{f_o}{\sqrt{3}} (u_2 - u_3) + \frac{\partial \Phi}{\partial x_1} = 0, \tag{27.78}$$

$$\frac{\partial u_2}{\partial t} - \frac{f_o}{\sqrt{3}} (u_3 - u_1) + \frac{\partial \Phi}{\partial x_2} = 0, \tag{27.79}$$

$$\frac{\partial u_3}{\partial t} - \frac{f_o}{\sqrt{3}} (u_1 - u_2) + \frac{\partial \Phi}{\partial x_3} = 0. \tag{27.80}$$

Spatial discretization results

$$\frac{\partial \Phi}{\partial t} + \frac{2}{3} \Phi_0 (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3) = 0, \quad (27.81)$$

$$\frac{\partial u_1}{\partial t} - \frac{f_0}{\sqrt{3}} (\overline{u_2^3} - \overline{u_3^{(2)}}) + \delta_1 \Phi = 0, \quad (27.82)$$

$$\frac{\partial u_2}{\partial t} - \frac{f_0}{\sqrt{3}} (\overline{u_3^{(1)}} - \overline{u_1^3}) + \delta_2 \Phi = 0, \quad (27.83)$$

$$\frac{\partial u_3}{\partial t} - \frac{f_0}{\sqrt{3}} (\overline{u_1^{(2)}} - \overline{u_2^{(1)}}) + \delta_3 \Phi = 0. \quad (27.84)$$

The arithmetic mean of the two nearest speed components in the desired direction was used to reconstruct the wind components for calculating the Coriolis acceleration. If you set a monochromatic plane wave for all fields, i.e

$$\psi(\mathbf{r}, t) = \hat{\psi} \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t) \quad (27.85)$$

for any field ψ with a complex amplitude $\hat{\psi}$, one obtains

$$-i\omega \hat{\Phi} + \frac{4i}{3d} \Phi_0 (s_1 \hat{u}_1 + s_2 \hat{u}_2 + s_3 \hat{u}_3) = 0, \quad (27.86)$$

$$-i\omega \hat{u}_1 - \frac{f_0}{\sqrt{3}} (c_3 \hat{u}_2 - c_2 \hat{u}_3) + \frac{2is_1}{d} \hat{\Phi} = 0, \quad (27.87)$$

$$-i\omega \hat{u}_2 - \frac{f_0}{\sqrt{3}} (c_1 \hat{u}_3 - c_3 \hat{u}_1) + \frac{2is_2}{d} \hat{\Phi} = 0, \quad (27.88)$$

$$-i\omega \hat{u}_3 - \frac{f_0}{\sqrt{3}} (c_2 \hat{u}_1 - c_1 \hat{u}_2) + \frac{2is_3}{d} \hat{\Phi} = 0. \quad (27.89)$$

It should be noted that there is a phase offset between the equations, which arises from the fact that the individual equations apply at different locations. This was edited out. In matrix form you get

$$\begin{pmatrix} -i\omega & \frac{4i}{3d} \Phi_0 s_1 & \frac{4i}{3d} \Phi_0 s_2 & \frac{4i}{3d} \Phi_0 s_3 \\ \frac{2is_1}{d} & -i\omega & -\frac{f_0}{\sqrt{3}} c_3 & \frac{f_0}{\sqrt{3}} c_2 \\ \frac{2is_2}{d} & \frac{f_0}{\sqrt{3}} c_3 & -i\omega & -\frac{f_0}{\sqrt{3}} c_1 \\ \frac{2is_3}{d} & -\frac{f_0}{\sqrt{3}} c_2 & \frac{f_0}{\sqrt{3}} c_1 & -i\omega \end{pmatrix} \begin{pmatrix} \hat{\Phi} \\ \hat{u}_1 \\ \hat{u}_2 \\ \hat{u}_3 \end{pmatrix} = 0. \quad (27.90)$$

Multiplying this by the imaginary unit i gives

$$\begin{pmatrix} \omega & -\frac{4}{3d} \Phi_0 s_1 & -\frac{4}{3d} \Phi_0 s_2 & -\frac{4}{3d} \Phi_0 s_3 \\ -\frac{2s_1}{d} & \omega & -\frac{if_0}{\sqrt{3}} c_3 & \frac{if_0}{\sqrt{3}} c_2 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}} c_3 & \omega & -\frac{if_0}{\sqrt{3}} c_1 \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}} c_2 & \frac{if_0}{\sqrt{3}} c_1 & \omega \end{pmatrix} \begin{pmatrix} \hat{\Phi} \\ \hat{u}_1 \\ \hat{u}_2 \\ \hat{u}_3 \end{pmatrix} = 0. \quad (27.91)$$

Nontrivial solutions exist if and only if the determinant of the coefficient matrix of this system of linear equations vanishes:

$$\begin{aligned}
& \begin{vmatrix} \omega & -\frac{4}{3d}\Phi_0 s_1 & -\frac{4}{3d}\Phi_0 s_2 & -\frac{4}{3d}\Phi_0 s_3 \\ -\frac{2s_1}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_3 & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & \omega & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \frac{if_0}{\sqrt{3}}c_1 & \omega \end{vmatrix} \stackrel{!}{=} 0 \\
& \Leftrightarrow \omega \begin{vmatrix} \omega & -\frac{if_0}{\sqrt{3}}c_3 & \frac{if_0}{\sqrt{3}}c_2 \\ \frac{if_0}{\sqrt{3}}c_3 & \omega & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{if_0}{\sqrt{3}}c_2 & \frac{if_0}{\sqrt{3}}c_1 & \omega \end{vmatrix} + \frac{4}{3d}\Phi_0 s_1 \begin{vmatrix} -\frac{2s_1}{d} & -\frac{if_0}{\sqrt{3}}c_3 & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & \frac{if_0}{\sqrt{3}}c_1 & \omega \end{vmatrix} \\
& - \frac{4}{3d}\Phi_0 s_2 \begin{vmatrix} -\frac{2s_1}{d} & \omega & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \omega \end{vmatrix} + \frac{4}{3d}\Phi_0 s_3 \begin{vmatrix} -\frac{2s_1}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_3 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & \omega \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \frac{if_0}{\sqrt{3}}c_1 \end{vmatrix} = 0 \quad (27.92)
\end{aligned}$$

$$\begin{aligned}
& \Leftrightarrow \omega^4 - \frac{\omega^2 f_0^2}{3} (c_1^2 + c_2^2 + c_3^2) + \frac{4}{3d}\Phi_0 s_1 \begin{vmatrix} -\frac{2s_1}{d} & -\frac{if_0}{\sqrt{3}}c_3 & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & \frac{if_0}{\sqrt{3}}c_1 & \omega \end{vmatrix} \\
& - \frac{4}{3d}\Phi_0 s_2 \begin{vmatrix} -\frac{2s_1}{d} & \omega & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \omega \end{vmatrix} + \frac{4}{3d}\Phi_0 s_3 \begin{vmatrix} -\frac{2s_1}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_3 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & \omega \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \frac{if_0}{\sqrt{3}}c_1 \end{vmatrix} = 0 \quad (27.93)
\end{aligned}$$

It applies

$$\begin{aligned}
& \frac{4}{3d}\Phi_0 s_1 \begin{vmatrix} -\frac{2s_1}{d} & -\frac{if_0}{\sqrt{3}}c_3 & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & \frac{if_0}{\sqrt{3}}c_1 & \omega \end{vmatrix} = -\frac{8\omega^2}{3d^2}\Phi_0 s_1^2 + \frac{8\Phi_0 f_0^2}{9d^2} (s_1 c_1 s_3 c_3 + s_1 c_1 s_2 c_2 + s_1 c_1 s_1 c_1) + \frac{8if_0}{3\sqrt{3}d} s_1 (s_3 c_2 - c_3 s_2) \\
& = -\frac{8\omega^2}{3d^2}\Phi_0 s_1^2 + \frac{8\Phi_0 f_0^2}{9d^2} s_1 c_1 (s_1 c_1 + s_2 c_2 + s_3 c_3) - \frac{8if_0}{3\sqrt{3}d} s_1 (s_2 c_3 - s_3 c_2). \quad (27.94)
\end{aligned}$$

The remaining two partial determinants arise analogously by cyclically exchanging the indices:

$$\begin{aligned}
& -\frac{4}{3d}\Phi_0 s_2 \begin{vmatrix} -\frac{2s_1}{d} & \omega & \frac{if_0}{\sqrt{3}}c_2 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & -\frac{if_0}{\sqrt{3}}c_1 \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \omega \end{vmatrix} = -\frac{8\omega^2}{3d^2}\Phi_0 s_2^2 + \frac{8\Phi_0 f_0^2}{9d^2} s_2 c_2 (s_1 c_1 + s_2 c_2 + s_3 c_3) - \frac{8if_0}{3\sqrt{3}d} s_2 (s_3 c_1 - s_1 c_3), \\
& \frac{4}{3d}\Phi_0 s_3 \begin{vmatrix} -\frac{2s_1}{d} & \omega & -\frac{if_0}{\sqrt{3}}c_3 \\ -\frac{2s_2}{d} & \frac{if_0}{\sqrt{3}}c_3 & \omega \\ -\frac{2s_3}{d} & -\frac{if_0}{\sqrt{3}}c_2 & \frac{if_0}{\sqrt{3}}c_1 \end{vmatrix} = -\frac{8\omega^2}{3d^2}\Phi_0 s_3^2 + \frac{8\Phi_0 f_0^2}{9d^2} s_3 c_3 (s_1 c_1 + s_2 c_2 + s_3 c_3) - \frac{8if_0}{3\sqrt{3}d} s_3 (s_1 c_2 - s_2 c_1). \quad (27.95)
\end{aligned}$$

So the characteristic polynomial is finally:

$$\boxed{\omega^4 - \omega^2 \left[\frac{f_0^2}{3} (c_1^2 + c_2^2 + c_3^2) + \frac{8\Phi_0}{3d^2} (s_1^2 + s_2^2 + s_3^2) \right] + \frac{8\Phi_0 f_0^2}{9d^2} (s_1 c_1 + s_2 c_2 + s_3 c_3)^2 = 0.} \quad (27.96)$$

For the case of well-resolved waves $|\mathbf{k}| \ll \frac{1}{d}$ apply

$$c_j \approx \mathbf{i}, \quad s_j \approx \frac{k_j d}{2}. \quad (27.97)$$

Putting this into Eq. (27.96), you get

$$\begin{aligned} \omega^4 - \omega^2 \left[f_o^2 + \frac{8\Phi_o}{3d^2} \left(\frac{k_1^2 d^2}{4} + \frac{k_2^2 d^2}{4} + \frac{k_3^2 d^2}{4} \right) \right] + \frac{8\Phi_o f_o^2}{9d^2} \underbrace{\left(\frac{k_1 d}{2} + \frac{k_1 d}{2} + \frac{k_1 d}{2} \right)^2}_{\approx 0} &\approx 0 \\ \Leftrightarrow \omega^4 - \omega^2 \left[f_o^2 + \frac{2\Phi_o}{3} (k_1^2 + k_2^2 + k_3^2) \right] &\approx 0. \\ \Leftrightarrow \omega^4 - \omega^2 [f_o^2 + \Phi \mathbf{k}^2] &\approx 0. \end{aligned} \quad (27.98)$$

The last step took advantage of the fact that $k_1^2 + k_2^2 + k_3^2 = \frac{3}{2} \mathbf{k}^2$. This can be made clear by: A. $\mathbf{k} \parallel \mathbf{i}_1$ assumes, because then $k_1 = k$, $k_2 = -k \sin(30^\circ) = -\frac{k}{2}$ and $k_3 = -\frac{k}{2}$. This leads to the two intertio-gravity modes

$$\omega^2 \approx f_o^2 + \Phi_o |\mathbf{k}|^2 \quad (27.99)$$

as well as geostrophic fashion

$$\omega \approx 0. \quad (27.100)$$

However, for less well-resolved waves, the term $\propto (s_1 c_1 + s_2 c_2 + s_3 c_3)^2$ causes the geostrophic mode to split into two submodes with $\omega \neq 0$. This is problematic and corresponds to the findings of Sect. 26.9.

27.4 Thuburn averaging

27.4.1 Requirements

In a planar triangular or hexagonal C-grid discretization, the velocity components are rotated by 120 or 60° with respect to each other, but the components are not defined at the same location. Therefore, the condition Eq. (27.18) not simply for the vector components, but only after interpolation to reference locations, for which the centers of the cells are used here. This interpolation is done using operators

$$\tilde{u}^{(i)} \quad (27.101)$$

with $1 \leq i \leq 3$, where u is any vector component. A separate averaging operator is permitted here for each spatial direction i . The conditions Eq. (27.18) can be expressed here in the form

$$\tilde{u}_1^{(1)} + \tilde{u}_2^{(2)} + \tilde{u}_3^{(3)} \stackrel{!}{=} 0, \quad \tilde{v}_1^{(1)} + \tilde{v}_2^{(2)} + \tilde{v}_3^{(3)} \stackrel{!}{=} 0 \quad (27.102)$$

note down. These equations are to be understood as requirements for vector fields $\mathbf{v}$. If gradient fields ∇a satisfy the condition Eq. (27.102) is not, so you have a problem, since the calculation of gradient fields is fixed on the C-grid. Therefore, the averaging of Eq. is used as a requirement for the averaging operator to be found. (27.22):

$$\widetilde{\delta_1 a}^{(1)} + \widetilde{\delta_2 a}^{(2)} + \widetilde{\delta_3 a}^{(3)} \stackrel{!}{=} 0 \quad (27.103)$$

27.4.2 Conclusions for the Helmholtz division

For the Helmholtz distribution Equations (27.55) - (27.60) follows by averaging in the relevant spatial directions

$$\widetilde{u}_1^{(1)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_3 \mathcal{Y}^{(1)}} - \widetilde{\partial_2 \mathcal{Y}^{(1)}} \right) + \widetilde{\partial_1 \mathcal{X}^{(1)}}, \quad (27.104)$$

$$\widetilde{u}_2^{(2)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_1 \mathcal{Y}^{(2)}} - \widetilde{\partial_3 \mathcal{Y}^{(2)}} \right) + \widetilde{\partial_2 \mathcal{X}^{(2)}}, \quad (27.105)$$

$$\widetilde{u}_3^3 = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_2 \mathcal{Y}^3} - \widetilde{\partial_1 \mathcal{Y}^3} \right) + \widetilde{\partial_3 \mathcal{X}^3}, \quad (27.106)$$

$$\widetilde{v}_1^{(1)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_2 \mathcal{X}^{(1)}} - \widetilde{\partial_3 \mathcal{X}^{(1)}} \right) + \widetilde{\partial_1 \mathcal{Y}^{(1)}}, \quad (27.107)$$

$$\widetilde{v}_2^{(2)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_3 \mathcal{X}^{(2)}} - \widetilde{\partial_1 \mathcal{X}^{(2)}} \right) + \widetilde{\partial_2 \mathcal{Y}^{(2)}}, \quad (27.108)$$

$$\widetilde{v}_3^3 = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_1 \mathcal{X}^3} - \widetilde{\partial_2 \mathcal{X}^3} \right) + \widetilde{\partial_3 \mathcal{Y}^3}. \quad (27.109)$$

This does not yet fulfill the equations (27.102) - (27.102), rather a preparatory averaging of the scalar fields is required:

$$\widetilde{u}_1^{(1)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_3 \widetilde{\mathcal{Y}^{(2)}}^{(1)}} - \widetilde{\partial_2 \widetilde{\mathcal{Y}^3}^{(1)}} \right) + \widetilde{\partial_1 \mathcal{X}^{(1)}} \quad (27.110)$$

$$\widetilde{u}_2^{(2)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_1 \widetilde{\mathcal{Y}^3}^{(2)}} - \widetilde{\partial_3 \widetilde{\mathcal{Y}^{(1)}}^{(2)}} \right) + \widetilde{\partial_2 \mathcal{X}^{(2)}} \quad (27.111)$$

$$\widetilde{u}_3^3 = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_2 \widetilde{\mathcal{Y}^{(1)}}^3} - \widetilde{\partial_1 \widetilde{\mathcal{Y}^{(2)}}^3} \right) + \widetilde{\partial_3 \mathcal{X}^3} \quad (27.112)$$

$$\widetilde{v}_1^{(1)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_2 \widetilde{\mathcal{X}^3}^{(1)}} - \widetilde{\partial_3 \widetilde{\mathcal{X}^{(2)}}^{(1)}} \right) + \widetilde{\partial_1 \mathcal{Y}^{(1)}} \quad (27.113)$$

$$\widetilde{v}_2^{(2)} = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_3 \widetilde{\mathcal{X}^{(1)}}^{(2)}} - \widetilde{\partial_1 \widetilde{\mathcal{X}^3}^{(2)}} \right) + \widetilde{\partial_2 \mathcal{Y}^{(2)}} \quad (27.114)$$

$$\widetilde{v}_3^3 = \frac{\mathbf{I}}{\sqrt{3}} \left(\widetilde{\partial_1 \widetilde{\mathcal{X}^{(2)}}^3} - \widetilde{\partial_2 \widetilde{\mathcal{X}^{(1)}}^3} \right) + \widetilde{\partial_3 \mathcal{Y}^3} \quad (27.115)$$

This implies

$$u_1 = \frac{\mathbf{I}}{\sqrt{3}} \left(\partial_3 \widetilde{\mathcal{Y}^{(2)}} - \partial_2 \widetilde{\mathcal{Y}^3} \right) + \partial_1 \mathcal{X}, \quad (27.116)$$

$$u_2 = \frac{\mathbf{I}}{\sqrt{3}} \left(\partial_1 \widetilde{\mathcal{Y}^3} - \partial_3 \widetilde{\mathcal{Y}^{(1)}} \right) + \partial_2 \mathcal{X}, \quad (27.117)$$

$$u_3 = \frac{\mathbf{I}}{\sqrt{3}} \left(\partial_2 \widetilde{\mathcal{Y}^{(1)}} - \partial_1 \widetilde{\mathcal{Y}^{(2)}} \right) + \partial_3 \mathcal{X}, \quad (27.118)$$

$$v_1 = \frac{\mathbf{I}}{\sqrt{3}} \left(\partial_2 \widetilde{\mathcal{X}^3} - \partial_3 \widetilde{\mathcal{X}^{(2)}} \right) + \partial_1 \mathcal{Y}, \quad (27.119)$$

$$v_2 = \frac{\mathbf{I}}{\sqrt{3}} \left(\partial_3 \widetilde{\mathcal{X}^{(1)}} - \partial_1 \widetilde{\mathcal{X}^3} \right) + \partial_2 \mathcal{Y}, \quad (27.120)$$

$$v_3 = \frac{\mathbf{I}}{\sqrt{3}} \left(\partial_1 \widetilde{\mathcal{X}^{(2)}} - \partial_2 \widetilde{\mathcal{X}^{(1)}} \right) + \partial_3 \mathcal{Y}. \quad (27.121)$$

27.4.3 Derivation of the averaging operator

Now the question arises as to what the averaging operator $\tilde{\psi}^{(j)}$ should actually look like. For the one in Eq. (27.73) operator applies

$$\begin{aligned}
 & \overline{\delta_1 \psi}^{(1)} + \overline{\delta_1 \psi}^{(2)} + \overline{\delta_1 \psi}^3 \\
 &= \psi(\mathbf{r}) \frac{2i}{d} \left[\sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_1 d}{2}\right) + \sin\left(\frac{k_2 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) + \sin\left(\frac{k_3 d}{2}\right) \cos\left(\frac{k_3 d}{2}\right) \right] \\
 &= \psi(\mathbf{r}) \frac{i}{d} \left[2 \sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_1 d}{2}\right) + 2 \sin\left(\frac{k_2 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) + 2 \sin\left(\frac{k_3 d}{2}\right) \cos\left(\frac{k_3 d}{2}\right) \right] \\
 &= \psi(\mathbf{r}) \frac{i}{d} [\sin(k_1 d) + \sin(k_2 d) + \sin(k_3 d)] \stackrel{\text{i. A.}}{\neq} 0.
 \end{aligned} \tag{27.122}$$

This operator satisfies the condition Eq. So (27.103) not. Therefore, a second averaging operator is defined

$$\overline{\psi}^{((1))} := \overline{\psi}^{(2,3)} = \overline{\psi}^{(2)} = \overline{\psi}^{(2)^3} = \psi(\mathbf{r}) \cos\left(\frac{k_2 d}{2}\right) \cos\left(\frac{k_3 d}{2}\right). \text{ (und zyklisch)} \tag{27.123}$$

This applies to this one

$$\begin{aligned}
 \overline{\delta_1 a}^{((1))} + \overline{\delta_2 a}^{((2))} + \overline{\delta_3 a}^{(3)} &= a(\mathbf{r}) \frac{2i}{d} \left[\sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) \cos\left(\frac{k_3 d}{2}\right) + \cos\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \cos\left(\frac{k_3 d}{2}\right) \right. \\
 &\quad \left. + \cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \right] \\
 &= a(\mathbf{r}) \frac{2i}{d} \left[\sin\left(\frac{k_1 d + k_2 d}{2}\right) \cos\left(\frac{k_3 d}{2}\right) + \cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \right] \\
 &= a(\mathbf{r}) \frac{2i}{d} \left[\sin\left(\frac{k_1 + k_2 + k_3}{2} d\right) - \cos\left(\frac{k_1 + k_2}{2} d\right) \sin\left(\frac{k_3}{2} d\right) \right. \\
 &\quad \left. + \cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \right].
 \end{aligned} \tag{27.124}$$

With $k_1 + k_2 + k_3 = 0$ follows

$$\begin{aligned}
 \overline{\delta_1 a}^{((1))} + \overline{\delta_2 a}^{((2))} + \overline{\delta_3 a}^{(3)} &= a(\mathbf{r}) \frac{2i}{d} \left[-\cos\left(\frac{k_1 + k_2}{2} d\right) \sin\left(\frac{k_3}{2} d\right) + \cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \right] \\
 &= a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_3}{2} d\right) \left[\cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) - \cos\left(\frac{k_1 + k_2}{2} d\right) \right] \\
 &= a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_3}{2} d\right) \left[\cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) - \cos\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) \right. \\
 &\quad \left. + \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \right] \\
 &= a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_1}{2} d\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \stackrel{\text{i. A.}}{\neq} 0.
 \end{aligned} \tag{27.125}$$

This operator also satisfies the condition Eq. So (27.103) not. However, one continues the calculation with $k_1 + k_2 + k_3 = 0$:

$$\begin{aligned}
\overline{\delta_1 a^{(1)}} + \overline{\delta_2 a^{(2)}} + \overline{\delta_3 a^{(3)}} &= a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \\
&= a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(-\frac{k_1 + k_2}{2} d\right) = -a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_1 + k_2}{2} d\right) \\
&= -a(\mathbf{r}) \frac{2i}{d} \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \left[\sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) + \cos\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \right] \\
&= -a(\mathbf{r}) \frac{2i}{d} \left[\sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_1 d}{2}\right)^2 \cos\left(\frac{k_2 d}{2}\right) + \sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) + \sin(k_1 d) - \sin(k_2 d) \cos\left(\frac{k_1 d}{2}\right)^2 - \sin(k_1 d) \cos\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) + \sin(k_1 d) - \sin(k_2 d) \cos(k_1) - \sin(k_1 d) \cos(k_2) + \sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 \right. \\
&\quad \left. + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) + \sin(k_1 d) - \sin[(k_1 + k_2) d] + \sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) + \sin(k_1 d) - \sin(-k_3 d) + \sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) + \sin(k_1 d) + \sin(k_3 d) + \sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \\
&= -\left(\overline{\delta_1 a^{(1)}} + \overline{\delta_2 a^{(2)}} + \overline{\delta_3 a^{(3)}}\right) - a(\mathbf{r}) \frac{i}{d} \left[\sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 \right] \tag{27.126}
\end{aligned}$$

Now you do the math

$$\begin{aligned}
\sin(k_2 d) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin(k_1 d) \sin\left(\frac{k_2 d}{2}\right)^2 &= \sin\left(\frac{k_2}{2} d + \frac{k_2}{2} d\right) \sin\left(\frac{k_1 d}{2}\right)^2 + \sin\left(\frac{k_1}{2} d + \frac{k_1}{2} d\right) \sin\left(\frac{k_2 d}{2}\right)^2 \\
&= 2 \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) + 2 \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_1 d}{2}\right) \\
&= \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \left[2 \sin\left(\frac{k_1 d}{2}\right) \cos\left(\frac{k_2 d}{2}\right) + 2 \cos\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \right] \\
&= \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_1 + k_2}{2} d\right) = \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(-\frac{k_3}{2} d\right) \\
&= -\sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right). \tag{27.127}
\end{aligned}$$

Thus follows

$$\begin{aligned}
\overline{\delta_1 a^{(1)}} + \overline{\delta_2 a^{(2)}} + \overline{\delta_3 a^{(3)}} &= -\left(\overline{\delta_1 a^{(1)}} + \overline{\delta_1 a^{(2)}} + \overline{\delta_1 a^{(3)}}\right) + a(\mathbf{r}) \frac{i}{d} \sin\left(\frac{k_1 d}{2}\right) \sin\left(\frac{k_2 d}{2}\right) \sin\left(\frac{k_3 d}{2}\right) \\
&\stackrel{\text{Glg. (27.125)}}{=} -\left(\overline{\delta_1 a^{(1)}} + \overline{\delta_1 a^{(2)}} + \overline{\delta_1 a^{(3)}}\right) + \frac{\mathbf{I}}{2} \left(\overline{\delta_1 a^{(1)}} + \overline{\delta_2 a^{(2)}} + \overline{\delta_3 a^{(3)}}\right) \\
&\Rightarrow \overline{\delta_1 a^{(1)}} + \overline{\delta_2 a^{(2)}} + \overline{\delta_3 a^{(3)}} = -\frac{\mathbf{I}}{2} \left(\overline{\delta_1 a^{(1)}} + \overline{\delta_1 a^{(2)}} + \overline{\delta_1 a^{(3)}}\right). \tag{27.128}
\end{aligned}$$

You now make the approach

$$\widetilde{a}^{(j)} = \beta \overline{a}^{(j)} + (\mathbf{1} - \beta) \overline{a}^{(j)} \quad (27.129)$$

with $\mathbf{o} \leq \beta \leq \mathbf{o}$. If you put Eq. (27.128), you get

$$\widetilde{\delta_1 a}^{(1)} + \widetilde{\delta_2 a}^{(2)} + \widetilde{\delta_3 a}^3 = \left(\beta - \frac{\mathbf{1}}{2} (\mathbf{1} - \beta) \right) \left(\overline{\delta_1 a}^{(1)} + \overline{\delta_1 a}^{(2)} + \overline{\delta_1 a}^3 \right) \stackrel{!}{=} \mathbf{o}. \quad (27.130)$$

This is fulfilled for

$$\begin{aligned} \beta - \frac{\mathbf{1}}{2} (\mathbf{1} - \beta) = \mathbf{o} &\Leftrightarrow \beta - \frac{\mathbf{1}}{2} + \frac{\beta}{2} = \frac{3\beta}{2} - \frac{\mathbf{1}}{2} = \mathbf{o} \\ &\Leftrightarrow \beta = \frac{\mathbf{1}}{3}. \end{aligned} \quad (27.131)$$

Therefore applies

$$\widetilde{a}^{(j)} = \frac{\mathbf{1}}{3} \overline{a}^{(j)} + \frac{2}{3} \overline{a}^{(j)}. \quad (27.132)$$

This operator is called the *Thuburn operator* because it was first used by Thuburn in [38].

27.4.4 Conclusions for the dispersion relation

The application of the Thuburn operator in the linearized shallow water equations on the hexagonal lattice equations (27.81) - (27.84) shows

$$\frac{\partial \Phi}{\partial t} + \frac{2}{3} \Phi_{\mathbf{o}} (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3) = \mathbf{o}, \quad (27.133)$$

$$\frac{\partial u_1}{\partial t} - \frac{f_{\mathbf{o}}}{\sqrt{3}} \left(\widetilde{u}_2^{(3)} - \widetilde{u}_3^{(2)} \right) + \delta_1 \Phi = \mathbf{o}, \quad (27.134)$$

$$\frac{\partial u_2}{\partial t} - \frac{f_{\mathbf{o}}}{\sqrt{3}} \left(\widetilde{u}_3^{(1)} - \widetilde{u}_1^{(3)} \right) + \delta_2 \Phi = \mathbf{o}, \quad (27.135)$$

$$\frac{\partial u_3}{\partial t} - \frac{f_{\mathbf{o}}}{\sqrt{3}} \left(\widetilde{u}_1^{(2)} - \widetilde{u}_2^{(1)} \right) + \delta_3 \Phi = \mathbf{o}. \quad (27.136)$$

From this it follows immediately

$$\frac{\partial}{\partial t} \left(\widetilde{u}_1^{(1)} + \widetilde{u}_2^{(2)} + \widetilde{u}_3^{(3)} \right) = \mathbf{o}. \quad (27.137)$$

The dispersion relation of this system of equations can be calculated analogously to the derivation of Eq. (27.96) by doing the substitution

$$c_1 \rightarrow a_1 := \frac{c_1 + 2c_2c_3}{3} \text{ (und zyklisch)} \quad (27.138)$$

carries out. This leads to

$$\omega^4 - \omega^2 \left[\frac{f_{\mathbf{o}}^2}{3} (a_1^2 + a_2^2 + a_3^2) + \frac{8\Phi_{\mathbf{o}}}{3d^2} (s_1^2 + s_2^2 + s_3^2) \right] + \frac{8\Phi_{\mathbf{o}}f_{\mathbf{o}}^2}{9d^2} (s_1a_1 + s_2a_2 + s_3a_3)^2 = \mathbf{o}. \quad (27.139)$$

If one sets $a = \exp(i\mathbf{k} \cdot \mathbf{r})$ in Eq. (27.103), you get

$$\frac{2i}{d} (a_1s_1 + a_2s_2 + a_3s_3) a = \mathbf{o} \Leftrightarrow a_1s_1 + a_2s_2 + a_3s_3 = \mathbf{o}. \quad (27.140)$$

Thus, Eq. (27.139) to

$$\omega^4 - \omega^2 \left[\frac{f_o^2}{3} (a_1^2 + a_2^2 + a_3^2) + \frac{8\Phi_o}{3d^2} (s_1^2 + s_2^2 + s_3^2) \right] = 0. \quad (27.141)$$

If you use Eq. (27.132) to reconstruct the tangential velocity components, thus creating a stationary geostrophic mode.

27.5 Checkerboard pattern

27.5.1 Reasons

On a regular hexagonal lattice with lattice constant d , a triangle has area

$$A_v = \frac{d}{2}l. \quad (27.142)$$

This applies

$$l = \cos(30^\circ) d = \frac{\sqrt{3}}{2}d, \quad (27.143)$$

from what

$$A_v = \frac{d^2 \sqrt{3}}{4} \quad (27.144)$$

follows. Thus, on a triangle (superscript t) that points upwards (index u), one can find the divergence according to Gauss's theorem in the form

$$D_u^{(t)} = -\frac{dv_1 + dv_2 + dv_3}{A_v} = -\frac{4}{\sqrt{3}d} (v_1 + v_2 + v_3) \quad (27.145)$$

calculate. The minus sign comes from the fact that in such a triangle the coordinate axes of the j -system point inwards. On a triangle that points downwards (index l), this is the other way around, it applies

$$D_l^{(t)} = \frac{dv_1 + dv_2 + dv_3}{A_v} = \frac{4}{\sqrt{3}d} (v_1 + v_2 + v_3). \quad (27.146)$$

This can be done in the form

$$D_{u,l}^{(t)} = \mp \frac{dv_1 + dv_2 + dv_3}{A_v} = \mp \frac{4}{\sqrt{3}d} (v_1 + v_2 + v_3) = \mp \frac{4}{\sqrt{3}d} \sum_{e \in t} v_e \quad (27.147)$$

summarize, where e denotes the edges of the triangle. Analogously, for the relative vorticity according to Stokes' theorem applies

$$\zeta_{u,l}^{(t)} = \pm \frac{du_1 + du_2 + du_3}{A_v} = \pm \frac{4}{\sqrt{3}d} \sum_{e \in t} u_e. \quad (27.148)$$

Let h now denote a hexagon. Then $u \in h$ denote the three upward-pointing triangles that overlap with the hexagon h under consideration and similarly $l \in h$ denote the three downward-pointing triangles that overlap with h . With these names you can

$$\frac{\sqrt{3}d}{4} \left(\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)} \right) = \sum_{l \in h} \sum_{e \in l} v_e + \sum_{u \in h} \sum_{e \in u} v_e = \sum_{l \in h} \left(\sum_{e \in l, e \in h} v_e + \sum_{e \in l, e \notin h} v_e \right) + \sum_{u \in h} \left(\sum_{e \in u, e \in h} v_e + \sum_{e \in u, e \notin h} v_e \right) \quad (27.149)$$

note down. During the last transformation step, the edges of the triangles were divided into those that are also edges of the hexagon under consideration ($e \in h$) and those that are not ($e \notin h$). Excluding results

$$\frac{\sqrt{3}d}{4} \left(\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)} \right) = \sum_{l \in h} \sum_{e \in l, e \in h} v_e + \sum_{l \in h} \sum_{e \in l, e \notin h} v_e + \sum_{u \in h} \sum_{e \in u, e \in h} v_e + \sum_{u \in h} \sum_{e \in u, e \notin h} v_e. \quad (27.150)$$

As can be seen, all velocity components with a positive sign contribute to $\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)}$. In the sums $\sum_{l \in h} \sum_{e \in l, e \in h}$ and $\sum_{u \in h} \sum_{e \in u, e \in h}$, each edge of the hexagon h occurs once. Therefore applies

$$\frac{\sqrt{3}d}{4} \left(\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)} \right) = \mathbf{2} \sum_{e \in h} v_e + \sum_{l \in h} \sum_{e \in l, e \notin h} v_e + \sum_{u \in h} \sum_{e \in u, e \notin h} v_e. \quad (27.151)$$

Those edges that do not border the hexagon under consideration each contribute once to $\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)}$:

$$\frac{\sqrt{3}d}{4} \left(\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)} \right) = \mathbf{2} \sum_{e \in h} v_e + \sum_{l \in h} \sum_{e \in l, e \notin h} v_e \quad (27.152)$$

At this point, consider the size $\tilde{v}_1^{(1)}$, which is defined in the center of the hexagon under consideration. This is a superposition of four velocity components, two of which lie on the $i-1$ axis and two perpendicular to it. The former contribute with the weight $\mathbf{1}/3$ to $\tilde{v}_1^{(1)}$, the latter with the weight $\mathbf{1}/6$. This can also be transferred cyclically to the other spatial directions. Therefore applies

$$\frac{\sqrt{3}d}{4} \left(\sum_{l \in h} D_l^{(t)} - \sum_{u \in h} D_u^{(t)} \right) = 6 \left(\tilde{v}_1^{(1)} + \tilde{v}_2^{(2)} + \tilde{v}_3^{(3)} \right). \quad (27.153)$$

If the condition $\tilde{v}_1^{(1)} + \tilde{v}_2^{(2)} + \tilde{v}_3^{(3)} = \mathbf{o}$ is not met, then the mean of the divergence of the three upward-pointing triangles is $\mathbf{i}$. A. not equal to the mean of the divergence of the downward triangles. This leads to the creation of a so-called *Checkerboard pattern* in the divergence. This noise propagates from there to other fields. It is therefore important to always adhere to the condition $\tilde{v}_1^{(1)} + \tilde{v}_2^{(2)} + \tilde{v}_3^{(3)} = \mathbf{o}$.

On the hexagonal grid, the train of thought can be transferred completely analogously to the relative vorticity, which is based on

$$\frac{\sqrt{3}d}{4} \left(\sum_{u \in h} \zeta_u^{(t)} - \sum_{l \in h} \zeta_l^{(t)} \right) = 6 \left(\tilde{u}_1^{(1)} + \tilde{u}_2^{(2)} + \tilde{u}_3^{(3)} \right) \quad (27.154)$$

leads. Failure to comply with the condition $\tilde{u}_1^{(1)} + \tilde{u}_2^{(2)} + \tilde{u}_3^{(3)} = \mathbf{o}$ also leads to a checkerboard pattern on the hexagonal grid (but here in the vorticity) and must therefore also be taken into account here.

27.5.2 Elimination

In the previous section it was shown that a checkerboard pattern exists on the hexagonal grid in the vorticity calculated on triangles if the condition $\tilde{u}_1^{(1)} + \tilde{u}_2^{(2)} + \tilde{u}_3^{(3)} = \mathbf{o}$ for the wind field $\mathbf{v}$ is not met. However, in order for this condition for the wind field to be fulfilled for all time steps, this must apply to the wind field in the initial state as well as to all forcings $\mathbf{w}$. However, simulations are usually carried out with momentum diffusion to avoid a build-up of kinetic energy on the grid scale. These diffusive terms break down gradients on the grid scale and can therefore also break down an existing checkerboard pattern as long as it is not too strong. Accordingly, the requirement $\tilde{u}_1^{(1)} + \tilde{u}_2^{(2)} + \tilde{u}_3^{(3)} = \mathbf{o}$ for the initial wind field $\mathbf{v}$ can be dispensed with. However, the following is important:

For all velocity tendencies $\mathbf{w}$ $\tilde{w}_1^{(1)} + \tilde{w}_2^{(2)} + \tilde{w}_3^{(3)} = \mathbf{o}$ must hold.

The analogous facts apply on the triangular grid.

27.6 Conclusions

27.6.1 Formulation of rotation

If you apply the Laplace operator to equations (27.116) - (27.118), you get

$$\Delta u_1 = \frac{1}{\sqrt{3}} \left(\partial_3 \Delta \tilde{\psi}^{(2)} - \partial_2 \Delta \tilde{\psi}^{(3)} \right) + \partial_1 \Delta \chi, \quad (27.155)$$

$$\Delta u_2 = \frac{1}{\sqrt{3}} \left(\partial_1 \Delta \tilde{\psi}^{(3)} - \partial_3 \Delta \tilde{\psi}^{(1)} \right) + \partial_2 \Delta \chi, \quad (27.156)$$

$$\Delta u_3 = \frac{1}{\sqrt{3}} \left(\partial_2 \Delta \tilde{\psi}^{(1)} - \partial_1 \Delta \tilde{\psi}^{(2)} \right) + \partial_3 \Delta \chi. \quad (27.157)$$

Since discretized partial derivatives and averaging operators swap, it follows immediately

$$\widetilde{\Delta u_1^{(1)}} + \widetilde{\Delta u_2^{(2)}} + \widetilde{\Delta u_3^{(3)}} = 0. \quad (27.158)$$

If you discretize the equations (27.62) - (27.64), you get

$$\Delta u_1 = \frac{1}{\sqrt{3}} (\partial_3 \zeta - \partial_2 \zeta) + \partial_1 D, \quad (27.159)$$

$$\Delta u_2 = \frac{1}{\sqrt{3}} (\partial_1 \zeta - \partial_3 \zeta) + \partial_2 D, \quad (27.160)$$

$$\Delta u_3 = \frac{1}{\sqrt{3}} (\partial_2 \zeta - \partial_1 \zeta) + \partial_3 D. \quad (27.161)$$

By comparison, one finds that there are three types of vorticities in the $\mathbf{i}$ system:

$$\zeta_1 := \Delta \tilde{\psi}^{(1)}, \quad \zeta_2 := \Delta \tilde{\psi}^{(2)}, \quad \zeta_3 := \Delta \tilde{\psi}^{(3)} \quad (27.162)$$

It therefore applies

$$\Delta u_1 = \frac{1}{\sqrt{3}} (\partial_3 \zeta_2 - \partial_2 \zeta_3) + \partial_1 D, \quad (27.163)$$

$$\Delta u_2 = \frac{1}{\sqrt{3}} (\partial_1 \zeta_3 - \partial_3 \zeta_1) + \partial_2 D, \quad (27.164)$$

$$\Delta u_3 = \frac{1}{\sqrt{3}} (\partial_2 \zeta_1 - \partial_1 \zeta_2) + \partial_3 D. \quad (27.165)$$

For the divergence, according to Eq. (27.33)

$$D = \frac{2}{3} (\partial_1 u_1 + \partial_2 u_2 + \partial_3 u_3). \quad (27.166)$$

If you insert this into the equations (27.163) - (27.165), you get

$$\Delta u_1 = \frac{1}{\sqrt{3}} (\partial_3 \zeta_2 - \partial_2 \zeta_3) + \frac{2}{3} (\partial_1 \partial_1 u_1 + \partial_1 \partial_2 u_2 + \partial_1 \partial_3 u_3), \quad (27.167)$$

$$\Delta u_2 = \frac{1}{\sqrt{3}} (\partial_1 \zeta_3 - \partial_3 \zeta_1) + \frac{2}{3} (\partial_2 \partial_1 u_1 + \partial_2 \partial_2 u_2 + \partial_2 \partial_3 u_3), \quad (27.168)$$

$$\Delta u_3 = \frac{1}{\sqrt{3}} (\partial_2 \zeta_1 - \partial_1 \zeta_2) + \frac{2}{3} (\partial_3 \partial_1 u_1 + \partial_3 \partial_2 u_2 + \partial_3 \partial_3 u_3). \quad (27.169)$$

For the vorticities ζ_i , the approaches are made, motivated by the equations (27.49) - (27.51)

$$\zeta_1 = \frac{2}{\sqrt{3}} (\delta_2 u_3 - \delta_3 u_2), \quad (27.170)$$

$$\zeta_2 = \frac{2}{\sqrt{3}} (\delta_3 u_1 - \delta_1 u_3), \quad (27.171)$$

$$\zeta_3 = \frac{2}{\sqrt{3}} (\delta_1 u_2 - \delta_2 u_1). \quad (27.172)$$

If you put Eq. (27.170) in Eq. (27.167), you get

$$\Delta u_1 = \frac{2}{3} (\delta_3 \delta_3 u_1 - \delta_3 \delta_1 u_3 - \delta_2 \delta_1 u_2 + \delta_2 \delta_2 u_1) + \frac{2}{3} (\delta_1 \delta_1 u_1 + \delta_1 \delta_2 u_2 + \delta_1 \delta_3 u_3) = \frac{2}{3} (\delta_1 \delta_1 u_1 + \delta_2 \delta_2 u_1 + \delta_3 \delta_3 u_1). \quad (27.173)$$

By cyclically swapping, the analogous statement is also obtained for the other components. The approaches of the equations (27.170) - (27.172) are therefore justified. Two neighboring triangles together form a rhombus (a parallelogram), according to Eq. (27.144) the area

$$A_r = 2A_v = 2 \frac{d^2 \sqrt{3}}{4} = \frac{d^2 \sqrt{3}}{2}. \quad (27.174)$$

Thus, ζ_i corresponds to the vorticity calculated using Stokes' theorem over a rhombus whose short axis of symmetry is parallel to the i -axis. On the hexagonal grid, the rhombuses form the natural sets on which Stokes' theorem must be evaluated. This is a deviation from the actually intuitive assumption that the vorticity must be calculated via the dual grid (the triangular grid).

As usual, divergence and vorticity appear in reversed roles on the triangular grid. The vorticity has the clear value there

$$\zeta = \frac{2}{3} (\delta_1 v_1 + \delta_2 v_2 + \delta_3 v_3) \quad (27.175)$$

However, three types of divergences occur there, each of which is calculated using Gauss's theorem over the respective rhombuses:

$$D_1 = \frac{2}{\sqrt{3}} (\delta_3 v_2 - \delta_2 v_3) \quad (27.176)$$

$$D_2 = \frac{2}{\sqrt{3}} (\delta_1 v_3 - \delta_3 v_1) \quad (27.177)$$

$$D_3 = \frac{2}{\sqrt{3}} (\delta_2 v_1 - \delta_1 v_2) \quad (27.178)$$

This is also achieved by the discretization of the vector Laplace operator according to Eq. (B.54) underlined which

$$\Delta \mathbf{v} = \nabla (\nabla \cdot \mathbf{v}) - \nabla \times (\nabla \times \mathbf{v}) \quad (27.179)$$

is. Applying this to the vector component u_1 gives

$$\Delta u_1 = \delta_1 D_h - \delta_{i,\perp} \zeta_t. \quad (27.180)$$

Here D_h is the divergence on hexagons and ζ_t is the vorticity on triangles. $\delta_{i,\perp}$ denotes the central difference quotient in the $\mathbf{j}_i$ -direction. This applies to this one

$$-\delta_{i,\perp} \zeta_t = \frac{\sqrt{3}}{d} (\zeta_{t,l} - \zeta_{t,u}). \quad (27.181)$$

From Eq. (27.163) follows

$$\begin{aligned}
\Delta u_1 &= \delta_1 D_h + \frac{\sqrt{3}}{d} (\zeta_{t,l} - \zeta_{t,u}) = \delta_1 D_h + \frac{\mathbf{I}}{\sqrt{3}} (\delta_3 \zeta_2 - \delta_2 \zeta_3) \\
&\Leftrightarrow \sqrt{3} \frac{\zeta_{t,l} - \zeta_{t,u}}{d} = \frac{\sqrt{3}}{3} (\delta_3 \zeta_2 - \delta_2 \zeta_3) \Leftrightarrow \sqrt{3} \frac{\zeta_{t,l} - \zeta_{t,u}}{d} = \frac{\sqrt{3}}{3} \frac{\zeta_{2,l} - \zeta_{2,u} - \zeta_{3,u} + \zeta_{3,l}}{d} \\
&\Leftrightarrow \sqrt{3} \frac{\zeta_{t,l} - \zeta_{t,u}}{d} = \frac{\sqrt{3}}{3} \frac{\zeta_{2,l} + \zeta_{3,l} - (\zeta_{2,u} - \zeta_{3,u})}{d} \\
&\Leftrightarrow \sqrt{3} \frac{\zeta_{t,l} - \zeta_{t,u}}{d} = \frac{\sqrt{3}}{3} \frac{\zeta_{1,l} + \zeta_{2,l} + \zeta_{3,l} - (\zeta_{1,u} + \zeta_{2,u} - \zeta_{3,u})}{d}.
\end{aligned} \tag{27.182}$$

The final equivalent transformation follows from the fact $\zeta_{1,l} = \zeta_{1,u}$. This is with the definitions

$$\zeta_{t,u} := \frac{\zeta_{1,u} + \zeta_{2,u} + \zeta_{3,u}}{3}, \tag{27.183}$$

$$\zeta_{t,l} := \frac{\zeta_{1,l} + \zeta_{2,l} + \zeta_{3,l}}{3} \tag{27.184}$$

fulfilled. The rotation on a triangle can therefore be calculated as the average of the three rhombuses that overlap with this triangle.

27.6.2 Another perspective on the superiority of the hexagonal grid over the triangular one

On the hexagonal C-lattice, gradient fields $\mathbf{u} = \nabla \psi$ satisfy the condition

$$\tilde{u}_1^{(1)} + \tilde{u}_2^{(2)} + \tilde{u}_3^3 = \mathbf{o}. \tag{27.185}$$

On the triangular C-lattice, a gradient field $\mathbf{v} = \nabla \psi$ naturally has components parallel to the basis elements $\mathbf{j}_i$. This fulfills

$$\tilde{v}_1^{(1)} + \tilde{v}_2^{(2)} + \tilde{v}_3^3 = \mathbf{o} \tag{27.186}$$

not, as one can easily see. Therefore, gradient fields on the triangular C-lattice produce according to Eq. (27.153) a checkerboard pattern in divergence, which would require unphysical numerical stabilizers such as divergence damping. Therefore, this grid was rightly excluded in Section 26.9.1. This finding was first put forward by Gassmann in [13].

The generalized Coriolis term

$$\mathbf{v} \times \boldsymbol{\eta} = \mathbf{v} \times (\mathbf{f} + \boldsymbol{\xi}) = \mathbf{v} \times (\mathbf{f} + \nabla \times \mathbf{v}) \quad (28.1)$$

requires special attention on a C-lattice. In particular, the following three questions must be answered:

1. Over which polygon must Stokes' theorem be evaluated to calculate the vorticity?
2. How must the tangential wind component on an edge be reconstructed from the normal wind components on the surrounding edges?
3. By what vorticity must the tangential wind component ultimately be multiplied to obtain a component of $\mathbf{v} \times \boldsymbol{\eta}$?

In this chapter, these questions will first be considered in the light of the shallow water equations (SWEs).. The SWEs are without friction

$$\frac{\partial \mathbf{v}}{\partial t} \stackrel{\text{Glg. (13.171)}}{=} -g \nabla (h + b) - f \mathbf{k} \times \mathbf{v} - \nabla k - \boldsymbol{\zeta} \mathbf{k} \times \mathbf{v} + \mu \mathbf{k}, \quad (28.2)$$

$$\frac{\partial h}{\partial t} \stackrel{\text{Glg. (13.172)}}{=} -\nabla \cdot (h \mathbf{v}), \quad (28.3)$$

where $\mathbf{v}$ is the velocity, g is the gravitational acceleration, h is the deflection of the surface from the rest position, f is the Coriolis parameter, $\mathbf{k}$ is the vertical unit vector, $k := \frac{1}{2} \mathbf{v}^2$ is the specific kinetic energy, $\boldsymbol{\zeta} := \mathbf{k} \cdot (\nabla \times \mathbf{v})$ the relative vorticity and μ a Lagrange multiplier which, in the case of a curved set such as a sphere, ensures that the right-hand side of the equation is tangent to that set. The red terms are the momentum advection terms, which are also the nonlinear terms. Thus, the linearized momentum equation of the SWEs is

$$\frac{\partial \mathbf{v}}{\partial t} = -g \nabla (h + b) - f \mathbf{k} \times \mathbf{v}. \quad (28.4)$$

If you project Eq. (28.2) to a normal vector $\mathbf{n}$ of an edge, one obtains

$$\frac{\partial v_n}{\partial t} = -g \frac{\partial (h + b)}{\partial n} - f \mathbf{n} \cdot (\mathbf{k} \times \mathbf{v}) - \frac{\partial k}{\partial n} - \boldsymbol{\zeta} \mathbf{n} \cdot (\mathbf{k} \times \mathbf{v}), \quad (28.5)$$

is there

$$v_n := \mathbf{n} \cdot \mathbf{v} \quad (28.6)$$

the normal velocity component at the edge. $\partial/\partial n$ denote partial derivatives perpendicular to the edge. With Eq. (A.159) is obtained

$$\mathbf{n} \cdot (\mathbf{k} \times \mathbf{v}) = \mathbf{v} \cdot (\mathbf{n} \times \mathbf{k}) \stackrel{\text{Glg. (A.149)}}{=} -\mathbf{v} \cdot (\mathbf{k} \times \mathbf{n}) = -\mathbf{v} \cdot \mathbf{t} = -v_t, \quad (28.7)$$

where $\mathbf{t} := \mathbf{k} \times \mathbf{n}$ is the tangential unit vector on the edge and

$$v_t := \mathbf{v} \cdot \mathbf{t} \quad (28.8)$$

the tangential velocity component at the edge. Therefore applies

$$\frac{\partial v_n}{\partial t} = -g \frac{\partial (h + b)}{\partial n} + (f + \boldsymbol{\zeta}) v_t - \frac{\partial k}{\partial n}. \quad (28.9)$$

The linear part of this is

$$\frac{\partial v_n}{\partial t} = -g \frac{\partial (h + b)}{\partial n} + f v_t. \quad (28.10)$$

The vorticity and divergence dynamics of the SWEs can be summarized in the equations (13.172) and (15.170):

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\mathbf{v}) = \mathbf{o}, \quad \frac{\partial (hq)}{\partial t} + \nabla \cdot (hq\mathbf{v}) = \mathbf{o} \quad (28.11)$$

From the second equation (this is a form of the barotropic vorticity equation) one can

$$\frac{d}{dt} \int_{4\pi} hq d\omega = \int_{4\pi} \frac{\partial (hq)}{\partial t} d\omega = - \int_{4\pi} \nabla \cdot (hq\mathbf{v}) d\omega \quad (28.12)$$

conclude. The integral over the divergence of the potential vorticity flux density over the unit sphere can be evaluated by adding a third dimension in the form of a thin spherical shell of thickness Δr . No potential vorticity flows through the vertical edges of this set, since in the SWEs $w = \mathbf{o}$. Thus follows

$$\frac{d}{dt} \int_{4\pi} hq d\omega = \mathbf{o}. \quad (28.13)$$

The global integral of the incompressible potential vorticity q is therefore constant.

28.1 Regular grid

The vorticity flow term of the shallow water equations is

$$-(f + \zeta) \mathbf{k} \times \mathbf{v}. \quad (28.14)$$

In this section we want to find a discretization that satisfies the Thuburn condition and thus according to Eq. (27.141) also has a geostrophic mode. If you project this onto the normal vector $\mathbf{n}$ of an edge, you get according to Eq. (28.7)

$$-[(f + \zeta) \mathbf{k} \times \mathbf{v}] \cdot \mathbf{n} = (f + \zeta) v_t. \quad (28.15)$$

This term is now linearized in the form

$$(f + \zeta) v_t \rightarrow f_{\circ} v_t + \zeta U_t, \quad (28.16)$$

here is

$$U_t := (\mathbf{k} \times \mathbf{n}) \cdot U\mathbf{i} \quad (28.17)$$

the projection of a homogeneous zonal base current U on the tangential direction. One now orientates oneself on the notations from Chap. 27. There, for the term $f v_t$ according to Eq. (27.134) the discretization

$$f_{\circ} v_t \rightarrow \frac{f_{\circ}}{\sqrt{3}} \left(\tilde{u}_2^{(3)} - \tilde{u}_3^{(2)} \right) \quad (28.18)$$

derived. According to Eq. (27.137) the Thuburn condition Eq. (27.102). For the term ζU_t one sets with

$$U_{t,1} = \mathbf{o}, \quad (28.19)$$

$$U_{t,2} = -\zeta_2 \frac{\sqrt{3}}{2} U, \quad (28.20)$$

$$U_{t,3} = -\zeta_3 \frac{\sqrt{3}}{2} U \quad (28.21)$$

at the edges in the x_i -direction initially

$$(\zeta U_t)_1 = 0, \quad (28.22)$$

$$(\zeta U_t)_2 = -\zeta_2 \frac{\sqrt{3}}{2} U, \quad (28.23)$$

$$(\zeta U_t)_3 = -\zeta_3 \frac{\sqrt{3}}{2} U \quad (28.24)$$

to. These terms must also satisfy the Thuburn condition. One expects to be checked

$$\widetilde{(\zeta U_t)}_1^{(1)} + \widetilde{(\zeta U_t)}_2^{(2)} + \widetilde{(\zeta U_t)}_3^{(3)} = -\frac{\sqrt{3}}{2} U \left(\tilde{\zeta}_2^{(2)} + \tilde{\zeta}_3^{(3)} \right) \stackrel{\text{i. A.}}{\neq} 0. \quad (28.25)$$

Inspired by Eq. (27.134) one modifies the approach of the equations (28.19) - (28.21)

$$(\zeta U_t)_1 = \frac{1}{\sqrt{3}} \left(-\zeta_2 \frac{U}{2} + \zeta_3 \frac{U}{2} \right), \quad (28.26)$$

$$(\zeta U_t)_2 = \frac{1}{\sqrt{3}} \left(-\zeta_3 \frac{U}{2} + \zeta_1 U \right), \quad (28.27)$$

$$(\zeta U_t)_3 = \frac{1}{\sqrt{3}} \left(-\zeta_1 U + \zeta_2 \frac{U}{2} \right). \quad (28.28)$$

From this it follows

$$\begin{aligned} \widetilde{(\zeta U_t)}_1^{(1)} + \widetilde{(\zeta U_t)}_2^{(2)} + \widetilde{(\zeta U_t)}_3^{(3)} &\propto \widetilde{\zeta_3 - \zeta_2}^{(1)} + \widetilde{2\zeta_1 - \zeta_3}^{(2)} + \widetilde{\zeta_2 - 2\zeta_1}^{(3)} \\ &= -\tilde{\zeta}_2^{(1)} + \tilde{\zeta}_3^{(1)} - \tilde{\zeta}_3^{(2)} + 2\tilde{\zeta}_1^{(2)} - 2\tilde{\zeta}_1^{(3)} + \tilde{\zeta}_2^{(3)} \stackrel{\text{i. A.}}{\neq} 0. \end{aligned} \quad (28.29)$$

This approach also does not satisfy the Thuburn condition. Rather, a preparatory averaging of the vorticities is required, which leads to the approach

$$(\zeta U_t)_1 = \frac{1}{\sqrt{3}} \left(-\bar{\zeta}_2^{(3)} \frac{U}{2} + \bar{\zeta}_3^{(2)} \frac{U}{2} \right), \quad (28.30)$$

$$(\zeta U_t)_2 = \frac{1}{\sqrt{3}} \left(-\bar{\zeta}_3^{(1)} \frac{U}{2} + \bar{\zeta}_1^{(3)} U \right), \quad (28.31)$$

$$(\zeta U_t)_3 = \frac{1}{\sqrt{3}} \left(-\bar{\zeta}_1^{(2)} U + \bar{\zeta}_2^{(1)} \frac{U}{2} \right). \quad (28.32)$$

This satisfies the Thuburn condition since averaging operators commute. An operator other than the simple averaging operator $\bar{\zeta}_i^{(j)}$ can also be used. With $\zeta \rightarrow \eta = \zeta + f$ the complete vorticity flow term on the regular C lattice can be expressed as follows.

28.2 Deformed grid

28.2.1 Coriolis acceleration

28.2.1.1 Homogeneous Coriolis parameter

It is not trivial how to extend the vorticity flow term to the deformed grid. To do this, we first start from the f-plane in order to be able to assume a homogeneous vorticity f_0 . Rather than attempting to generalize the Thuburn condition to the deformed grid, the closely related statement is used as a basic requirement that a geostrophic mode should exist. Furthermore, the discretization should be energy-conserving.

- 28.2.1.2 Inhomogeneous Coriolis parameter
- 28.2.2 Using full vorticity
 - 28.2.2.1 Modification to comply with the Thuburn condition

29 MOMENTUM DIFFUSION AND DISSIPATION ON THE HEXAGONAL C-LATTICE

The aim of this chapter is to discretize the momentum diffusion and dissipation on the three-dimensional deformed C-lattice.

29.1 Regular grid

First of all, the aim is to discretize the momentum diffusion within the framework of the shallow water equations on the two-dimensional regular hexagonal lattice. In the two-dimensional case, according to Eq. (8.50) for the frictional acceleration

$$\frac{\partial \mathbf{v}_{\text{diff}}}{\partial t} = \frac{1}{h} \nabla \cdot \left[{}_2K \begin{pmatrix} S_{1,1} & S_{1,2} \\ S_{2,1} & S_{2,2} \end{pmatrix} \right] = \frac{1}{h} \nabla \cdot \left[K \begin{pmatrix} {}_2 \frac{\partial v_1}{\partial x_1} & \frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \\ \frac{\partial v_2}{\partial x_1} + \frac{\partial v_1}{\partial x_2} & {}_2 \frac{\partial v_2}{\partial x_2} \end{pmatrix} \right]. \quad (29.1)$$

Here, the density ρ was replaced by the layer thickness h , K is a general mass-weighted diffusion coefficient. The three-dimensional divergence $\nabla \cdot \mathbf{v}$ disappears in the incompressible case. As an approach for discretization one uses

$$\frac{\partial \mathbf{v}_{\text{diff}}^T}{\partial t} = (\delta_1, \delta_2, \delta_3) \cdot \tau = (\delta_1, \delta_2, \delta_3) \cdot \begin{pmatrix} \tau_{1,1} & \tau_{1,2} & \tau_{1,3} \\ \tau_{2,1} & \tau_{2,2} & \tau_{2,3} \\ \tau_{3,1} & \tau_{3,2} & \tau_{3,3} \end{pmatrix} \quad (29.2)$$

The aim of this section is to clearly determine the $\tau_{i,j}$. Motivated by Eq. (29.1) requires the symmetry of τ , so

$$\tau_{i,j} = \tau_{j,i}. \quad (29.3)$$

The tensor τ is developed in several modifying interactions. You start first

$$\tau = K \begin{pmatrix} {}_2 \delta_1 u_1 & \delta_2 u_1 + \delta_1 u_2 & \delta_3 u_1 + \delta_1 u_3 \\ \delta_2 u_1 + \delta_1 u_2 & {}_2 \delta_2 u_2 & \delta_3 u_2 + \delta_2 u_3 \\ \delta_3 u_1 + \delta_1 u_3 & \delta_3 u_2 + \delta_2 u_3 & {}_2 \delta_3 u_3 \end{pmatrix}. \quad (29.4)$$

From this it follows

$$\begin{aligned} \frac{\partial u_{1,\text{diff}}}{\partial t} &= K [\delta_1 ({}_2 \delta_1 u_1) + \delta_2 (\delta_2 u_1 + \delta_1 u_2) + \delta_3 (\delta_3 u_1 + \delta_1 u_3)] \\ &= K (\delta_{1,1} u_1 + \delta_{1,1} u_1 + \delta_{2,2} u_1 + \delta_{3,3} u_1 + \delta_{2,1} u_2 + \delta_{3,1} u_3) \\ &= K [\delta_{1,1} u_1 + \delta_{2,2} u_1 + \delta_{3,3} u_1 + \delta_1 (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3)] = K \left(\frac{3}{2} \Delta u_1 + \frac{3}{2} \delta_1 D \right). \end{aligned} \quad (29.5)$$

It follows from this

$$\tau = K \begin{pmatrix} \frac{4}{3} \delta_1 u_1 & \frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) & \frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) \\ \frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) & \frac{4}{3} \delta_2 u_2 & \frac{2}{3} (\delta_3 u_2 + \delta_2 u_3) \\ \frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) & \frac{2}{3} (\delta_3 u_2 + \delta_2 u_3) & \frac{4}{3} \delta_3 u_3 \end{pmatrix} \quad (29.6)$$

for frictional acceleration

$$\frac{\partial u_{1,\text{diff}}}{\partial t} = K (\Delta u_1 + \delta_1 D). \quad (29.7)$$

The term proportional to $\delta_1 D$ does not occur in the shallow water equations, since these describe an incompressible medium, and should therefore be eliminated or at least reduced if possible. The terms that are not on the diagonal must not be modified in order not to destroy the symmetry of the tensor. Therefore one starts with a parameter $0 \leq a \leq 1$

$$\begin{aligned}
 \tau &= K \begin{pmatrix} \frac{4}{3}\delta_1 u_1 - aD & \frac{2}{3}(\delta_2 u_1 + \delta_1 u_2) & \frac{2}{3}(\delta_3 u_1 + \delta_1 u_3) \\ \frac{2}{3}(\delta_2 u_1 + \delta_1 u_2) & \frac{4}{3}\delta_2 u_2 - aD & \frac{2}{3}(\delta_3 u_2 + \delta_2 u_3) \\ \frac{2}{3}(\delta_3 u_1 + \delta_1 u_3) & \frac{2}{3}(\delta_3 u_2 + \delta_2 u_3) & \frac{4}{3}\delta_3 u_3 - aD \end{pmatrix} \\
 &= K \begin{pmatrix} \frac{2}{3}(2-a)\delta_1 u_1 - a\frac{2}{3}(\delta_2 u_2 + \delta_3 u_3) & \frac{2}{3}(\delta_2 u_1 + \delta_1 u_2) & \frac{2}{3}(\delta_3 u_1 + \delta_1 u_3) \\ \frac{2}{3}(\delta_2 u_1 + \delta_1 u_2) & \frac{2}{3}(2-a)\delta_2 u_2 - a\frac{2}{3}(\delta_1 u_1 + \delta_3 u_3) & \frac{2}{3}(\delta_3 u_2 + \delta_2 u_3) \\ \frac{2}{3}(\delta_3 u_1 + \delta_1 u_3) & \frac{2}{3}(\delta_3 u_2 + \delta_2 u_3) & \frac{2}{3}(2-a)\delta_3 u_3 - a\frac{2}{3}(\delta_1 u_1 + \delta_2 u_2) \end{pmatrix}.
 \end{aligned} \tag{29.8}$$

It now follows from this

$$\frac{\partial u_{1,\text{diff}}}{\partial t} = K[\Delta u_1 + (1-a)\delta_1 D]. \tag{29.9}$$

The factor $1-a$ should be as close to zero as possible, so a should be as close to one as possible. According to Eq. (8.66) applies to the dissipation rate

$$\begin{aligned}
 \frac{3}{2}h\varepsilon &= \frac{2}{3}(2-a)(\delta_1 u_1)^2 - a\frac{2}{3}(\delta_1 u_1 \delta_2 u_2 + \delta_1 u_1 \delta_3 u_3) + \frac{2}{3}(\delta_1 u_2 \delta_2 u_1 + \delta_1 u_2 \delta_1 u_2) + \frac{2}{3}(\delta_1 u_3 \delta_3 u_1 + \delta_1 u_3 \delta_1 u_3) \\
 &+ \frac{2}{3}(\delta_2 u_1 \delta_3 u_1 + \delta_2 u_1 \delta_1 u_2) + \frac{2}{3}(2-a)(\delta_2 u_2)^2 - a\frac{2}{3}(\delta_2 u_2 \delta_1 u_1 + \delta_2 u_2 \delta_3 u_3) + \frac{2}{3}(\delta_2 u_3 \delta_3 u_2 + \delta_2 u_3 \delta_2 u_3) \\
 &+ \frac{2}{3}(\delta_3 u_1 \delta_3 u_1 + \delta_3 u_1 \delta_1 u_3) + \frac{2}{3}(\delta_3 u_2 \delta_3 u_2 + \delta_3 u_2 \delta_2 u_3) + \frac{2}{3}(2-a)(\delta_3 u_3)^2 - a\frac{2}{3}(\delta_3 u_3 \delta_1 u_1 + \delta_3 u_3 \delta_2 u_2) \\
 &= \frac{2}{3}(2-a)(\delta_1 u_1)^2 - a\frac{2}{3}(\delta_1 u_1 \delta_2 u_2 + \delta_1 u_1 \delta_3 u_3) + \frac{2}{3}(\delta_2 u_1 + \delta_1 u_2)^2 + \frac{2}{3}(\delta_3 u_1 + \delta_1 u_3)^2 \\
 &+ \frac{2}{3}(2-a)(\delta_2 u_2)^2 - a\frac{2}{3}(\delta_2 u_2 \delta_1 u_1 + \delta_2 u_2 \delta_3 u_3) + \frac{2}{3}(\delta_3 u_2 + \delta_2 u_3)^2 \\
 &+ \frac{2}{3}(2-a)(\delta_3 u_3)^2 - a\frac{2}{3}(\delta_3 u_3 \delta_1 u_1 + \delta_3 u_3 \delta_2 u_2).
 \end{aligned} \tag{29.10}$$

The **red** marked terms arise from the non-diagonal elements and are all square and therefore non-negative. applies to the remaining terms

$$\begin{aligned}
 &\frac{2}{3}(2-a)(\delta_1 u_1)^2 - a\frac{2}{3}(\delta_1 u_1 \delta_2 u_2 + \delta_1 u_1 \delta_3 u_3) + \frac{2}{3}(2-a)(\delta_2 u_2)^2 - a\frac{2}{3}(\delta_2 u_2 \delta_1 u_1 + \delta_2 u_2 \delta_3 u_3) \\
 &+ \frac{2}{3}(2-a)(\delta_3 u_3)^2 - a\frac{2}{3}(\delta_3 u_3 \delta_1 u_1 + \delta_3 u_3 \delta_2 u_2) \\
 &= \frac{2}{3}(2-a)(\delta_1 u_1)^2 + \frac{2}{3}(2-a)(\delta_2 u_2)^2 + \frac{2}{3}(2-a)(\delta_3 u_3)^2 - a\frac{4}{3}(\delta_1 u_1 \delta_2 u_2 + \delta_1 u_1 \delta_3 u_3 + \delta_2 u_2 \delta_3 u_3) \\
 &\stackrel{!}{=} a\frac{2}{3}(\delta_1 u_1 - \delta_2 u_2)^2 + a\frac{2}{3}(\delta_1 u_1 - \delta_3 u_3)^2 + a\frac{2}{3}(\delta_2 u_2 - \delta_3 u_3)^2.
 \end{aligned} \tag{29.11}$$

The requirement in the last step is based on wanting to obtain a non-negative dissipation rate. It turns out

$$\frac{2}{3}(2-a) = \frac{4}{3}a \Leftrightarrow \frac{4}{3} - a\frac{2}{3} = \frac{4}{3}a \Rightarrow \frac{4}{3} = \frac{6}{3}a \Leftrightarrow a = \frac{2}{3}. \tag{29.12}$$

With this choice of a , the terms on the main diagonal also contribute non-negatively to the dissipation rate and it holds

$$\varepsilon \geq 0. \tag{29.13}$$

The result for the friction tensor is therefore:

$$\tau = K \begin{pmatrix} \frac{4}{9} [2\delta_1 u_1 - (\delta_2 u_2 + \delta_3 u_3)] & \frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) & \frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) \\ \frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) & \frac{4}{9} [2\delta_2 u_2 - (\delta_1 u_1 + \delta_3 u_3)] & \frac{2}{3} (\delta_3 u_2 + \delta_2 u_3) \\ \frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) & \frac{2}{3} (\delta_3 u_2 + \delta_2 u_3) & \frac{4}{9} [2\delta_3 u_3 - (\delta_1 u_1 + \delta_2 u_2)] \end{pmatrix}. \quad (29.14)$$

The generalization

$$\tau = \begin{pmatrix} K_c \frac{4}{9} [2\delta_1 u_1 - (\delta_2 u_2 + \delta_3 u_3)] & K_1 \frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) & K_2 \frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) \\ K_1 \frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) & K_c \frac{4}{9} [2\delta_2 u_2 - (\delta_1 u_1 + \delta_3 u_3)] & K_3 \frac{2}{3} (\delta_3 u_2 + \delta_2 u_3) \\ K_2 \frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) & K_3 \frac{2}{3} (\delta_3 u_2 + \delta_2 u_3) & K_c \frac{4}{9} [2\delta_3 u_3 - (\delta_1 u_1 + \delta_2 u_2)] \end{pmatrix} \quad (29.15)$$

does not destroy any of the verified statements.

29.1.1 Modification to comply with the Thuburn condition

The divergence of the tensor Eq. (29.15) does not yet satisfy the Thuburn condition. Motivated by section 27.6.1, one therefore makes the approach for the frictional acceleration on the edge e

$$\begin{aligned} h_e \frac{\partial u_{e,\text{diff}}}{\partial t} &= [\nabla (K_c E_{c(e)})]_e + \frac{1}{l_e} \left(\frac{1}{3} \sum_{r \in t_1} K_r F_{r(e)} - \frac{1}{3} \sum_{r \in t_2} K_r F_{r(e)} \right) \\ &= [\nabla (K_c E_{c(e)})]_e + \frac{1}{3l_e} \left(\sum_{r \in t_1} K_r F_{r(e)} - \sum_{r \in t_2} K_r F_{r(e)} \right). \end{aligned} \quad (29.16)$$

Here E_c and F_r are *deformations*, which are localized in the cell centers and at the edges, respectively. The E_c are located on the diagonal of the stress tensor, they are referred to as *shear deformations*. The F_r are not located on the diagonal of the stress tensor, they are called *shear deformation*. Here you allow that both can depend not only on their position but also on the edge on which you want to calculate the acceleration, i.e. $E_{c(e)}$ or $F_{r(e)}$. The triangle t_1 is located with respect to the edge e in the direction $\mathbf{k} \times \mathbf{n}_e$, the edge t_2 in the direction $-\mathbf{k} \times \mathbf{n}_e$. K_c and K_r are nonnegative diffusion coefficients, which are left open in this chapter. O.B.d. A. assume that $\mathbf{n}_e$ is aligned parallel to $\mathbf{i}_1$.

On the regular grid one obtains for the shear deformation

$$\begin{aligned} E_{c(e)} &= \frac{4}{9} [2\delta_1 u_1 - (\delta_2 u_2 + \delta_3 u_3)] = \frac{4}{9} [3\delta_1 u_1 - (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3)] = \frac{4}{3} \delta_1 u_1 - \frac{4}{9} (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3) \\ &= -\frac{4}{9} (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3) + \frac{4}{3} \delta_1 u_1 = -\frac{2}{3} \frac{2}{3} (\delta_1 u_1 + \delta_2 u_2 + \delta_3 u_3) + \frac{4}{3} \delta_1 u_1 \\ &\stackrel{\text{Glg. (27.33)}}{=} -\frac{2}{3} D + \frac{4}{3} \delta_1 u_1 \end{aligned} \quad (29.17)$$

For the shear deformations, according to Eq. (29.15)

$$\begin{aligned} &\delta_2 \left[\frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) \right] + \delta_3 \left[\frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) \right] \stackrel{!}{=} \frac{1}{3} \delta_y (F_{1(e)} + F_{2(e)} + F_{3(e)}) \\ &\stackrel{\text{Glg. (27.31)}}{=} \frac{1}{3\sqrt{3}} (\delta_2 - \delta_3) (F_{1(e)} + F_{2(e)} + F_{3(e)}) \end{aligned} \quad (29.18)$$

apply. The choice of $F_{1(e)}$ is arbitrary because this term is first added and then subtracted again. It is therefore obvious to choose

$$F_{1(e)} = \zeta_1. \quad (29.19)$$

First, one treats Eq. (29.18) in the form

$$\delta_2 \left[\frac{2}{3} (\delta_2 u_1 + \delta_1 u_2) \right] + \delta_3 \left[\frac{2}{3} (\delta_3 u_1 + \delta_1 u_3) \right] = \frac{1}{\sqrt{3}} (\delta_2 F_{3(e)} - \delta_3 F_{2(e)}). \quad (29.20)$$

This gives you

$$F_{\mathbf{z}(e)} = -\frac{\mathbf{2}}{\sqrt{3}} (\delta_3 u_1 + \delta_1 u_3) = \frac{\mathbf{2}}{\sqrt{3}} (-\delta_3 u_1 - \delta_1 u_3) = \frac{\mathbf{2}}{\sqrt{3}} [(\delta_3 u_1 - \delta_1 u_3) - \mathbf{2}\delta_3 u_1] \stackrel{\text{Glg. (27.171)}}{=} \zeta_2 - \frac{\mathbf{4}}{\sqrt{3}} \delta_3 u_1, \quad (29.21)$$

$$F_{\mathbf{3}(e)} = \frac{\mathbf{2}}{\sqrt{3}} (\delta_2 u_1 + \delta_1 u_2) = \frac{\mathbf{2}}{\sqrt{3}} [(\delta_1 u_2 - \delta_2 u_1) + \mathbf{2}\delta_2 u_1] \stackrel{\text{Glg. (27.172)}}{=} \zeta_3 + \frac{\mathbf{4}}{\sqrt{3}} \delta_2 u_1. \quad (29.22)$$

Analogous to section 27.6.1, the averaged shear deformations are now used, which is based on Eq. (29.18) leads. The procedure for calculating the gradient of the component u_i is presented in Section 29.2.0.1 in the context of the deformed grid.

29.2 Deformed grid

In this section the results of the previous section are generalized to the deformed hexagonal C-lattice. Here too one remains within the framework of the shallow water equations. Essentially you can use the same formulas as on the regular grid, but the velocity gradients can be noted slightly differently. Because of

$$\begin{aligned} F_{\mathbf{z}(e)} + F_{\mathbf{3}(e)} &= \zeta_2 - \frac{\mathbf{4}}{\sqrt{3}} \delta_3 u_1 + \zeta_3 + \frac{\mathbf{4}}{\sqrt{3}} \delta_2 u_1 = \zeta_2 + \zeta_3 + \mathbf{4} \frac{\mathbf{1}}{\sqrt{3}} (\delta_2 - \delta_3) u_1 = \zeta_2 + \zeta_3 + \mathbf{4} \delta_y u_1 \\ &= \zeta_2 + \mathbf{2} \delta_y u_1 + \zeta_3 + \mathbf{2} \delta_y u_1 \end{aligned} \quad (29.23)$$

you can also see the deformations in the form

$$E_{c(e)} = -\frac{\mathbf{2}}{\mathbf{3}} D + \frac{\mathbf{4}}{\mathbf{3}} \delta_x u_1 \Big|_c, \quad (29.24)$$

$$F_{\mathbf{1}(e)} = \zeta_1, \quad (29.25)$$

$$F_{\mathbf{2}(e)} = \zeta_2 + \mathbf{2} \delta_y u_1 \Big|_2, \quad (29.26)$$

$$F_{\mathbf{3}(e)} = \zeta_3 + \mathbf{2} \delta_y u_1 \Big|_3 \quad (29.27)$$

write down. The speed gradients are calculated via cells or rhombuses.

29.2.0.1 Calculation of velocity gradients

29.3 Three-dimensional expansion

29.4 Dissipation

For the dissipation rate ε_{hex} can simply

$$\varepsilon_{\text{hex}} = -\rho \frac{\partial \mathbf{v}_{\text{diff}}}{\partial t} \cdot \mathbf{v} \quad (29.28)$$

be set. Although this does not correspond exactly to the molecular dissipation rate Eq. (8.66), but the global integrals over both approaches are according to Eq. (8.96) identical. This creates energetic self-consistency.

Radiation is treated in models using separate simulations, so-called *radiation transport models*. This takes place in the following steps; the procedure may be slightly modified in the specific implementation:

- First, the densities of the components of the air are transmitted to the radiation model.
- The radiation properties of the matter are then calculated using these densities and tabulated spectra of the substances.
- Now the spectral radiance is calculated by solving the radiation transfer equation.
- By spectrally integrating the convergence of the radiation flux density, thermal power densities are determined, which are transmitted back to the dynamic core. This shows heating rates.

Since solving the radiation transfer equation would lead to a global linear system of equations, the atmosphere is divided into non-interacting columns that have at least the horizontal extent of a grid cell.

Data assimilation is about determining a model state from observations.

31.1 Objective analysis

Until the second half of the 20th century, meteorologists had to draw weather maps manually based on the available data, which is called *analysis*. The initial states of the first operational model runs were also determined in this way [25]. This was time-consuming, inefficient and error-prone. Therefore, people quickly began to automate this process, which is known as *objective analysis*. The analysis is objective because it no longer depends on the person who creates it. Such analyzes essentially involve interpolations and conversions of the measured variables into model variables.

31.2 Optimal interpolation

A disadvantage of interpolations is that they can become very inaccurate if there are no measurement data in the nearby area. At the beginning of operational numerical weather forecasting in the 1950s, there were only conventional measurements, most of them in Europe and the USA. There were hardly any weather observations in the southern hemisphere. An obvious solution is to use a climatological background state or the previous model run as a replacement for measurements in regions where hardly any measurements are taken. This allows the information from the areas with many observations to propagate to the regions with few observations using the physical laws simulated by the model.

The so-called *optimum interpolation* is about combining information from the observation data and a background state in an optimal way. This means that the result (the analysis) should be as close as possible to the real atmospheric state at the time of analysis.¹ For this purpose, a cost function J is used, which contains two terms:

- A portion J_B that represents the difference between the analysis and the background state.
- A portion J_y representing the difference between the analysis and the observations.

Write it down as a formula

$$J(\mathbf{x}) = J_B(\mathbf{x}, \mathbf{x}_B) + J_y(\mathbf{x}, \mathbf{y}). \quad (31.1)$$

31.2.1 An observation

31.2.1.1 A model degree of freedom

First, imagine that you only have one observation y and the model consists of only a single number x . The approach J' for J is based on the Euclidean norm and noted

$$J'(x) = \sqrt{J'_B(x, x_B)^2 + J'_y(x, y)^2} = \sqrt{a_B(x - x_B)^2 + a_y[x - \hat{I}(y)]^2}. \quad (31.2)$$

Here a_B, a_y are two weighting factors

$$a_B + a_y = 1. \quad (31.3)$$

Since the cost function is to be minimized and the root increases strictly monotonically, the notation of the cost function is simplified to:

$$J(x) = J_B(x, x_B) + J_y(x, y) = \frac{1}{2}a_B(x - x_B)^2 + \frac{1}{2}a_y[x - \hat{I}(y)]^2. \quad (31.4)$$

The factor $\frac{1}{2}$ is by convention and does not change the minimum of the cost function. Since in the case of conventional observations there are usually more model degrees of freedom than measured values, the replacement leads

$$\text{Modell} - \text{interpolierte Beobachtung} \rightarrow \text{Beobachtung} - \text{interpoliertes Modell} \quad (31.5)$$

$$\Rightarrow x - \hat{I}(y) \rightarrow y - \hat{h}(x) \quad (31.6)$$

¹This is not necessarily the state that leads to the best prediction.

to a minor problem. Here $\hat{h}$ is an i. A. nonlinear operator, the so-called *observation operator*. The cost function is therefore:

$$J(x) = \frac{1}{2}a_B(x - x_B)^2 + \frac{1}{2}a_y \left[y - \hat{h}(x) \right]^2. \quad (31.7)$$

The minimum of the cost function is satisfied

$$\nabla J = 0. \quad (31.8)$$

This equation is also necessary and sufficient for the minimum in the multidimensional case: Since J is square, ∇J is linear with constant terms that can be made to disappear by a coordinate transformation. The matrix defining ∇J is still symmetric. Since the entries on the main diagonal are all non-zero, this matrix is invertible. So there is only one x with $\nabla J(x) = 0$. Because of $\lim_{|x| \rightarrow \infty} J = \infty$ this is a minimum.

In order to be able to work on the problem with linear algebra, $\hat{h}$ is linearized at the point x_B , i.e

$$\hat{h}(x) = \hat{h}(x_B) + \hat{H}(x - x_B) + \mathcal{O}[(x - x_B)^2], \quad (31.9)$$

here is

$$\hat{H}(x) := \hat{h}'(x_B) \quad (31.10)$$

the derivative of $\hat{h}$ at location x_B . Putting this into Eq. (31.7) is obtained by neglecting an approximate sign

$$J(x) = \frac{1}{2}a_B(x - x_B)^2 + \frac{1}{2}a_y \left[y - \hat{h}(x_B) - \hat{H}(x - x_B) \right]^2. \quad (31.11)$$

The derivation from this is:

$$J'(x) = a_B(x - x_B) - a_y \hat{H} \left[y - \hat{h}(x_B) - \hat{H}(x - x_B) \right]. \quad (31.12)$$

With only one measurement and one model variable, $\hat{H}$ is simply a number,

$$\hat{H} = H. \quad (31.13)$$

The cost function should be dimensionless. From a dimensional analysis one obtains

$$[a_B] = \frac{1}{[x^2]}, \quad [a_y] = \frac{1}{[y^2]}. \quad (31.14)$$

A useful approach for the weighting factors is the inverse variances:

$$a_B = \frac{1}{\sigma_B^2}, \quad a_y = \frac{1}{\sigma_y^2} \quad (31.15)$$

Here σ_B is the standard deviation of the background state and σ_y is the standard deviation of the measurement y . This can also be justified more formally by assuming that both the error of the background state and of the measurement are normally distributed, i.e

$$P(x, y) \propto \exp \left[-\frac{(x - x_B)^2}{2\sigma_B^2} \right] \exp \left[-\frac{(y - \hat{h}(x))^2}{2\sigma_B^2} \right] = \exp \left[-\frac{(x - x_B)^2}{2\sigma_B^2} - \frac{(y - \hat{h}(x))^2}{2\sigma_B^2} \right]. \quad (31.16)$$

$P(x, y)$ is the probability density for x assuming that y has occurred. You maximize this by minimizing the negative

logarithm, so

$$P(x, y) \text{ maximal} \Rightarrow \frac{(x - x_B)^2}{2\sigma_B^2} + \frac{(y - \hat{h}(x))^2}{2\sigma_y^2} \text{ minimal.} \quad (31.17)$$

From Eq. (31.12) is obtained using Eq. (31.8)

$$\begin{aligned} \frac{1}{\sigma_B^2} (x - x_B) - \frac{H}{\sigma_y^2} [y - \hat{h}(x_B) - H(x - x_B)] &= \frac{1}{\sigma_B^2} (x - x_B) - \frac{H}{\sigma_y^2} [y - \hat{h}(x_B)] + \frac{H^2}{\sigma_y^2} (x - x_B) = 0 \\ \Rightarrow \left(\frac{1}{\sigma_B^2} + \frac{H^2}{\sigma_y^2} \right) (x - x_B) - \frac{H}{\sigma_y^2} [y - \hat{h}(x_B)] &= 0 \\ \Rightarrow x = x_B + \frac{H}{\sigma_y^2 \left(\frac{1}{\sigma_B^2} + \frac{H^2}{\sigma_y^2} \right)} [y - \hat{h}(x_B)] &= x_B + \frac{H}{\frac{\sigma_y^2}{\sigma_B^2} + H^2} [y - \hat{h}(x_B)]. \end{aligned} \quad (31.18)$$

Two interesting borderline cases follow from this:

- In the case $\frac{\sigma_y^2}{\sigma_B^2} \rightarrow \infty$, which corresponds to very imprecise measurements y , $x = x_B$. In this case, the analysis is determined only from the background state.
- In the case $\frac{\sigma_B^2}{\sigma_y^2} \rightarrow \infty$, which corresponds to a very imprecise background state x_B , applies

$$x = x_B + \frac{H}{H^2} [y - \hat{h}(x_B)] = x_B + \frac{y - \hat{h}(x_B)}{H}. \quad (31.19)$$

In this case, the analysis is determined only from the measurements.

31.2.1.2 Multiple degrees of model freedom

Now assume that a model state is not determined by a single number x , but by a state vector $\mathbf{x}$ of length N . For this case, the cost function generalizes to Eq. (31.11) to

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}_B)^T B^{-1} (\mathbf{x} - \mathbf{x}_B) + \frac{1}{2} \frac{1}{\sigma_y^2} [y - \hat{h}(\mathbf{x}_B) - H(\mathbf{x} - \mathbf{x}_B)]^2. \quad (31.20)$$

H ist ein $1 \times N$ -Vektor. $B \in \mathbb{R}^{N \times N}$ ist die Kovarianzmatrix der Fehler des Hintergrundzustandes. Diese Matrix hat Diagonalform, auf ihrer Hauptdiagonalen stehen die Varianzen des Hintergrundzustandes:

$$B = \begin{pmatrix} \sigma_{o,B}^2 & 0 & \dots & 0 \\ 0 & \sigma_{1,B}^2 & 0 & \vdots \\ \vdots & \dots & \ddots & 0 \\ 0 & \dots & 0 & \sigma_{N-1,B}^2 \end{pmatrix} \quad (31.21)$$

From this it follows

$$B^{-1} = \begin{pmatrix} \frac{1}{\sigma_{o,B}^2} & 0 & \dots & 0 \\ 0 & \frac{1}{\sigma_{1,B}^2} & 0 & \vdots \\ \vdots & \dots & \ddots & 0 \\ 0 & \dots & 0 & \frac{1}{\sigma_{N-1,B}^2} \end{pmatrix}. \quad (31.22)$$

Thus you get

$$\frac{1}{2} (\mathbf{x} - \mathbf{x}_B)^T B^{-1} (\mathbf{x} - \mathbf{x}_B) = \sum_{i=0}^{N-1} \frac{(x_i - x_{i,B})^2}{2\sigma_{i,B}^2}. \quad (31.23)$$

You get from this

$$(\nabla J)_i = \frac{(x_i - x_{i,B})}{\sigma_{i,B}^2} - \frac{H_i}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) - \mathbf{H}(\mathbf{x} - \mathbf{x}_B) \right]. \quad (31.24)$$

This can be done in the compact form

$$\nabla J = B^{-1} (\mathbf{x} - \mathbf{x}_B) - \frac{\mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) - \mathbf{H}(\mathbf{x} - \mathbf{x}_B) \right]. \quad (31.25)$$

note down. From Eq. (31.8) follows in this case

$$\begin{aligned} B^{-1} (\mathbf{x} - \mathbf{x}_B) &= \frac{\mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) - \mathbf{H}(\mathbf{x} - \mathbf{x}_B) \right] \\ \Rightarrow B^{-1} (\mathbf{x} - \mathbf{x}_B) + \frac{\mathbf{H}^T}{\sigma_y^2} [\mathbf{H}(\mathbf{x} - \mathbf{x}_B)] &= \frac{\mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) \right] \\ \Rightarrow \left(B^{-1} + \frac{\mathbf{H}^T \mathbf{H}}{\sigma_y^2} \right) (\mathbf{x} - \mathbf{x}_B) &= \frac{\mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) \right] \\ \Rightarrow \left(\mathbf{I} + B \frac{\mathbf{H}^T \mathbf{H}}{\sigma_y^2} \right) (\mathbf{x} - \mathbf{x}_B) &= \frac{B \mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) \right] \\ \Rightarrow \mathbf{x} - \mathbf{x}_B &= \left(\mathbf{I} + B \frac{\mathbf{H}^T \mathbf{H}}{\sigma_y^2} \right)^{-1} \frac{B \mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) \right] \end{aligned}$$

$$\Rightarrow \mathbf{x} = \mathbf{x}_B + \left(B \frac{\mathbf{H}^T \mathbf{H}}{\sigma_y^2} + \mathbf{I} \right)^{-1} \frac{B \mathbf{H}^T}{\sigma_y^2} \left[y - \hat{h}(\mathbf{x}_B) \right]. \quad (31.26)$$

31.2.2 Any number of observations

Now assume that there are not one, but M observations. The cost function Eq. (31.20) generalizes to this case

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}_B)^T B^{-1} (\mathbf{x} - \mathbf{x}_B) + \frac{1}{2} \left(\mathbf{y} - \hat{h}(\mathbf{x}_B) - \mathbf{H}(\mathbf{x} - \mathbf{x}_B) \right)^T R^{-1} \left(\mathbf{y} - \hat{h}(\mathbf{x}_B) - \mathbf{H}(\mathbf{x} - \mathbf{x}_B) \right). \quad (31.27)$$

Here R is the covariance matrix of the errors of the observations. Since these are mainly statistical (and not systematic) errors, one can assume that they have a diagonal shape. It applies

$$(\mathbf{y} - \mathbf{H}\mathbf{x})^T R^{-1} (\mathbf{y} - \mathbf{H}\mathbf{x}) = \mathbf{y}^T R^{-1} \mathbf{y} - \mathbf{y}^T R^{-1} \mathbf{H}\mathbf{x} - \mathbf{x}^T \mathbf{H}^T R^{-1} \mathbf{y} + \mathbf{x}^T \mathbf{H}^T R^{-1} \mathbf{H}\mathbf{x}. \quad (31.28)$$

Now you do the math

$$\mathbf{y}^T R^{-1} \mathbf{H}\mathbf{x} = (R^{-1} \mathbf{H}\mathbf{x})^T \mathbf{y} = \mathbf{x}^T \mathbf{H}^T R^{-1} \mathbf{y}. \quad (31.29)$$

It was used that R^{-1} is orthogonal. Therefore applies

$$\begin{aligned}
(\mathbf{y} - H\mathbf{x})^T R^{-1} (\mathbf{y} - H\mathbf{x}) &= \mathbf{y}^T R^{-1} \mathbf{y} - \mathbf{2} \mathbf{x}^T H^T R^{-1} \mathbf{y} + \mathbf{x}^T H^T R^{-1} H \mathbf{x} \\
&= \mathbf{y}^T R^{-1} \mathbf{y} - \mathbf{2} \mathbf{x}^T H^T R^{-1} \mathbf{y} + (\mathbf{x}^T H^T R^{-1} H)^T \cdot \mathbf{x} \\
&= \mathbf{y}^T R^{-1} \mathbf{y} - \mathbf{2} \mathbf{x}^T H^T R^{-1} \mathbf{y} + (H^T R^{-1} H \mathbf{x}) \cdot \mathbf{x}.
\end{aligned} \tag{31.30}$$

It was taken into account that because of

$$(H^T R^{-1} H)^T = H^T R^{-1} H \tag{31.31}$$

the matrix $H^T R^{-1} H$ is orthogonal. If one forms the gradient of Eq. (31.30) (with respect to $\mathbf{x}$), one obtains

$$\nabla \left[(\mathbf{y} - H\mathbf{x})^T R^{-1} (\mathbf{y} - H\mathbf{x}) \right] = -\mathbf{2} H^T R^{-1} \mathbf{y} + \mathbf{2} H^T R^{-1} H \mathbf{x} = -\mathbf{2} H^T R^{-1} (\mathbf{y} - H\mathbf{x}). \tag{31.32}$$

From this it follows

$$\nabla J = B^{-1} (\mathbf{x} - \mathbf{x}_B) - H^T R^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B) - H(\mathbf{x} - \mathbf{x}_B)). \tag{31.33}$$

From Eq. So (31.8) follows

$$\begin{aligned}
B^{-1} (\mathbf{x} - \mathbf{x}_B) - H^T R^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B) - H(\mathbf{x} - \mathbf{x}_B)) &= \mathbf{0} \\
\Leftrightarrow (\mathbf{x} - \mathbf{x}_B) - B H^T R^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B) - H(\mathbf{x} - \mathbf{x}_B)) &= \mathbf{0} \\
\Leftrightarrow (B H^T R^{-1} H + \mathbf{1}) (\mathbf{x} - \mathbf{x}_B) - B H^T R^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B)) &= \mathbf{0}
\end{aligned}$$

$$\Leftrightarrow (B H^T R^{-1} H + \mathbf{1}) (\mathbf{x} - \mathbf{x}_B) = B H^T R^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B)). \tag{31.34}$$

This is the system of linear equations valid for $\mathbf{x}$. You can further transform this into:

$$\mathbf{x} = \mathbf{x}_B + (B H^T R^{-1} H + \mathbf{1})^{-1} B H^T R^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B)). \tag{31.35}$$

The Matrix

$$K := (B H^T R^{-1} H + \mathbf{1})^{-1} B H^T R^{-1} \tag{31.36}$$

is called *gain matrix*. To calculate the right-hand side of this equation, one must invert an $N \times N$ matrix.

You can simplify the expression for the gain matrix a little. Let $A \in \mathbb{R}^{N \times M}$. Then applies

$$\begin{aligned}
A &= A (H A + \mathbf{1}) (H A + \mathbf{1})^{-1} \\
\Leftrightarrow A &= (A H A + A) (H A + \mathbf{1})^{-1} \\
\Leftrightarrow A &= (A H + \mathbf{1}) A (H A + \mathbf{1})^{-1} \\
\Leftrightarrow (A H + \mathbf{1})^{-1} A &= A (H A + \mathbf{1})^{-1}.
\end{aligned}$$

Now define it

$$A := B H^T R^{-1}, \tag{31.37}$$

follows

$$K = (BH^T R^{-1} H + \mathbf{1})^{-1} BH^T R^{-1} = BH^T R^{-1} (HBH^T R^{-1} + \mathbf{1})^{-1}. \quad (31.38)$$

To calculate the right-hand side of this equation, an $M \times M$ -matrix must now be inverted, which for $M < N$ is more efficient than Eq. (31.36) is. You can take this further

$$K = BH^T (HBH^T + R)^{-1} \quad (31.39)$$

simplify. Putting this into Eq. (31.35), you get

$$\mathbf{x} = \mathbf{x}_B + BH^T (HBH^T + R)^{-1} (\mathbf{y} - \hat{h}(\mathbf{x}_B)). \quad (31.40)$$

31.2.3 Special problems in the treatment of the wind field

The wind field can be assimilated as part of the OI. However, with coarse model resolutions, this has the disadvantage that the wind obtained in this way is often further away from the balance equation than is usual on the synoptic scale and thus triggers sound and gravity waves that are too strong. These then trigger prediction errors. Therefore, it may make sense to determine the wind field not based on measurements, but by solving the balance equation. This is an example of OI maximizing the quality of analysis rather than prediction.

31.2.4 Consideration of hydrostatics

If one assumes hydrostatics, i.e. the validity of the basic hydrostatic equation Eq. (13.122), the thermodynamic state of the atmosphere is simplified considerably: usually two thermodynamic quantities q_1 , q_2 are sufficient to determine this. If an equation of the form is valid

$$\frac{\partial q_1}{\partial z} = f(q_2) \quad (31.41)$$

However, one can replace the determination of the quantity q_1 in the entire atmosphere by its determination on a surface, for example the earth's surface or a pressure surface. Requiring the exact validity of a statement about the result of data assimilation is called *strong constraint*.

31.3 3D Var

The inversion of the $M \times M$ -matrix $HBH^T + R$ is very complex if the number of individual observations is large. It is important to remember that a radar image, for example, consists of a very large number of individual observations. This is a disadvantage of OI. This could be avoided by replacing Eq. (31.6) undoes. This is not directly possible with remote sensing data because, for example, spectral radiance on a satellite cannot easily be converted into temperatures. A solution to this is presented in this section.

The *3D-Var method* is about solving Eq. (31.40) can be solved iteratively without explicitly calculating the gain matrix. Define

$$\delta \mathbf{x} := \mathbf{x} - \mathbf{x}_B, \quad (31.42)$$

$$\mathbf{d}_B := \mathbf{y} - \hat{h}(\mathbf{x}_B), \quad (31.43)$$

$$(31.44)$$

Eq. (31.34) is then

$$(BH^T R^{-1} H + \mathbf{1}) \delta \mathbf{x} = BH^T R^{-1} \mathbf{d}_B. \quad (31.45)$$

Multiplying by B^{-1} gives you

$$(H^T R^{-1} H + B^{-1}) \delta \mathbf{x} = H^T R^{-1} \mathbf{d}_B. \quad (31.46)$$

So here an $N \times N$ matrix has to be inverted. From this one would expect that for $N < M$, i.e. if there are more observations than model degrees of freedom, this equation is more efficient than Eq. (31.40).

31.3.1 Iterative solution process

31.3.2 Outer and inner loop

31.3.2.1 The outer loop

31.3.2.2 The inner loop

31.3.3 Weak constraints

Another advantage of 3D-Var over OI is that it can easily request additional conditions by including them in the cost function. This is called *weak constraint*. The procedure presented in section 31.2.4 can be formulated as a weak constraint by using a term

$$J \propto \frac{1}{2} \int_A \left(\frac{\partial p}{\partial z} + g\rho \right)^2 d^3r \quad (31.47)$$

included in the cost function.

31.3.3.1 Balance equation

The horizontal wind is closely linked to the thermodynamic quantities on the synoptic scale due to the approximate validity of the geostrophic balance and the balance equation. It can therefore be viewed as a diagnostic variable. It directly from geostrophy in the form of Eq. (13.187) is not possible in the tropics due to the divergence problem presented in Sect. 13.10.1. Therefore, one can instead use the balance equation (15.137) or the linearized balance equation Eq. Use (15.138). This filters both sound and gravity waves, as both are associated with divergences.

Analogous to the case of hydrostatics, it is again possible to either demand the validity of the balance equation exactly or, what is easier, to include it in the cost function.

31.4 4D Var

4D-Var is based on 3D-Var, but also takes the time dimension into account. To do this, the cost function J is generalized in the form

$$J = J_{\text{3D-Var}} + \sum_{n=1}^N J_n, \quad (31.48)$$

here N is the number of time steps involved (except the analysis time itself) and J_n is the cost function at step n . $J_{\text{3D-Var}}$ is as in Eq. (31.27) defined. Let $\mathbf{Y}_n$ be the vector of observations at time step n . At each time step, this vector can have a different magnitude and a different meaning. Let $\mathbf{X}_n$ be the state vector of the model atmosphere at time step n , which comes from the analysis state $\mathbf{X}$ via

$$\mathbf{X}_n = \mathbf{M}_n \mathbf{X}, \quad (31.49)$$

is determined. Here $\mathbf{M}_n$ is the integration of the model from the analysis time to time step n . To linearize this integration, one calculates a so-called *tangential linear model operator* $\mathbf{M}$, which is a matrix. It then applies

$$\mathbf{M}_n \approx \mathbf{M}^n, \quad (31.50)$$

which becomes more and more inaccurate as n increases. Therefore applies

$$J_n = (\mathbf{Y}_n - \mathbf{H}_n \mathbf{M}^n \mathbf{X})^T \mathbf{A}_{O,n} (\mathbf{Y}_n - \mathbf{H}_n \mathbf{M}^n \mathbf{X}). \quad (31.51)$$

31.4.1 Outer and inner loop

31.4.1.1 The outer loop

31.4.1.2 The inner loop

31.5 Interpolation of another model

If the initial state of another model exists (for example on a length-latitude grid), it is entirely possible to simply interpolate this onto the desired model grid and convert it into the prognostic variables. Here, the analysis of the other model is interpreted as „observation“ and the assumption is made that the error of the data assimilation of the other model is negligible compared to the error of the prediction of the own model. This assumption is often justified, and even if it is not justified, it may make sense to still use this method in order to use the computing capacity freed up by the simplicity of this procedure for model running.

Part VII

Development of a dynamic core

The term *dynamic core* is often not precisely defined, but this is what will be done here. For this purpose, various subcomponents are defined:

- The *reversible part of the dynamic core* solves the equations of a dry adiabatic atmosphere without molecular and numerical diffusion terms. For models in which this part of the dynamic core does not exactly comply with the second law of thermodynamics, it is better to call this part *primary part of the dynamic core*.
- The *irreversible part of the dynamic core* deals with molecular and numerical diffusive flows. These can be heat, mass or momentum flows. For models in which the previously defined part of the dynamic core does not exactly comply with the second law of thermodynamics, it is better to call this part *secondary part of the dynamic core*. Together with the previously defined part, this part forms the *dry dynamic core*.
- The *extended dynamic core* handles the advection of tracers and ensures that negative tracer densities do not occur. These can be water components, aerosols and/or trace gases.

33.1 Horizontal grid

33.1.1 Constants of the hexagonal lattice

First you write an icosahedron into a sphere. This consists of 20 triangles, so the number of corners is E

$$E = \frac{3 \cdot 20}{5} = 12, \quad (33.1)$$

since each corner is touched by five polygons. The number K of edges is

$$K = \frac{3 \cdot 20}{2} = 30. \quad (33.2)$$

Now each triangle is divided n times into four triangles each, where $n \in \mathbb{N}$. Subsequently exist

$$D = 20 \cdot 4^n \quad (33.3)$$

Triangles. The dual grid of the resulting grid is the hexagonal grid. This consists of

$$N = N_5 + N_6 \quad (33.4)$$

Polygons, where N_5 denotes the number of pentagons and N_6 denotes the number of hexagons. Pentagons only form at the twelve vertices of the icosahedron, so $N_5 = 12$ is independent of n . The number of vertices of this grid is

$$\frac{5N_5 + 6N_6}{3} = D = 20 \cdot 4^n, \quad (33.5)$$

since each corner is touched by three polygons; this is equal to the number of triangles. So follow

$$5N_5 + 6N_6 = 60 + 6N_6 = 60 \cdot 4^n \Rightarrow N_6 = 10(4^n - 1) \Rightarrow N = 10(4^n - 1) + 12. \quad (33.6)$$

This is the number of scalar degrees of freedom per model level $N_S^{(H)}$. The number $N_V^{(H)}$ of vector degrees of freedom per model level is given by

$$N_V^{(H)} = \frac{5N_5 + 6N_6}{2} = \frac{60 \cdot 4^n}{2} = 30 \cdot 4^n. \quad (33.7)$$

The number of layers N_L is arbitrary

$$N_L = 2 + 6 \cdot n \quad (33.8)$$

set. The total number of horizontal vectors is $N_L \cdot N_V^{(H)}$, to which the number of vertical vectors $N_S^{(H)} \cdot (N_L + 1)$ must be added to get the total number

index	geographical latitude	geographical longitude
0	$\frac{\pi}{2}$	0
1	$\arctan\left(\frac{1}{2}\right)$	0
2	$\arctan\left(\frac{1}{2}\right)$	$\frac{2\pi}{5}$
3	$\arctan\left(\frac{1}{2}\right)$	$2\frac{2\pi}{5}$
4	$\arctan\left(\frac{1}{2}\right)$	$3\frac{2\pi}{5}$
5	$\arctan\left(\frac{1}{2}\right)$	$4\frac{2\pi}{5}$
6	$-\arctan\left(\frac{1}{2}\right)$	$\frac{2\pi}{10}$
7	$-\arctan\left(\frac{1}{2}\right)$	$\frac{2\pi}{10} + \frac{2\pi}{5}$
8	$-\arctan\left(\frac{1}{2}\right)$	$\frac{2\pi}{10} + 2\frac{2\pi}{5}$
9	$-\arctan\left(\frac{1}{2}\right)$	$\frac{2\pi}{10} + 3\frac{2\pi}{5}$
10	$-\arctan\left(\frac{1}{2}\right)$	$\frac{2\pi}{10} + 4\frac{2\pi}{5}$
11	$-\frac{\pi}{2}$	0

Table 33.1: Corners of the icosahedron inscribed in the unit sphere.

$$N_V = N_L \cdot N_V^{(H)} + N_S^{(H)} \cdot (N_L + 1) \quad (33.9)$$

of the vectors. For the total number of scalars N_S applies

$$N_S = N_L \cdot N_S^{(H)} = N_L [10(4^n - 1) + 12]. \quad (33.10)$$

Apply on the dual grid (the triangular grid).

$${}^{(D)}N_S^{(H)} = 20 \cdot 4^n, \quad {}^{(D)}N_S = 20 \cdot 4^n (N_L + 1), \quad (33.11)$$

$${}^{(D)}N_V^{(H)} = 30 \cdot 4^n, \quad {}^{(D)}N_V = 30 \cdot 4^n (N_L + 1) + 20 \cdot 4^n \cdot N_L. \quad (33.12)$$

33.1.2 Grid generation on the unit sphere

33.1.3 Grid optimization

33.2 Vertical grid

In order to make communication easier, the following specifications are made:

- A *Layer* is a layer of grid cells.
- A *Level* is the edge of a layer.
- The numbering starts at zero at the top of the atmosphere. If there are n layers, then there are $n + 1$ levels.
- All variables are placed in the middle of the layers, vertical components of vector fields in the levels. Such a vertical lattice structure is called a *Lorenz lattice*.
- The radial component of a vector field points positively upwards.

Let a grid with n layers be given. According to section 24.2, central difference quotients are second order, while other types of difference quotients are only first order. That's why you specify for the z coordinates of the levels that they should be in the middle of the scalar grid points of the neighboring layers, i.e

$$z_{\text{Level}} = \frac{z_{\text{Layer darüber}} + z_{\text{Layer darunter}}}{2}. \quad (33.13)$$

The z coordinates of the scalar grid points (z_{Layer}) must first be determined. It makes sense to make the layers as thick as possible so that the resolution is as homogeneous as possible. Near the earth's surface, the grid boxes must follow the orography. Since this leads to numerical overhead, it is useful not to do this above a certain height $\tilde{z}$. This size is a compromise between accuracy and computing time. The height $\tilde{z}$ is set indirectly by the user. This determines the height H of the model atmosphere and the number N_L of layers. In addition, it specifies a number $1 \leq N_{L,0} \leq N_L$ of layers that should follow the orography. $\tilde{z}$ is then a horizontal scalar field, which is given by

$$\tilde{z}(\varphi, \lambda) = h(\varphi, \lambda) + \frac{N_{L,0}}{N_L} (H - h(\varphi, \lambda)) \quad (33.14)$$

is fixed in terms of orography $h = h(\varphi, \lambda)$.¹ From this one calculates preliminary positions $z_{w,\text{pre},i}$ of vertical vectors, where i is the layer index:

$$z_{w,\text{pre},i} = \begin{cases} H - i \frac{H-\tilde{z}}{N_L-N_{L,0}}, & \text{falls } i < N_{L,0}, \\ h + (N_L - i) \frac{\tilde{z}-h}{N_{L,0}}, & \text{sonst.} \end{cases} \quad (33.15)$$

The scalar grid points are then placed in the middle of two adjacent vertical vectors before Eq. (33.13) is applied to finally determine the position of the levels. For the horizontal vector points it is specified that they are also placed vertically in the middle of the two adjacent boxes, i.e

$$z_{\text{Vektor}, h} = \frac{z_{\text{Skalar}, \text{Herkunft}} + z_{\text{Skalar}, \text{Ziel}}}{2}. \quad (33.16)$$

The same procedure is followed for dual scalar fields, here the determining variable is the position $z_{j,i}$ of the dual scalar grid points, where j is the horizontal index and i is the layer again. For this size you lay

$$z_{j,i} = \frac{1}{3} \sum_{j' \in \text{APC}(j)} z_{j',w,i} \quad (33.17)$$

fixed, so it is the average of the z positions of the vertical vectors of the three surrounding cells.

33.2.1 Functional determinant of a generalized vertical coordinate

The starting point are spherical coordinates with a generalized vertical coordinate ζ , which depends on the horizontal coordinates. The transformation to global coordinates is

$$x = r(\zeta, \varphi, \lambda) \cos(\varphi) \cos(\lambda), \quad y = r(\zeta, \varphi, \lambda) \cos(\varphi) \sin(\lambda), \quad z = r(\zeta, \varphi, \lambda) \sin(\varphi). \quad (33.18)$$

The covariant basis elements of this coordinate system

$$\mathbf{j}_\eta = \frac{\partial r}{\partial \zeta} \mathbf{e}_r, \quad \mathbf{j}_\varphi = r \mathbf{e}_\varphi + \frac{\partial r}{\partial \varphi} \mathbf{e}_r, \quad \mathbf{j}_\lambda = r \cos(\varphi) \mathbf{e}_\lambda + \frac{\partial r}{\partial \lambda} \mathbf{e}_r. \quad (33.19)$$

This follows for the six relevant scalar products of the basic elements

$$\mathbf{j}_\eta \cdot \mathbf{j}_\eta = \left(\frac{\partial r}{\partial \zeta} \right)^2, \quad \mathbf{j}_\eta \cdot \mathbf{j}_\varphi = \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi}, \quad \mathbf{j}_\eta \cdot \mathbf{j}_\lambda = \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda}, \quad (33.20)$$

$$\mathbf{j}_\varphi \cdot \mathbf{j}_\varphi = r^2 + \left(\frac{\partial r}{\partial \varphi} \right)^2, \quad \mathbf{j}_\varphi \cdot \mathbf{j}_\lambda = \frac{\partial r}{\partial \varphi} \frac{\partial r}{\partial \lambda}, \quad \mathbf{j}_\lambda \cdot \mathbf{j}_\lambda = r^2 \cos^2(\varphi) + \left(\frac{\partial r}{\partial \lambda} \right)^2. \quad (33.21)$$

For the determinant of the metric tensor follows by expansion after the first line

¹The idea that h is a function of horizontal coordinates is incorrect when thinking about buildings, plants and canyons. However, these structures are small-scale. Only when the horizontal model resolution reaches the order of ten meters does one have to take it into account.

$$\begin{aligned}
g &= \begin{vmatrix} \left(\frac{\partial r}{\partial \zeta}\right)^2 & \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi} & \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda} \\ \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi} & r^2 + \left(\frac{\partial r}{\partial \varphi}\right)^2 & \frac{\partial r}{\partial \varphi} \frac{\partial r}{\partial \lambda} \\ \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda} & \frac{\partial r}{\partial \varphi} \frac{\partial r}{\partial \lambda} & r^2 \cos^2(\varphi) + \left(\frac{\partial r}{\partial \lambda}\right)^2 \end{vmatrix} \\
&= \left(\frac{\partial r}{\partial \zeta}\right)^2 \left[r^4 \cos^2(\varphi) + r^2 \left(\frac{\partial r}{\partial \lambda}\right)^2 + \left(\frac{\partial r}{\partial \varphi}\right)^2 r^2 \cos^2(\varphi) + \left(\frac{\partial r}{\partial \varphi}\right)^2 \left(\frac{\partial r}{\partial \lambda}\right)^2 - \left(\frac{\partial r}{\partial \varphi}\right)^2 \left(\frac{\partial r}{\partial \lambda}\right)^2 \right] \\
&\quad - \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi} \left[\frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi} r^2 \cos^2(\varphi) + \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi} \left(\frac{\partial r}{\partial \lambda}\right)^2 - \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda} \frac{\partial r}{\partial \varphi} \frac{\partial r}{\partial \lambda} \right] \\
&\quad + \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda} \left[\frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \varphi} \frac{\partial r}{\partial \varphi} \frac{\partial r}{\partial \lambda} - \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda} r^2 - \frac{\partial r}{\partial \zeta} \frac{\partial r}{\partial \lambda} \left(\frac{\partial r}{\partial \varphi}\right)^2 \right] \\
&= \left(\frac{\partial r}{\partial \zeta}\right)^2 r^4 \cos^2(\varphi). \tag{33.22}
\end{aligned}$$

The terms marked in color cancel each other out. For the functional determinant one obtains

$$\sqrt{g} = \left| \frac{\partial r}{\partial \zeta} \right| r^2 \cos(\varphi). \tag{33.23}$$

If one uses the linearly interplred level index for η , it follows

$$\sqrt{g} \stackrel{\text{Modell}}{=} \Delta z r^2 \cos(\varphi). \tag{33.24}$$

The *shallow-atmosphere* approximation assumes $r = a = \text{const.}$, where a is the radius of the Earth. This factor can be ignored as a constant and obtained

$$\sqrt{g} \stackrel{\text{shallow-atmosphere-Modell}}{=} \Delta z \cos(\varphi). \tag{33.25}$$

33.2.2 SLEVE

33.2.3 Alternative to terrain-following coordinates

33.3 fields

33.3.1 nomenclature

Let $\psi : A \rightarrow \mathbb{R}^n$ with $n \in \{1, 2, 3\}$ be a doubly continuously differentiable scalar or vector field. The discretization of ψ is written in the form

$$\psi \rightarrow \psi_{h,v}^{(\tau)}, \tag{33.26}$$

here $h \in \mathbb{N}$ is the horizontal index, $v \in \mathbb{N}$ is the vertical index and $\tau \in \mathbb{N}$ is the index defining the time step. If one or more of the indices are not important for consideration, they will be ignored in the notation. If no different definitions are introduced at the respective location, c denotes cells, e edges, dc dual cells and de dual edges. In the vertical, the layers are numbered from $k = 1$ to $k = N_L$, the levels are numbered from $k = \frac{1}{2}$ to $k = N_L + \frac{1}{2}$ (with a distance of one).

33.3.2 Excellent points

The following sets of points play a special role:

1. the centers of the cells (index c)
2. the midpoints of the dual cells (index d)
3. the midpoints of the dual edges from the primary grid perspective (index e)
4. the midpoints of the dual edges from the perspective of the dual grid (index de)

Both the layers and the levels are important. Each element of these eight point sets is assigned a volume $V_{l,k}$ with $l \in \{c, d, e, de\}$. You have to make a difference between the primary and dual grids at the edges, even if they are the same points. Normal vectors are denoted by $\mathbf{n}_e$ and $\mathbf{n}_{de}$, respectively.

33.3.3 Types of fields

Let ψ be a scalar field and $\mathbf{v} = \mathbf{u} + w\mathbf{k}$ a vector field. The following types of fields are defined:

1. scalar field:

$$\psi_{c,k} := \frac{1}{V_{c,k}} \int_{V_{c,k}} \psi d^3r \quad (33.27)$$

2. horizontal vector field:

$$u_{e,k} := \frac{1}{V_{e,k}} \int_{V_{e,k}} \mathbf{v} \cdot \mathbf{n}_e d^3r \quad (33.28)$$

3. vertical vector field:

$$w_{c,k+1/2} := \frac{1}{V_{c,k+1/2}} \int_{V_{c,k+1/2}} \mathbf{v} \cdot \mathbf{k} d^3r \quad (33.29)$$

4. horizontal dual vector field:

$$u_{e,k+1/2} := \frac{1}{V_{e,k+1/2}} \int_{V_{e,k+1/2}} \mathbf{v} \cdot \mathbf{n}_{de} d^3r \quad (33.30)$$

5. vertical dual vector field:

$$w_{d,k} := \frac{1}{V_{d,k}} \int_{V_{d,k}} \mathbf{v} \cdot \mathbf{k} d^3r \quad (33.31)$$

6. horizontal rotation field: identical to horizontal dual vector fields
7. vertical rotation field:

$$w_{e,k} := \frac{1}{V_{e,k}} \int_{V_{e,k}} \mathbf{v} \cdot \mathbf{k} d^3r \quad (33.32)$$

According to Sect. 27.6.1, rotation fields are necessary.

The notation did not distinguish between the quantity $V \in \mathbb{R}^3$ and its volume $|V|$, and this will continue to be done if it is clear what is meant.

33.3.4 Slope

The slope of a coordinate surface is denoted by

$$\mathbf{J} := \nabla_h z|_k. \quad (33.33)$$

This is a horizontal vector field. $\mathbf{J}$ is called *Slope*.

33.4 Averaging operators

Let $x, a \in \{c, d, e, de\}$ and $\mathcal{V}_{a,k}$ be a discretized field. Then you define

$$\overline{\mathcal{V}_{a,k}}^{(x)} := \frac{1}{V_{x,k}} \sum_{y \in a, k'} \mathcal{V}_{y,k'} |V_{x,k} \cap V_{y,k'}| \quad (33.34)$$

as an averaging operator. The weighting factors $\frac{|V_{x,k} \cap V_{y,k'}|}{V_{x,k}}$ correspond to the relative overlap of the corresponding sets. It applies

$$\sum_{y \in a, k'} \frac{|V_{x,k} \cap V_{y,k'}|}{V_{x,k}} = 1. \quad (33.35)$$

Vertical averaging is also defined analogously. So a single averaging operator is either exclusively horizontal or vertical.

33.4.1 Reconstruction of the horizontal covariant measure

33.4.1.1 Shallow atmosphere

In the vertical, the covariant measures are prognostic variables and therefore do not need to be reconstructed. However, horizontally you need

$$\mathbf{v} \cdot \mathbf{e}_h = u_h, \quad (33.36)$$

where $\mathbf{e}_h$ is the horizontal covariant unit vector. To determine u_h from u and the vertical covariant components w , one first considers a two-dimensional xz coordinate system. For the sake of simplicity, one assumes a coordinate surface of the shape

$$z(x) = Jx = \tan(a)x \quad (33.37)$$

where a is the angle between the coordinate surface and the x-axis. In this case applies

$$\mathbf{e}_h = \begin{pmatrix} \cos(a) \\ \sin(a) \end{pmatrix}. \quad (33.38)$$

Note this for the vector field

$$\mathbf{v} = \begin{pmatrix} u \\ w \end{pmatrix}, \quad (33.39)$$

follows

$$\mathbf{v} \cdot \mathbf{e}_h = u \cos(a) + w \sin(a). \quad (33.40)$$

A horizontal length along a coordinate line L' increases by a factor when tilted by the angle a

$$L' = L \cos(a) \Leftrightarrow L = \frac{L'}{\cos(a)}. \quad (33.41)$$

In a numerical implementation, it is often more efficient to absorb this horizontal length magnification factor into the vector field component. This gives you

$$\mathbf{v} \cdot \mathbf{e}_h|_{\text{GK}} = u + w \tan(a) = u + Jw, \quad (33.42)$$

where the index GK stands for *geometry-corrected*. In three dimensions this relation does not change because the horizontal wind component perpendicular to u does not interfere with these calculations. On a C-grid you have to average the vertical wind component to the edge:

$$v_{h,e,\text{GK}} = u_e + J_e \overline{w_c^{(e)}}. \quad (33.43)$$

In the three-dimensional case, further vertical interpolation of the vertical wind is necessary:

$$v_{h,e,k,\text{GK}} = u_{e,k} + J_{e,k} \overline{\overline{w_{c,k+\frac{1}{2}}}}^{(e)}{}^{(k)} \quad (33.44)$$

It applies

$$\begin{aligned} \overline{\overline{w_{c,k+\frac{1}{2}}}}^{(e)}{}^{(k)} &= \frac{1}{2} \left(w_{c,k+\frac{1}{2}} + w_{o(e),k+\frac{1}{2}} \right)^{(k)} = \frac{1}{2} \left(w_{c,k+\frac{1}{2}} + w_{o(e),k+\frac{1}{2}} \right)^{(k)} = \frac{1}{2} \left(\overline{w_{c,k+\frac{1}{2}}}^{(k)} + \overline{w_{o(e),k+\frac{1}{2}}}^{(k)} \right) \\ &= \overline{\overline{w_{c,k+\frac{1}{2}}}}^{(k)}{}^{(e)}. \end{aligned} \quad (33.45)$$

The order of the averaging does not play any role here.

33.4.1.2 Deep atmosphere

In the deep atmosphere, only the averaging order $\overline{\overline{w_{c,k+\frac{1}{2}}}}^{(e)}$ is permitted. The averaging on the edge (e) is still the arithmetic mean of the two values averaged on the cell centers. The weights from Eq. are used for vertical averaging at the centers. (26.72):

$$\overline{\overline{w_{c,k+\frac{1}{2}}}}^{(k)} = \frac{A_{c,k-1/2} \Delta z_{c,k-1/2} w_{c,k-\frac{1}{2}} + A_{c,k+1/2} \Delta z_{c,k+1/2} w_{c,k+\frac{1}{2}}}{2 V_{c,k}} \quad (33.46)$$

Here the vertical areas also depend on the vertical index.

33.4.2 Scalar product on the C-grid in terrain-following coordinates

The dot product turns two vector fields into a scalar field and should therefore also be considered in the context of the averaging operators.

33.4.2.1 Shallow atmosphere

In Section 26.7 it was assumed that the discretizations of gradient and divergence are fixed, and the discretization of the three-dimensional dot product on the C-grid Eq. (26.66). Here we proceed the other way around and assume the discretization of the scalar product. One generalizes Eq. (26.66) to the following terrain coordinates:

$$\left(\mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)} \right)_{c,k} = \sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta z_{c,k}} \Delta z_{e,k} u_{e,k}^{(1)} u_{e,k}^{(2)} + \frac{\Delta z_{c,k-1/2}}{2 \Delta z_{c,k}} w_u^{(1)} w_u^{(2)} + \frac{\Delta z_{c,k+1/2}}{2 \Delta z_{c,k}} w_l^{(1)} w_l^{(2)} \quad (33.47)$$

This can be viewed as an averaging operator from the edges to the cell centers:

$$\overline{\mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)}}^{(c)} = \sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta z_{c,k}} \Delta z_{e,k} u_{e,k}^{(1)} u_{e,k}^{(2)} \quad (33.48)$$

33.4.2.2 Deep atmosphere

In the deep atmosphere you take the substitutions

$$A_c \Delta z_{c,k} \rightarrow V_{c,k}, \quad (33.49)$$

$$\Delta z_{e,k} l_{e,k} \rightarrow A_{e,k}, \quad (33.50)$$

$$d_e \rightarrow d_{e,k} \quad (33.51)$$

before. The vertical component is based on Eq. (26.72). This leads to

$$\left(\mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)} \right)_{c,k} = \sum_{e \in c} \frac{A_{e,k} d_e}{2 V_{c,k}} u_{e,k}^{(1)} u_{e,k}^{(2)} + \frac{A_{c,k-1/2} \Delta z_{c,k-1/2}}{2 V_{c,k}} w_u^{(1)} w_u^{(2)} + \frac{A_{c,k+1/2} \Delta z_{c,k+1/2}}{2 V_{c,k}} w_l^{(1)} w_l^{(2)}. \quad (33.52)$$

Similarly, the averaging operator is from the edges to the cell centers

$$\overline{\mathbf{u}^{(1)} \mathbf{u}^{(2)}}^{(c,k)} = \sum_{e \in c} \frac{A_{e,k} d_{e,k}}{2V_{c,k}} u_{e,k}^{(1)} u_{e,k}^{(2)}. \quad (33.53)$$

33.4.3 Reconstruction of the vertical contravariant measure

33.4.3.1 Shallow atmosphere

In the horizontal, the contravariant measures are prognostic variables and therefore do not need to be reconstructed. However, vertically you need

$$\mathbf{v} \cdot \mathbf{e}^{(v)} = v^{(v)}, \quad (33.54)$$

where $\mathbf{e}^{(v)}$ is the vertical contravariant unit vector. To determine $v^{(v)}$ from w and the horizontal contravariant components u , one first considers a two-dimensional xz coordinate system; in the y direction the system is homogeneous. For the sake of simplicity, one assumes a coordinate surface of the shape

$$z(x) = Jx = \tan(a) x \quad (33.55)$$

where a is the angle between the coordinate surface and the x-axis. In this case applies

$$\mathbf{e}^{(v)} = \begin{pmatrix} -\sin(a) \\ \cos(a) \end{pmatrix}. \quad (33.56)$$

Note this for the vector field

$$\mathbf{v} = \begin{pmatrix} u \\ w \end{pmatrix}, \quad (33.57)$$

follows

$$\mathbf{v} \cdot \mathbf{e}^{(v)} = -u \sin(a) + w \cos(a). \quad (33.58)$$

A horizontal coordinate surface A' increases by a factor when tilted by the angle a

$$A' = A \cos(a) \Leftrightarrow A = \frac{A'}{\cos(a)}. \quad (33.59)$$

In a numerical implementation, it is often more efficient to absorb this horizontal area magnification factor into the vector field component. This gives you

$$\mathbf{v} \cdot \mathbf{e}^{(v)}|_{\text{GK}} = w - u \tan(a) = w - Ju, \quad (33.60)$$

where the index GK stands for *geometry-corrected*. In the three-dimensional case, the product Ju is generalized to a dot product:

$$\mathbf{v} \cdot \mathbf{e}^{(v)}|_{\text{GK}} = w - \mathbf{J} \cdot \mathbf{v}_h \quad (33.61)$$

On a C-grid this becomes

$$v_{c,\text{GK}}^{(v)} = w_c - \overline{J_e u_e}^{(c)}. \quad (33.62)$$

If you use an L-grid vertically, further vertical interpolation is necessary.

$$v_{c,k+\frac{1}{2},\text{GK}}^{(v)} = w_{c,k+\frac{1}{2}} - \overline{\overline{J_{e,k} u_{e,k}}^{(c)}}^{(k+\frac{1}{2})}. \quad (33.63)$$

It applies

$$\begin{aligned}
\overline{\overline{J_{e,k}u_{e,k}}^{(c)}}^{(k+\frac{1}{2})} &= \sum_{e \in c} \frac{l_e d_e}{2A_c \Delta z_{c,k}} \overline{\Delta z_{e,k} J_{e,k} u_{e,k}}^{(k+\frac{1}{2})} = \sum_{e \in c} \frac{l_e d_e}{2A_c} \overline{\frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}}^{(k+\frac{1}{2})} \\
&= \sum_{e \in c} \frac{l_e d_e}{2A_c} \frac{\mathbf{I}}{2 \Delta z_{c,k+1/2}} \left(\Delta z_{c,k} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k} + \Delta z_{c,k+1} \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} u_{e,k+1} \right) \\
&= \sum_{e \in c} \frac{l_e d_e}{2A_c} \frac{\mathbf{I}}{2 \Delta z_{c,k+1/2}} (\Delta z_{e,k} J_{e,k} u_{e,k} + \Delta z_{e,k+1} J_{e,k+1} u_{e,k+1}) \\
&= \sum_{e \in c} \frac{l_e d_e}{2A_c} \frac{\Delta z_{e,k+1/2}}{\Delta z_{c,k+1/2}} \frac{\Delta z_{e,k} J_{e,k} u_{e,k} + \Delta z_{e,k+1} J_{e,k+1} u_{e,k+1}}{2 \Delta z_{e,k+1/2}} \\
&= \sum_{e \in c} \frac{l_e d_e}{2A_c} \frac{\Delta z_{e,k+1/2}}{\Delta z_{c,k+1/2}} \overline{J_{e,k} u_{e,k}}^{(k+1/2)} = \overline{J_{e,k} u_{e,k}}^{(k+1/2)(c)}. \tag{33.64}
\end{aligned}$$

Here too, the order of the averaging operators does not play any role.

33.4.3.2 Deep atmosphere

In the deep atmosphere will

$$v_{c,k+\frac{1}{2},\text{GK}}^{(v)} := w_{c,k+\frac{1}{2}} - \overline{\overline{J_{e,k}u_{e,k}}^{(c)}}^{(k+\frac{1}{2})}. \tag{33.65}$$

defined. Only this order of averaging operators is permitted. If you formulate this, you get with Eq. (33.53)

$$\overline{\overline{J_{e,k}u_{e,k}}^{(c)}}^{(k+\frac{1}{2})} = \frac{\mathbf{I}}{2} \left(\sum_{e \in c} \frac{A_{e,k} d_{e,k}}{2V_{c,k}} J_{e,k}^{(1)} u_{e,k}^{(2)} + \sum_{e \in c} \frac{A_{e,k+1} d_{e,k+1}}{2V_{c,k+1}} J_{e,k+1}^{(1)} u_{e,k+1}^{(2)} \right). \tag{33.66}$$

33.4.4 Divergence in terrain-following coordinates

33.4.4.1 Shallow atmosphere

Since we now know the vertical contravariant mass flux density, we can use Eq. (26.63) to

$$(\nabla \cdot \mathbf{v})_{c,k} = \frac{\mathbf{I}}{A_c \Delta z_{c,k}} \left(\sum_{e \in c} l_e \Delta z_{e,k} u_{e,k} + A_c v_{c,k-1/2,\text{GK}}^{(v)} - A_c v_{c,k+1/2,\text{GK}}^{(v)} \right) \tag{33.67}$$

generalize. The replacement was

$$w_{k+1/2} \rightarrow v_{c,k+1/2,\text{GK}}^{(v)} \tag{33.68}$$

and the layer thickness was made dependent on the horizontal position. If you put Eq. (33.63) in Eq. (33.67), you get

$$\begin{aligned}
(\nabla \cdot \mathbf{v})_{c,k} &= \frac{\mathbf{I}}{A_c \Delta z_{c,k}} \left[\sum_{e \in c} l_e \Delta z_{e,k} u_{e,k} + A_c \left(w_{c,k-1/2} - \overline{J_{e,k} u_{e,k}}^{(c)(k-\frac{1}{2})} \right) - A_c \left(w_{c,k+1/2} - \overline{J_{e,k} u_{e,k}}^{(c)(k+\frac{1}{2})} \right) \right] \\
&= \sum_{e \in c} \frac{l_e \Delta z_{e,k}}{A_c \Delta z_{c,k}} u_{e,k} + \frac{w_{c,k-1/2}}{\Delta z_{c,k}} - \frac{\overline{J_{e,k} u_{e,k}}^{(c)(k-\frac{1}{2})}}{\Delta z_{c,k}} - \frac{w_{c,k+1/2}}{\Delta z_{c,k}} + \frac{\overline{J_{e,k} u_{e,k}}^{(c)(k+\frac{1}{2})}}{\Delta z_{c,k}} \\
&\stackrel{\text{Glg. (33.48)}}{=} \frac{w_{c,k-1/2} - w_{c,k+1/2}}{\Delta z_{c,k}} + \sum_{e \in c} \frac{l_e \Delta z_{e,k}}{A_c \Delta z_{c,k}} u_{e,k} \\
&\quad - \frac{\sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta z_{c,k}} \Delta z_{e,k} J_{e,k} u_{e,k}^{(k-\frac{1}{2})}}{\Delta z_{c,k}} - \frac{\sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta z_{c,k}} \Delta z_{e,k} J_{e,k} u_{e,k}^{(k+\frac{1}{2})}}{\Delta z_{c,k}} \\
&= \frac{w_{c,k-1/2} - w_{c,k+1/2}}{\Delta z_{c,k}} + \sum_{e \in c} \frac{l_e \Delta z_{e,k}}{A_c \Delta z_{c,k}} u_{e,k} - \frac{\sum_{e \in c} \frac{l_e d_e}{2 A_c} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}^{(k-\frac{1}{2})}}{\Delta z_{c,k}} - \frac{\sum_{e \in c} \frac{l_e d_e}{2 A_c} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}^{(k+\frac{1}{2})}}{\Delta z_{c,k}} \\
&= \frac{w_{c,k-1/2} - w_{c,k+1/2}}{\Delta z_{c,k}} + \sum_{e \in c} \frac{l_e \Delta z_{e,k} u_{e,k} - \frac{l_e d_e}{2} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}^{(k-\frac{1}{2})} + \frac{l_e d_e}{2} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}^{(k+\frac{1}{2})}}{A_c \Delta z_{c,k}} \\
&= \frac{w_{c,k-1/2} - w_{c,k+1/2}}{\Delta z_{c,k}} + \sum_{e \in c} l_e \frac{\Delta z_{e,k} u_{e,k} - \frac{d_e}{2} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}^{(k-\frac{1}{2})} + \frac{d_e}{2} \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k}^{(k+\frac{1}{2})}}{A_c \Delta z_{c,k}} \\
&= \frac{w_{c,k-1/2} - w_{c,k+1/2}}{\Delta z_{c,k}} \\
&\quad + \sum_{e \in c} l_e \frac{\Delta z_{e,k} u_{e,k} - \frac{d_e}{4} \left(\frac{\Delta z_{e,k-1}}{\Delta z_{c,k-1}} J_{e,k-1} u_{e,k-1} + \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k} \right) + \frac{d_e}{4} \left(\frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k} + \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} u_{e,k+1} \right)}{A_c \Delta z_{c,k}}
\end{aligned}$$

$$\begin{aligned}
\Rightarrow (\nabla \cdot \mathbf{v})_{c,k} &= \left[\sum_{e \in c} \left(l_e \frac{\Delta z_{e,k} u_{e,k}}{A_c \Delta z_{c,k}} \right) + \frac{w_{c,k-1/2} - w_{c,k+1/2}}{\Delta z_{c,k}} \right] \\
&\quad - \frac{\mathbf{I}}{2} \sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta z_{c,k}} \left[\left(\frac{\Delta z_{e,k-1}}{\Delta z_{c,k-1}} J_{e,k-1} u_{e,k-1} + \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k} \right) \right. \\
&\quad \left. - \left(\frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} u_{e,k} + \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} u_{e,k+1} \right) \right]. \quad (33.69)
\end{aligned}$$

The terms in the first line correspond to Eq. (26.63), the terms in the last two equations are the orographic correction terms. These disappear in the case $\mathbf{J} = \mathbf{o}$. The terms marked **blue** cancel each other out and can be ignored.

33.4.4.2 Deep atmosphere

In the deep atmosphere, Eq. (33.67) to

$$(\nabla \cdot \mathbf{v})_{c,k} = \frac{\mathbf{I}}{V_{c,k}} \left(\sum_{e \in c} A_{e,k} u_{e,k} + A_{c,k-1/2} v_{c,k-1/2}^{(v)} - A_{c,k+1/2} v_{c,k+1/2}^{(v)} \right). \quad (33.70)$$

If you put Eq. (33.63), you get

$$\begin{aligned}
(\nabla \cdot \mathbf{v})_{c,k} &= \frac{\mathbf{I}}{V_{c,k}} \left(\sum_{e \in c} A_{e,k} u_{e,k} + A_{c,k-1/2} v_{c,k-1/2, \text{GK}}^{(v)} - A_{c,k+1/2} v_{c,k+1/2, \text{GK}}^{(v)} \right) \\
&= \frac{\mathbf{I}}{V_{c,k}} \left[\sum_{e \in c} (A_{e,k} u_{e,k}) + A_{c,k-1/2} w_{c,k-1/2} - A_{c,k+1/2} w_{c,k+1/2} \right] \\
&\quad - \frac{\mathbf{I}}{V_{c,k}} \sum_{e \in c} \left[A_{c,k-1/2} \frac{\mathbf{I}}{2} \left(\frac{A_{e,k} d_{e,k}}{2 V_{c,k}} J_{e,k} u_{e,k} + \frac{A_{e,k-1} d_{e,k-1}}{2 V_{c,k-1}} J_{e,k-1} u_{e,k-1} \right) \right. \\
&\quad \left. - A_{c,k+1/2} \frac{\mathbf{I}}{2} \left(\frac{A_{e,k} d_{e,k}}{2 V_{c,k}} J_{e,k} u_{e,k} + \frac{A_{e,k+1} d_{e,k+1}}{2 V_{c,k+1}} J_{e,k+1} u_{e,k+1} \right) \right]
\end{aligned}$$

$$\begin{aligned}
\Rightarrow (\nabla \cdot \mathbf{v})_{c,k} &= \frac{\mathbf{I}}{V_{c,k}} \left[\sum_{e \in c} (A_{e,k} u_{e,k}) + A_{c,k-1/2} w_{c,k-1/2} - A_{c,k+1/2} w_{c,k+1/2} \right] \\
&\quad + \frac{\mathbf{I}}{V_{c,k}} \sum_{e \in c} \left[- A_{c,k-1/2} \left(\frac{A_{e,k} d_{e,k}}{4 V_{c,k}} J_{e,k} u_{e,k} + \frac{A_{e,k-1} d_{e,k-1}}{4 V_{c,k-1}} J_{e,k-1} u_{e,k-1} \right) \right. \\
&\quad \left. + A_{c,k+1/2} \left(\frac{A_{e,k} d_{e,k}}{4 V_{c,k}} J_{e,k} u_{e,k} + \frac{A_{e,k+1} d_{e,k+1}}{4 V_{c,k+1}} J_{e,k+1} u_{e,k+1} \right) \right]. \quad (33.71)
\end{aligned}$$

The in Eq. (33.69) possible simplification is not applicable here.

33.5 Ellipsoidal modification of the grid

34 REVERSIBLE DYNAMICS

The aim of this chapter is to derive how differential and algebraic operators and boundary conditions are to be discretized. To do this, consider the atmosphere $\mathcal{A} \subseteq \mathbb{R}^3$ as an open set and use the reversible equations of dry air with the boundary conditions as the system of equations.

$$\mathbf{v} \cdot \mathbf{n} = 0 \quad (34.1)$$

at the top and

$$\mathbf{v} = 0 \quad (34.2)$$

at the bottom.

34.1 Prognostic variables and equations

As prognostic variables

- is the mass density ρ in the centers of the boxes,
- the potential temperature density $\tilde{\theta}$ in the centers of the boxes,
- is the horizontal velocity u at the edges of the cells
- the vertical velocity w in the levels as well
- the temperature T in the centers of the boxes as a semi-prognostic variable

chosen. The Hamilton function H is then written as a function of $\rho, \tilde{\theta}$ and $\mathbf{v}$,

$$H = H(\rho, \tilde{\theta}, \mathbf{v}). \quad (34.3)$$

The prognostic equations for this case were derived in Section 10.1.2, they are

$$\frac{\partial \mathbf{v}}{\partial t} = -c^{(p)} \theta \nabla \Pi - \nabla k + \mathbf{v} \times \boldsymbol{\eta} - \nabla \varphi, \quad (34.4)$$

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}), \quad (34.5)$$

$$\frac{\partial \tilde{\theta}}{\partial t} = -\nabla \cdot (\tilde{\theta} \mathbf{v}), \quad (34.6)$$

$$T = f(\rho, \tilde{\theta}). \quad (34.7)$$

The function f in Eq. (34.7) is the thermal equation of state of ideal gases, $\boldsymbol{\eta} := \boldsymbol{\xi} + \mathbf{f}$ is the absolute vorticity.

34.2 Discretization of Poisson brackets

The Poisson brackets are global integrals. One therefore defines a discrete integral operator according to the substitution

$$\int_{\mathcal{A}} \psi(\mathbf{r}) d^3 r \rightarrow \sum_{i=1}^N \psi_i V_i, \quad (34.8)$$

here $\psi(\mathbf{r})$ is an integrable scalar or vector field, ψ_i is the value of the discretized version of ψ in grid box i , V_i is the volume of grid box i and N is the number of grid boxes. The Poisson brackets are calculated according to the basic approach

$$\frac{dF[\mathbf{u}]}{dt} = \frac{d}{dt} \int_A f(\mathbf{u}(t)) d^3r = \int_A \frac{\delta F}{\delta \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial t} d^3r \rightarrow \sum_{c,k} \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial t} \right)_{c,k} V_{c,k} \quad (34.9)$$

discretized. First the Hamilton functional is needed. One discretizes Eq. (10.81) in the form

$$H(\varrho, \tilde{s}, \mathbf{v}) = \sum_{c,k} \left[\frac{1}{2} \varrho_{c,k} (\mathbf{v} \cdot \mathbf{v})_{c,k} + \varrho_{c,k} \mathcal{P}_{c,k} + \tilde{I}_{c,k} \right] V_{c,k}. \quad (34.10)$$

This is divided into two parts

$$H_{\text{kin}}(\mathbf{v}) = \sum_{c,k} \frac{1}{2} \varrho_{c,k} (\mathbf{v} \cdot \mathbf{v})_{c,k} V_{c,k}, \quad (34.11)$$

$$H_{I'}(\varrho, \tilde{s}) = \sum_{c,k} \left(\varrho_{c,k} \mathcal{P}_{c,k} + \tilde{I}_{c,k} \right) V_{c,k}. \quad (34.12)$$

The proportion of kinetic energy can be divided even further:

$$H_{\text{kin}}^{(u)}(u) = \sum_{c,k} \frac{1}{2} \varrho_{c,k} \sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta \mathcal{Z}_{c,k}} \Delta \mathcal{Z}_{e,k} u_{e,k}^2 V_{c,k} = \sum_{c,k} \sum_{e \in c} \frac{\varrho_{c,k} l_e d_e \Delta \mathcal{Z}_{e,k}}{4} u_{e,k}^2, \quad (34.13)$$

$$\begin{aligned} H_{\text{kin}}^{(w)}(w) &= \sum_{c,k} \frac{1}{2} \varrho_{c,k} \left(\frac{\Delta \mathcal{Z}_{c,k-1/2}}{2 \Delta \mathcal{Z}_{c,k}} w_u^2 + \frac{\Delta \mathcal{Z}_{c,k+1/2}}{2 \Delta \mathcal{Z}_{c,k}} w_l^2 \right) V_{c,k} \\ &= \sum_{c,k} \left(\frac{\varrho_{c,k} \Delta \mathcal{Z}_{c,k-1/2}}{4} w_{c,k+1/2}^2 + \frac{\varrho_{c,k} \Delta \mathcal{Z}_{c,k+1/2}}{4} w_{c,k+1/2}^2 \right) A_c \end{aligned} \quad (34.14)$$

An alternative formulation of kinetic energy is

$$H_{\text{kin}}^*(\mathbf{v}) := \sum_{c,k} \frac{1}{2} (\varrho \mathbf{v} \cdot \mathbf{v})_{c,k} V_{c,k}, \quad (34.15)$$

$$H_{\text{kin}}^{(u,*)}(u) := \sum_{c,k} \sum_{e \in c} \frac{l_e d_e \Delta \mathcal{Z}_{e,k}}{4} \widetilde{\varrho}_{c,k}^{(e)} u_{e,k}^2, \quad (34.16)$$

$$H_{\text{kin}}^{(w,*)}(w) := \sum_{c,k} \left(\frac{\Delta \mathcal{Z}_{c,k-1/2}}{4} \widetilde{\varrho}_{c,k}^{(k-1/2)} w_{c,k-1/2}^2 + \frac{\Delta \mathcal{Z}_{c,k+1/2}}{4} \widetilde{\varrho}_{c,k}^{(k+1/2)} w_{c,k+1/2}^2 \right) A_c. \quad (34.17)$$

Here $\widetilde{\varrho}_{c,k}^{(e)}$ is an averaging operator on the edges and $\widetilde{\varrho}_{c,k}^{(k+1/2)}$ is an averaging operator on the points where w is placed. These operators must

$$\sum_{e,k} \widetilde{\varrho}_{c,k}^{(e)} V_{e,k} = \sum_{c,k} \varrho_{c,k} V_{c,k}, \quad (34.18)$$

$$\sum_{c,k} \widetilde{\varrho}_{c,k}^{(k+1/2)} V_{c,k+1/2} = \sum_{c,k} \varrho_{c,k} V_{c,k} \quad (34.19)$$

in order not to endanger mass conservation.

34.2.1 Discretization of functional derivatives

Eq. (A.122) is discretized in the form

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \sum_{c,k} [f(\mathbf{u}_{c,k} + \varepsilon \mathbf{h}_{c,k}) - f(\mathbf{u}_{c,k})] V_{c,k} \stackrel{!}{=} \sum_{c,k} \left(\frac{\delta F}{\delta \mathbf{u}} \right)_{c,k} \cdot \mathbf{h}_{c,k} V_{c,k}. \quad (34.20)$$

The functional derivative is the discrete function that fulfills this for all auxiliary functions $\mathbf{h}_{c,k}$. $\mathbf{h}$ is a tuple of state variables. It can also be summed over volumes other than $V_{c,k}$.

For the functional derivatives according to the thermodynamic quantities one obtains

$$\left(\frac{\delta H_{\text{kin}}}{\delta \rho}\right)_{c,k} = \frac{\mathbf{I}}{2} (\mathbf{v} \cdot \mathbf{v})_{c,k}, \quad \left(\frac{\delta H_{I'}}{\delta \rho}\right)_{c,k} = \mathcal{P}_{c,k} + \frac{\partial \tilde{I}_{c,k}}{\partial \rho}, \quad \left(\frac{\delta H_{I'}}{\delta q_1}\right)_{c,k} = \frac{\partial \tilde{I}_{c,k}}{\partial q_1}. \quad (34.21)$$

The equations (34.16) - (34.17) can be written in the form

$$H_{\text{kin}}^{(u,\star)}(u) := \sum_{c,k} \sum_{e \in c} V_{e,k} \widetilde{\rho}_{c,k}^{(e)} \frac{u_{e,k}^2}{2}, \quad (34.22)$$

$$\begin{aligned} H_{\text{kin}}^{(w,\star)}(w) &:= \sum_{c,k} \left(\frac{\Delta \mathcal{Z}_{c,k-1/2}}{4} \widetilde{\rho}_{c,k}^{(k-1/2)} w_{c,k-1/2}^2 + \frac{\Delta \mathcal{Z}_{c,k+1/2}}{4} \widetilde{\rho}_{c,k}^{(k+1/2)} w_{c,k+1/2}^2 \right) A_c \\ &= \sum_{c,k} \left(\frac{\Delta \mathcal{Z}_{c,k-1/2}}{4} \widetilde{\rho}_{c,k}^{(k-1/2)} w_{c,k-1/2}^2 + \frac{\Delta \mathcal{Z}_{c,k+1/2}}{4} \widetilde{\rho}_{c,k}^{(k+1/2)} w_{c,k+1/2}^2 \right) A_c \\ &= \sum_{c,k} \widetilde{\rho}_{c,k}^{(k+1/2)} \frac{w_{c,k+1/2}^2}{2} V_{c,k+1/2} \end{aligned} \quad (34.23)$$

rewrite. There were

$$V_{e,k} = \frac{l_e d_e \Delta \mathcal{Z}_{e,k}}{2} \quad (34.24)$$

and

$$V_{c,k+1/2} = A_c \Delta \mathcal{Z}_{c,k+1/2} \quad (34.25)$$

used. This implies

$$\left(\frac{\delta H_{\text{kin}}^{\star}}{\delta \rho}\right)_{c,k} = \frac{\mathbf{I}}{2} (\mathbf{v} \cdot \mathbf{v})_{c,k}, \quad (34.26)$$

since the functional derivative can also be evaluated at the boundaries of the boxes and then interpolated back to the center points using a scalar product.

34.2.1.1 Shallow atmosphere

From Eq. (34.13) follows

$$\frac{H_{\text{kin}}^{(u)}(u + \varepsilon h) - H_{\text{kin}}^{(u)}(u)}{\varepsilon} = \sum_{c,k} \sum_{e \in c} \frac{\rho_{c,k} l_e d_e \Delta \mathcal{Z}_{e,k}}{2} u_{e,k} h_{e,k} + O(h^2) = \sum_{c,k} \sum_{e \in c} \rho_{c,k} u_{e,k} h_{e,k} V_{e,k} + O(h^2). \quad (34.27)$$

The sum over cells can be rewritten as a sum over edges

$$\begin{aligned} \frac{H_{\text{kin}}^{(u)}(u + \varepsilon h) - H_{\text{kin}}^{(u)}(u)}{\varepsilon} &= \sum_{e,k} \left(\rho_{c_1(e),k} + \rho_{c_2(e),k} \right) u_{e,k} h_{e,k} V_{e,k} + O(h^2) \\ &= 2 \sum_{e,k} \frac{\rho_{c_1(e),k} + \rho_{c_2(e),k}}{2} u_{e,k} h_{e,k} V_{e,k} + O(h^2) \end{aligned} \quad (34.28)$$

The prefactor two stands for the two spatial directions under consideration. The two cells bordering the edge e were labeled c_o and c_i . Therefore applies

$$\left(\frac{\delta H}{\delta \mathbf{v}} \right)_{e,k} = \frac{\varrho_{c_1(e),k} + \varrho_{c_2(e),k}}{2} u_{e,k}. \quad (34.29)$$

Analogously it follows from Eq. (34.14)

$$\begin{aligned} \frac{H_{\text{kin}}^{(w)}(w + \varepsilon h) - H_{\text{kin}}^{(w)}(w)}{\varepsilon} &= \sum_{c,k} \left(\frac{\varrho_{c,k} \Delta z_{c,k-1/2}}{2} w_{c,k-1/2} h_{c,k-1/2} + \frac{\varrho_{c,k} \Delta z_{c,k+1/2}}{2} w_{c,k+1/2} h_{c,k+1/2} \right) A_c \\ &= \sum_{c,k} \left(\frac{\varrho_{c,k}}{2} w_{c,k+1/2} h_{c,k+1/2} + \frac{\varrho_{c,k+1}}{2} w_{c,k+1/2} h_{c,k+1/2} \right) \Delta z_{c,k+1/2} A_c. \end{aligned} \quad (34.30)$$

An index shift was made. With $V_{c,k+1/2} = A_c \Delta z_{c,k+1/2}$ you get

$$\frac{H_{\text{kin}}^{(w)}(w + \varepsilon h) - H_{\text{kin}}^{(w)}(w)}{\varepsilon} = \sum_{c,k} \frac{\varrho_{c,k} + \varrho_{c,k+1}}{2} w_{c,k+1/2} h_{c,k+1/2} V_{c,k+1/2}. \quad (34.31)$$

Thus follows

$$\left(\frac{\delta H}{\delta \mathbf{v}} \right)_{c,k+1/2} = \frac{\varrho_{c,k} + \varrho_{c,k+1}}{2} w_{c,k+1/2}. \quad (34.32)$$

Using the modified operator $H_{\text{kin}}^*(\mathbf{v})$ from Eq. (34.15), you get

$$\left(\frac{\delta H^*}{\delta \mathbf{v}} \right)_{e,k} = \widetilde{\varrho}_{c,k}^{(e)} u_{e,k}, \quad (34.33)$$

$$\left(\frac{\delta H^*}{\delta \mathbf{v}} \right)_{c,k+1/2} = \widetilde{\varrho}_{c,k}^{(k+1/2)} w_{c,k+1/2}. \quad (34.34)$$

34.2.1.2 Deep atmosphere

Eq. (34.27) generalizes with

$$V_{e,k} := A_{e,k} \frac{d_{e,k}}{2} \quad (34.35)$$

to the deep atmosphere as follows:

$$\frac{H_{\text{kin}}^{(u)}(u + \varepsilon h) - H_{\text{kin}}^{(u)}(u)}{\varepsilon} = \sum_{c,k} \sum_{e \in c} \frac{\varrho_{c,k} d_{e,k} A_{e,k}}{2} u_{e,k} h_{e,k} + O(h^2) = \sum_{c,k} \sum_{e \in c} \varrho_{c,k} u_{e,k} h_{e,k} V_{e,k} + O(h^2) \quad (34.36)$$

Now write down the sum over cells again as a sum over edges:

$$\begin{aligned} \frac{H_{\text{kin}}^{(u)}(u + \varepsilon h) - H_{\text{kin}}^{(u)}(u)}{\varepsilon} &= \sum_{e,k} \left(\varrho_{c_1(e),k} + \varrho_{c_2(e),k} \right) u_{e,k} h_{e,k} V_{e,k} + O(h^2) \\ &= 2 \sum_{e,k} \frac{\varrho_{c_1(e),k} + \varrho_{c_2(e),k}}{2} u_{e,k} h_{e,k} V_{e,k} + O(h^2) \end{aligned} \quad (34.37)$$

This also applies in the deep atmosphere

$$\left(\frac{\delta H}{\delta \mathbf{v}} \right)_{e,k} = \frac{\varrho_{c_1(e),k} + \varrho_{c_2(e),k}}{2} u_{e,k}. \quad (34.38)$$

The procedure is analogous to Eq. (34.27):

$$\begin{aligned}
\frac{H_{\text{kin}}^{(w)}(w + \varepsilon h) - H_{\text{kin}}^{(w)}(w)}{\varepsilon} &= \sum_{c,k} \left(\frac{\varrho_{c,k} A_{c,k-1/2} \Delta z_{c,k-1/2}}{2 V_{c,k}} w_{c,k-1/2} h_{c,k-1/2} + \frac{\varrho_{c,k} A_{c,k+1/2} \Delta z_{c,k+1/2}}{2 V_{c,k}} w_{c,k+1/2} h_{c,k+1/2} \right) V_{c,k} \\
&= \sum_{c,k} \frac{\varrho_{c,k} A_{c,k-1/2} \Delta z_{c,k-1/2}}{2} w_{c,k-1/2} h_{c,k-1/2} + \frac{\varrho_{c,k} A_{c,k+1/2} \Delta z_{c,k+1/2}}{2} w_{c,k+1/2} h_{c,k+1/2} \\
&= \sum_{c,k} \frac{\varrho_{c,k+1} A_{c,k+1/2} \Delta z_{c,k+1/2}}{2} w_{c,k+1/2} h_{c,k+1/2} + \frac{\varrho_{c,k} A_{c,k+1/2} \Delta z_{c,k+1/2}}{2} w_{c,k+1/2} h_{c,k+1/2} \\
&= \sum_{c,k} \left(\frac{\varrho_{c,k+1}}{2} w_{c,k+1/2} h_{c,k+1/2} + \frac{\varrho_{c,k}}{2} w_{c,k+1/2} h_{c,k+1/2} \right) \Delta z_{c,k+1/2} A_{c,k+1/2} \quad (34.39)
\end{aligned}$$

With $V_{c,k+1/2} = A_c \Delta z_{c,k+1/2}$ you get

$$\frac{H_{\text{kin}}^{(w)}(w + \varepsilon h) - H_{\text{kin}}^{(w)}(w)}{\varepsilon} = \sum_{c,k} \frac{\varrho_{c,k} + \varrho_{c,k+1}}{2} w_{c,k+1/2} h_{c,k+1/2} V_{c,k+1/2}. \quad (34.40)$$

Thus follows

$$\left(\frac{\delta H}{\delta \mathbf{v}} \right)_{c,k+1/2} = \frac{\varrho_{c,k} + \varrho_{c,k+1}}{2} w_{c,k+1/2}. \quad (34.41)$$

The equations (34.33) - (34.34) also apply in the deep atmosphere.

34.2.2 Gradient on the C-grid in terrain-following coordinates

In Section 26.7 the requirement $\mathbf{v} \cdot \nabla \psi \stackrel{!}{=} \nabla \cdot (\psi \mathbf{v}) - \psi \nabla \cdot \mathbf{v}$ was assumed in order to derive a discretization of the scalar product, the discretizations of „Scalar field x vector field“, gradient and divergence assumed. In section 33.4.2 the scalar product was generalized to terrain-following coordinates. From this, the vertical contravariant measure could be reconstructed in Section 33.4.3. This was used in Sect. 33.4.4 to derive the shape of the divergence in terrain-following coordinates. Now the gradient must be generalized to coordinates following the terrain. For this you use

$$\mathbf{v} \cdot \nabla \psi \equiv \nabla \cdot (\psi \mathbf{v}) - \psi \nabla \cdot \mathbf{v} \quad (34.42)$$

as the equation defining the gradient.

34.2.2.1 Shallow atmosphere

From Eq. (33.69) follow

$$\begin{aligned}
\psi \nabla \cdot \mathbf{v} &= \left[\sum_{e \in c} \left(l_e \frac{\Delta z_{e,k} \psi_{c,k} u_e}{A_c \Delta z_{c,k}} \right) + \frac{\psi_{c,k} w_{c,k-1/2} - \psi_{c,k} w_{c,k+1/2}}{\Delta z_{c,k}} \right] \\
&\quad - \sum_{e \in c} \frac{l_e d_e}{4 A_c \Delta z_{c,k}} \left(\frac{\Delta z_{e,k-1}}{\Delta z_{c,k-1}} J_{e,k-1} \psi_{c,k} u_{e,k-1} - \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} \psi_{c,k} u_{e,k+1} \right) \quad (34.43)
\end{aligned}$$

and

$$\begin{aligned}
\nabla \cdot (\psi \mathbf{v}) &= \left[\sum_{e \in c} \left(l_e \frac{\Delta z_{e,k} (\psi_{o(e),k} + \psi_{c,k}) u_e}{2 A_c \Delta z_{c,k}} \right) + \frac{(\psi_{c,k-1} + \psi_{c,k}) w_{c,k-1/2} - (\psi_{c,k+1} + \psi_{c,k}) w_{c,k+1/2}}{2 \Delta z_{c,k}} \right] \\
&\quad - \sum_{e \in c} \frac{l_e d_e}{4 A_c \Delta z_{c,k}} \left(\frac{\Delta z_{e,k-1}}{\Delta z_{c,k-1}} J_{e,k-1} \frac{\psi_{c,k-1} + \psi_{o(e),k-1}}{2} u_{e,k-1} - \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} \frac{\psi_{c,k+1} + \psi_{o(e),k+1}}{2} u_{e,k+1} \right). \quad (34.44)
\end{aligned}$$

If you take Eq. (34.43) from Eq. (34.44), you get

$$\begin{aligned}
\mathbf{v} \cdot \nabla \psi &= \nabla \cdot (\psi \mathbf{v}) - \psi \nabla \cdot \mathbf{v} \\
&= \left[\sum_{e \in c} \left(l_e \frac{\Delta z_{e,k} (\psi_{o(e),k} - \psi_{c,k}) u_e}{2 A_c \Delta z_{c,k}} \right) + \frac{(\psi_{c,k-1} - \psi_{c,k}) w_{c,k-1/2} - (\psi_{c,k+1} - \psi_{c,k}) w_{c,k+1/2}}{2 \Delta z_{c,k}} \right] \\
&\quad - \sum_{e \in c} \frac{l_e d_e}{4 A_c \Delta z_{c,k}} \left(\frac{\Delta z_{e,k-1}}{\Delta z_{c,k-1}} J_{e,k-1} \frac{\psi_{c,k-1} + \psi_{o(e),k-1} - 2 \psi_{c,k}}{2} \mathbf{u}_{e,k-1} - \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} \frac{\psi_{c,k+1} + \psi_{o(e),k+1} - 2 \psi_{c,k}}{2} \mathbf{u}_{e,k+1} \right) \\
&\stackrel{\text{Glg. (33.47)}}{=} \sum_{e \in c} \frac{l_e d_e}{2 A_c \Delta z_{c,k}} \Delta z_{e,k} (\nabla \psi)_e u_e + \frac{\Delta z_{c,k-1/2}}{2 \Delta z_{c,k}} (\nabla \psi)_{c,k-1/2} w_{c,k-1/2} - \frac{\Delta z_{c,k+1/2}}{2 \Delta z_{c,k}} (\nabla \psi)_{c,k+1/2} w_{c,k+1/2}.
\end{aligned} \tag{34.45}$$

The terms marked **red** only appear on the left side, but not on the right. $\nabla \psi$ can therefore no longer be defined in coordinates following the terrain in such a way that this equation is fulfilled. One could eliminate these terms by calculating the contravariant flux densities only via a one-sided vertical reconstruction, which would be a contradiction to the requirement of mass conservation, since in this case the flux through a surface would depend on which side the surface is viewed from. So the problem cannot be solved exactly.

Nevertheless, conservation of total energy can still be achieved. For this it is necessary that the identity

$$\int_A \psi \nabla \cdot \mathbf{v} d^3 r = - \int_A \mathbf{v} \cdot \nabla \psi d^3 r \tag{34.46}$$

transferred to the discretization. For this calculation, the orientations $\gamma_{e(c)}$ of the vectors must also be taken into account. It will

$$\gamma_{e(c)} := \begin{cases} \mathbf{1}, & \text{falls der Vektor bei } e \text{ in Bezug auf } c \text{ nach au\ss en zeigt,} \\ -\mathbf{1}, & \text{sonst} \end{cases} \tag{34.47}$$

defined. Thus you get

$$\begin{aligned}
\int_A \psi \nabla \cdot \mathbf{v} d^3 r &\rightarrow \sum_{c,k} (\psi \nabla \cdot \mathbf{v})_{c,k} A_c \Delta z_{c,k} \\
&= \sum_{c,k} \left[\sum_{e \in c} \left(l_e \Delta z_{e,k} \psi_{c,k} \gamma_{e(c)} u_e \right) + A_c \left(\psi_{c,k} w_{c,k-1/2} - \psi_{c,k} w_{c,k+1/2} \right) \right. \\
&\quad \left. - \sum_{e \in c} \frac{l_e d_e}{4} \left(\frac{\Delta z_{e,k-1}}{\Delta z_{c,k-1}} J_{e,k-1} \psi_{c,k} u_{e,k-1} - \frac{\Delta z_{e,k+1}}{\Delta z_{c,k+1}} J_{e,k+1} \psi_{c,k} u_{e,k+1} \right) \right].
\end{aligned} \tag{34.48}$$

With an index shift follows

$$\begin{aligned}
\sum_{c,k} (\psi \nabla \cdot \mathbf{v})_{c,k} A_c \Delta z_{c,k} &= \sum_{c,k} \left[\sum_{e \in c} \left(l_e \Delta z_{e,k} \psi_{c,k} \gamma_{e(c)} u_e \right) + A_c \left(\psi_{c,k} w_{c,k-1/2} - \psi_{c,k} w_{c,k+1/2} \right) \right. \\
&\quad \left. - \sum_{e \in c} \frac{l_e d_e}{4} \left(\frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k+1} u_{e,k} - \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k-1} u_{e,k} \right) \right] \\
&= \sum_{c,k} \left[\sum_{e \in c} \left(l_e \Delta z_{e,k} \psi_{c,k} \gamma_{e(c)} u_e \right) + A_c \left(\psi_{c,k} w_{c,k-1/2} - \psi_{c,k} w_{c,k+1/2} \right) \right. \\
&\quad \left. - \sum_{e \in c} \frac{l_e d_e}{4} \left(\frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k+1} u_{e,k} - \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k} u_{e,k} - \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k-1} u_{e,k} + \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k} u_{e,k} \right) \right]
\end{aligned}$$

$$\begin{aligned}
&= \sum_{e,k} \sum_{c \in e} l_e \Delta z_{e,k} \psi_{c,k} \gamma_{e(c)} u_e + \sum_{c,k+1/2} A_c \left(\psi_{c,k} w_{c,k-1/2} - \psi_{c,k} w_{c,k+1/2} \right) \\
&- \sum_{e,k} \sum_{c \in e} \frac{l_e d_e}{4} \left(\frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k+1} u_{e,k} - \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k} u_{e,k} - \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k-1} u_{e,k} + \frac{\Delta z_{e,k}}{\Delta z_{c,k}} J_{e,k} \psi_{c,k} u_{e,k} \right) \\
&= \sum_{e,k} \sum_{c \in e} l_e \Delta z_{e,k} \psi_{c,k} \gamma_{e(c)} u_e - \sum_{c,k+1/2} A_c \Delta z_{c,k+1/2} w_{c,k+1/2} \frac{\psi_{c,k} - \psi_{c,k+1}}{\Delta z_{c,k+1/2}} \\
&- \sum_{e,k} \sum_{c \in e} \frac{l_e d_e}{4} \left(\frac{\Delta z_{e,k}}{\Delta z_{c,k}} \Delta z_{c,k+1/2} J_{e,k} \frac{\psi_{c,k+1} - \psi_{c,k}}{\Delta z_{c,k+1/2}} u_{e,k} + \frac{\Delta z_{e,k}}{\Delta z_{c,k}} \Delta z_{c,k-1/2} J_{e,k} u_{e,k} \frac{\psi_{c,k} - \psi_{c,k-1}}{\Delta z_{c,k-1/2}} \right) \\
&= \sum_{e,k} -l_e d_e \Delta z_{e,k} u_e \sum_{c \in e} -\frac{\psi_{c,k} \gamma_{e(c)}}{d_e} - \sum_{c,k+1/2} A_c \Delta z_{c,k+1/2} w_{c,k+1/2} \frac{\psi_{c,k} - \psi_{c,k+1}}{\Delta z_{c,k+1/2}} \\
&- \sum_{e,k} l_e d_e \Delta z_{e,k} u_{e,k} J_{e,k} \sum_{c \in e} \frac{1}{4} \left(\frac{\Delta z_{c,k+1/2}}{\Delta z_{c,k}} \frac{\psi_{c,k+1} - \psi_{c,k}}{\Delta z_{c,k+1/2}} + \frac{\Delta z_{c,k-1/2}}{\Delta z_{c,k}} \frac{\psi_{c,k} - \psi_{c,k-1}}{\Delta z_{c,k-1/2}} \right) \\
&= \sum_{e,k} -l_e d_e \Delta z_{e,k} u_e \sum_{c \in e} -\frac{\psi_{c,k} \gamma_{e(c)}}{d_e} - \sum_{c,k+1/2} A_c \Delta z_{c,k+1/2} w_{c,k+1/2} (\nabla_z \psi)_{c,k+1/2} \\
&+ \sum_{e,k} l_e d_e \Delta z_{e,k} u_{e,k} J_{e,k} \frac{1}{2} \overline{\left(\frac{\Delta z_{c,k-1/2}}{\Delta z_{c,k}} (\nabla_z \psi)_{c,k-1/2} + \frac{\Delta z_{c,k+1/2}}{\Delta z_{c,k}} (\nabla_z \psi)_{c,k+1/2} \right)}^{(e)} \\
&= \sum_{e,k} -l_e d_e \Delta z_{e,k} u_e \sum_{c \in e} -\frac{\psi_{c,k} \gamma_{e(c)}}{d_e} - \sum_{c,k+1/2} A_c \Delta z_{c,k+1/2} w_{c,k+1/2} (\nabla_z \psi)_{c,k+1/2} \\
&+ \sum_{e,k} l_e d_e \Delta z_{e,k} u_{e,k} J_{e,k} \overline{(\nabla_z \psi)_{c,k+1/2}}^{(k)(e)} \\
&= \sum_{e,k} -l_e d_e \Delta z_{e,k} u_e \left[\sum_{c \in e} \left(-\frac{\psi_{c,k} \gamma_{e(c)}}{d_e} \right) - J_{e,k} \overline{(\nabla_z \psi)_{c,k+1/2}}^{(k)(e)} \right] - \sum_{c,k+1/2} A_c \Delta z_{c,k+1/2} w_{c,k+1/2} (\nabla_z \psi)_{c,k+1/2} \\
&= - \left\{ 2 \sum_{e,k} V_{e,k} u_e \left[\sum_{c \in e} \left(-\frac{\psi_{c,k} \gamma_{e(c)}}{d_e} \right) - J_{e,k} \overline{(\nabla_z \psi)_{c,k+1/2}}^{(k)(e)} \right] + \sum_{c,k+1/2} V_{c,k+1/2} w_{c,k+1/2} (\nabla_z \psi)_{c,k+1/2} \right\}. \tag{34.49}
\end{aligned}$$

The factor 2 stands for the two spatial directions in the horizontal. This results in the discretization

$$(\nabla \psi)_{e,k} = \frac{1}{d_e} \sum_{c \in e} \left(-\psi_{c,k} \gamma_{e(c)} \right) - J_{e,k} \overline{(\nabla_z \psi)_{c,k+1/2}}^{(k)(e)} \tag{34.50}$$

of the gradient in terrain-following coordinates.

34.2.2.2 Deep atmosphere

Even in the deep atmosphere, the discretized product rule of the Nabla operator is not locally valid in coordinates following the terrain. Here, according to Eq. (33.71)

$$\begin{aligned}
\int_A \mathcal{V} \nabla \cdot \mathbf{v} d^3 r &\rightarrow \sum_{c,k} (\mathcal{V} \nabla \cdot \mathbf{v})_{c,k} V_{c,k} = \sum_{c,k} \left\{ \left[\sum_{e \in c} \left(A_{e,k} \mathcal{V}_{c,k} u_{e,k} \right) + A_{c,k-1/2} \mathcal{V}_{c,k} w_{c,k-1/2} - A_{c,k+1/2} \mathcal{V}_{c,k} w_{c,k+1/2} \right] \right. \\
&+ \sum_{e \in c} \left[-A_{c,k-1/2} \left(\frac{A_{e,k} d_{e,k}}{4 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + \frac{A_{e,k-1} d_{e,k-1}}{4 V_{c,k-1}} J_{e,k-1} \mathcal{V}_{c,k} u_{e,k-1} \right) \right. \\
&\left. \left. + A_{c,k+1/2} \left(\frac{A_{e,k} d_{e,k}}{4 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + \frac{A_{e,k+1} d_{e,k+1}}{4 V_{c,k+1}} J_{e,k+1} \mathcal{V}_{c,k} u_{e,k+1} \right) \right] \right\}. \quad (34.51)
\end{aligned}$$

Except for the correction terms for the coordinates following the terrain, the product rule of the Nabla operator is also locally valid here; the derivation in Sect. 26.7.5 still applies. In addition, a global integral disappears over a divergence here too, the reason for this is the same as in the shallow atmosphere. One can therefore limit the partial integration to the terms of the terrain-following correction:

$$\begin{aligned}
&\sum_{c,k} \sum_{e \in c} \left[-A_{c,k-1/2} \left(\frac{A_{e,k} d_{e,k}}{4 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + \frac{A_{e,k-1} d_{e,k-1}}{4 V_{c,k-1}} J_{e,k-1} \mathcal{V}_{c,k} u_{e,k-1} \right) \right. \\
&\left. + A_{c,k+1/2} \left(\frac{A_{e,k} d_{e,k}}{4 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + \frac{A_{e,k+1} d_{e,k+1}}{4 V_{c,k+1}} J_{e,k+1} \mathcal{V}_{c,k} u_{e,k+1} \right) \right] \\
&= \sum_{c,k} \sum_{e \in c} \left[-A_{c,k-1/2} \left(\frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + \frac{V_{e,k-1}}{2 V_{c,k-1}} J_{e,k-1} \mathcal{V}_{c,k} u_{e,k-1} \right) \right. \\
&\left. + A_{c,k+1/2} \left(\frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + \frac{V_{e,k+1}}{2 V_{c,k+1}} J_{e,k+1} \mathcal{V}_{c,k} u_{e,k+1} \right) \right] \\
&= \sum_{c,k} \sum_{e \in c} \left[-A_{c,k-1/2} \frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} - A_{c,k-1/2} \frac{V_{e,k-1}}{2 V_{c,k-1}} J_{e,k-1} \mathcal{V}_{c,k} u_{e,k-1} \right. \\
&\left. + A_{c,k+1/2} \frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + A_{c,k+1/2} \frac{V_{e,k+1}}{2 V_{c,k+1}} J_{e,k+1} \mathcal{V}_{c,k} u_{e,k+1} \right] \\
&= \sum_{c,k} \sum_{e \in c} \left(-A_{c,k-1/2} \frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} - A_{c,k+1/2} \frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k+1} u_{e,k} \right. \\
&\left. + A_{c,k+1/2} \frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k} u_{e,k} + A_{c,k-1/2} \frac{V_{e,k}}{2 V_{c,k}} J_{e,k} \mathcal{V}_{c,k-1} u_{e,k} \right) \\
&= \sum_{c,k} \sum_{e \in c} J_{e,k} u_{e,k} \left(-\frac{A_{c,k-1/2}}{2 V_{c,k}} \mathcal{V}_{c,k} - \frac{A_{c,k+1/2}}{2 V_{c,k}} \mathcal{V}_{c,k+1} + \frac{A_{c,k+1/2}}{2 V_{c,k}} \mathcal{V}_{c,k} + \frac{A_{c,k-1/2}}{2 V_{c,k}} \mathcal{V}_{c,k-1} \right) V_{e,k} \\
&= \sum_{c,k} \sum_{e \in c} J_{e,k} u_{e,k} \left(\frac{A_{c,k-1/2}}{2 V_{c,k}} \Delta \mathcal{Z}_{c,k-1/2} \frac{\mathcal{V}_{c,k-1} - \mathcal{V}_{c,k}}{\Delta \mathcal{Z}_{c,k-1/2}} + \frac{A_{c,k+1/2}}{2 V_{c,k}} \Delta \mathcal{Z}_{c,k+1/2} \frac{\mathcal{V}_{c,k} - \mathcal{V}_{c,k+1}}{\Delta \mathcal{Z}_{c,k+1/2}} \right) V_{e,k} \\
&= \sum_{c,k} \sum_{e \in c} J_{e,k} u_{e,k} \overline{(\nabla_z \mathcal{V})}_{c,k+1/2}^{(k)} V_{e,k} = - \sum_{c,k} \sum_{e \in c} -J_{e,k} u_{e,k} \overline{(\nabla_z \mathcal{V})}_{c,k+1/2}^{(k)} V_{e,k} \\
&= - \sum_{c,k} \sum_{e \in c} -J_{e,k} 2 u_{e,k} \frac{1}{2} \overline{(\nabla_z \mathcal{V})}_{c,k+1/2}^{(k)} V_{e,k} = - \sum_{e,k} J_{e,k} u_{e,k} V_{e,k} \left(-2 \sum_{c \in e} \frac{1}{2} \overline{(\nabla_z \mathcal{V})}_{c,k+1/2}^{(k)} \right) \\
&= -2 \sum_{e,k} u_{e,k} V_{e,k} \left(-J_{e,k} \overline{(\nabla_z \mathcal{V})}_{c,k+1/2}^{(k)} \right) \quad (34.52)
\end{aligned}$$

Therefore this also applies in the deep atmosphere

$$(\nabla \psi)_{e,k} = \frac{1}{d_{e,k}} \sum_{c \in e} \left(-\psi_{c,k} \gamma_{e(c)} \right) - J_{e,k} \overline{(\nabla_z \psi)_{c,k+1/2}}^{(k)(e)}, \quad (34.53)$$

where only this order of the averaging operators is permitted here.

34.2.3 Three-dimensional extension of the helicity bracket

$$\sum_{e,k} \bar{\rho}_c^{(e)} v_e \frac{\partial v_{e,k}}{\partial t} = \sum_{e,k} \bar{\rho}_c^{(e)} v_e \overline{\rho_w \cdot \eta_t^{(e)}}^{(k)} \quad (34.54)$$

34.2.4 Verification of conservation of energy

Since the Hamilton function does not explicitly depend on time, it is equal to the total energy. If you put in Eq. (10.66) $F = H$ is obtained

$$\frac{dH}{dt} = \{H, H\} = \{H, Z_a, H\} + \{H, H\}_\ell + \{H, H\}_{\tilde{s}}. \quad (34.55)$$

Still apply

$$\{H, Z_a, H\} \stackrel{\text{Glg. (10.54)}}{=} 0, \quad \{H, H\}_\ell \stackrel{\text{Glg. (10.50)}}{=} 0, \quad \{H, H\}_{\tilde{s}} \stackrel{\text{Glg. (10.51)}}{=} 0. \quad (34.56)$$

This implies conservation of energy

$$H = \text{const.} \quad (34.57)$$

In order to transfer energy conservation to spatial discretization, three requirements must be taken into account:

1. The helicity bracket $\{H, Z_a, H\} = \{K, Z_a, H\}$ is energetically inactive.
2. The following applies: $\{H, H\}_\ell = \{K, H\}_\ell + \{I', H\}_\ell = 0$.
3. We have $\{H, H\}_{\tilde{s}} = \{K, H\}_{\tilde{s}} + \{I', H\}_{\tilde{s}} = 0$.

The first point corresponds to the fact that the generalized Coriolis force does no work, which was already discussed in Chap. 28 was detected. The second and third statements have the same mathematical requirement. Add to this the equations (10.78) - (10.79), which results in

$$\int_A \underbrace{-\rho \mathbf{v} \cdot \nabla \varphi}_A \underbrace{-c_d^{(p)} \rho \theta \mathbf{v} \cdot \nabla \Pi}_B \underbrace{-\rho \nabla \cdot (\rho \mathbf{v})}_A \underbrace{-c_d^{(p)} \Pi \nabla \cdot (\rho \theta \mathbf{v})}_B d^3r = 0 \quad (34.58)$$

leads. The integrals over the terms A and B cancel each other out. The following two facts were used:

1. The calculation rule $\nabla \cdot (\psi \mathbf{v}) = \mathbf{v} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{v}$.
2. Global integrals over $\nabla \cdot (\psi \mathbf{v})$ disappear with Gauss' theorem due to kinematic boundary conditions.

Both facts also apply in discretization. The evidence for this has already been provided:

1. The definition of the gradient in section 34.2.2 ensures that $\nabla \cdot (\psi \mathbf{v}) = \mathbf{v} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{v}$ also applies in the discretization.
2. The fact that global integrals disappear over divergences has already been proven in Sect. 26.5.

Another aspect should be pointed out here: one discretizes Eq. (34.58), θ only occurs at the edges of the lattice, not in the cell centers. You can freely choose the value of θ on the edge, as long as you also do this in the pressure gradient acceleration. This will be used in Section 34.4 to calculate θ on the edge in such a way that the accuracy

of the flow operator $-\nabla \cdot (\rho \theta \mathbf{v})$ is increased. The θ -conservation itself is not violated by this, since what flows out of one grid box continues to flow into the neighboring one.

Pressure gradient and gravitational acceleration as well as the generalized Coriolis force are covered here. The gradient of kinetic energy, however, cancels out in the Poisson brackets because, although it transports kinetic energy, it does not create or destroy any energy. This will be repeated here. To see this, write down the momentum equation in the form

$$\frac{\partial \mathbf{v}}{\partial t} = -\nabla k + \mathbf{l}, \quad (34.59)$$

where pressure gradient and gravitational acceleration were combined in the term $\mathbf{l}$. The Coriolis force can be ignored here. Scalar multiplication by $\mathbf{v}$ yields

$$\mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v} \cdot \nabla k + \mathbf{v} \cdot \mathbf{l} \quad \Leftrightarrow \quad \frac{\partial k}{\partial t} = -\mathbf{v} \cdot \nabla k + \mathbf{v} \cdot \mathbf{l}.$$

Multiplying this by the mass density ρ gives

$$\rho \frac{\partial k}{\partial t} = -\rho \mathbf{v} \cdot \nabla k + \rho \mathbf{v} \cdot \mathbf{l}. \quad (34.60)$$

The continuity equation is:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}). \quad (34.61)$$

Multiplying this by the specific kinetic energy k gives

$$k \frac{\partial \rho}{\partial t} = -k \nabla \cdot (\rho \mathbf{v}). \quad (34.62)$$

If you add the equations (34.60) and (34.62), you get

$$\frac{\partial (\rho k)}{\partial t} = -\nabla \cdot (\rho k \mathbf{v}) + \mathbf{v} \cdot \mathbf{l}. \quad (34.63)$$

This means that only the global integral over $\mathbf{v} \cdot \mathbf{l}$ contributes to the evolution of the total kinetic energy of the atmosphere. The derivation only includes calculation rules for $\frac{\partial}{\partial t}$ and the rule $\nabla \cdot (\psi \mathbf{v}) = \mathbf{v} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{v}$, which is already considered to be fulfilled. The acceleration $-\nabla k$ does not influence the energetic integrals even in the discretization.

Thus, the location discretization developed in this chapter is energetically self-consistent.

34.2.4.1 Recording a hydrostatic background state

A hydrostatic background state as described in Sect. 13.7.5 can be used without destroying energy conservation. It must be ensured that:

$$0 = -c^{(p)} \overline{\theta \nabla \Pi} - \nabla \varphi \quad (34.64)$$

also applies discretely. The corresponding terms then have each other in the discretization.

However, this is only the case without orography. However, if mountains are present, the horizontal components of the gradients do not cancel each other out exactly, resulting in a small error in the conservation of energy. However, in the interaction of spatial and time discretization, the advantages of the hydrostatic background state outweigh the disadvantages. The most important advantage here is that the horizontal orographic correction components of $-c^{(p)} \theta \nabla \Pi$ and $-\nabla \varphi$ are two quantities that almost completely cancel each other out, i.e.

$$-c^{(p)} \overline{\theta_{c,k}}^{(e)} J_{e,k} \overline{(\nabla_z \Pi)_{c,k+1/2}}^{(k)} - J_{e,k} \overline{(\nabla_z \varphi)_{c,k+1/2}}^{(k)} \approx 0. \quad (34.65)$$

The remaining difference is largely a discretization error. This becomes smaller if you use a hydrostatic background state, since then only

$$-c^{(p)}\overline{\theta_{c,k}}^{(e)}J_{e,k}(\overline{\nabla_z\Pi'})_{c,k+1/2}^{(k)} - c^{(p)}\overline{\theta'_{c,k}}^{(e)}J_{e,k}(\overline{\nabla_z\Pi})_{c,k+1/2}^{(k)} \quad (34.66)$$

must be calculated.

34.3 Boundary conditions

34.3.1 Upper boundary condition

The kinematic boundary condition $\boldsymbol{v} \cdot \boldsymbol{n} = 0$ is used as the upper boundary condition in the context of reversible dynamics. This corresponds to the model

$$w_{c,1/2} = 0 \quad (34.67)$$

for all cells c .

34.3.2 Lower boundary condition

The lower boundary condition in the context of reversible dynamics is the no-slip boundary condition $\boldsymbol{v} = 0$. Since there are only vertical vector components there, this corresponds

$$w_{c,N_L+\frac{1}{2}} = 0 \quad (34.68)$$

for all cells c .

34.4 Ways to increase order

Within the framework of the formalism developed so far, there are three possible approaches to increasing the convergence order:

1. Modification of the kinetic energy functional including interpolation of the density $\widetilde{\rho}_{c,k}^{(e)}$ and the edge.
2. Interpolation from θ to the edge (see section 34.4.1).
3. Increase the number of edges taken into account when calculating the vorticity flow term.

These remaining freedoms are not sufficient to increase the convergence order of the overall model.

34.4.1 Higher-order tracer advection

The accuracy of the discretization can be increased by not using θ via the arithmetic mean

$$\widetilde{\theta}^{(e)} = \frac{\theta_{c_1(e)} + \theta_{c_2(e)}}{2}, \quad (34.69)$$

what is second order is interpolated to the edge, but in a more complex way. The vertical index k is omitted here because two-dimensionality is assumed in this section and $c_1(e)$, $c_2(e)$ are, as usual, the two lines that border the edge e .

34.4.1.1 One-dimensional flow

First of all, this is viewed one-dimensionally. To do this, one assumes the true location dependence $\theta = \theta(x)$ and assumes that the values of θ are known in the scalar grid points i , which are positioned at locations $x_i = i\Delta x$, i.e

$$\theta_i = \theta(x_i). \quad (34.70)$$

A suitable approximation for $\widetilde{\theta}^{(e)}$ is now sought, i.e. θ at position $x = \frac{\Delta x}{2}$. To do this, first replace the location dependence $\theta(x)$ by $\mu^{(n)}(x)$, where n stands for the convergence order.

For $n = 2$ you do the approach

$$\mu^{(2)}(\mathbf{o}) = \theta(\mathbf{o}), \quad (34.71)$$

$$\mu^{(2)}(\Delta x) = \theta(\Delta x). \quad (34.72)$$

Since you have two linear equations for $\mu^{(2)}$, you do an approach with two coefficients, i.e

$$\mu^{(2)}(x) = a + bx. \quad (34.73)$$

If you insert this into the equations (34.71) - (34.72), you get

$$a = \theta(\mathbf{o}), \quad (34.74)$$

$$a + b\Delta x = \theta(\Delta x). \quad (34.75)$$

This leads to

$$a = \theta_{c_1(e)}, \quad (34.76)$$

$$b = \frac{\theta(\Delta x) - \theta(\mathbf{o})}{\Delta x} = \frac{\theta_{c_2(e)} - \theta_{c_1(e)}}{\Delta x}. \quad (34.77)$$

In order to calculate $\tilde{\theta}^{(e,2)}$ from this, where the superscript two stands for the order, an integration must be carried out over the time interval $[\mathbf{o}, \Delta t]$, where Δt is the length of a time step. You calculate:

$$\tilde{\theta}^{(e,2)} = a + b \frac{\Delta x}{2} = \theta_{c_1(e)} + \frac{\theta(\Delta x) - \theta(\mathbf{o})}{2} = \frac{\theta(\mathbf{o}) + \theta(\Delta x)}{2} \quad (34.78)$$

To obtain a third-order approximation ($n = 3$), one includes the second derivative of θ in the grid cell $c_1(e)$ in the reconstruction of θ , i.e

$$\mu^{(3)}(x) = a + bx + cx^2. \quad (34.79)$$

Follow from this

$$f_{\mathbf{o}} = a, \quad (34.80)$$

$$f_1 = a + b\Delta x + c\Delta x^2, \quad (34.81)$$

$$f_{-1} = a - b\Delta x + c\Delta x^2, \quad (34.82)$$

what is happening

$$a = f_{\mathbf{o}}, \quad (34.83)$$

$$f_{-1} + f_1 = 2a + 2c\Delta x^2 = 2(f_{\mathbf{o}} + c\Delta x^2) \Rightarrow \frac{f_{-1} + f_1}{2} - f_{\mathbf{o}} = c\Delta x^2 \Rightarrow c = \frac{f_{-1} - 2f_{\mathbf{o}} + f_1}{2\Delta x^2}, \quad (34.84)$$

$$f_1 - f_{-1} = 2b\Delta x \Rightarrow b = \frac{f_1 - f_{-1}}{2\Delta x} \quad (34.85)$$

can be reshaped. From this it follows

$$\mu^{(3)}(x) = f_{\mathbf{o}} + \frac{f_1 - f_{-1}}{2\Delta x}x + \frac{f_{-1} - 2f_{\mathbf{o}} + f_1}{2\Delta x^2}x^2. \quad (34.86)$$

The value of this function on the edge ($x = \frac{\Delta x}{2}$) is therefore

$$\begin{aligned}
\mu^{(3)}\left(\frac{\Delta x}{2}\right) &= f_0 + \frac{f_1 - f_{-1}}{4} + \frac{f_{-1} - 2f_0 + f_1}{8} = \frac{8f_0 + 2f_1 - 2f_{-1} + f_{-1} - 2f_0 + f_1}{8} \\
&= \frac{6f_0 + 3f_1 - f_{-1}}{8} = \frac{4f_0 + 4f_1 + 2f_0 - f_1 - f_{-1}}{8} = \frac{f_0 + f_1}{2} + \frac{2f_0 - f_1 - f_{-1}}{8} \\
&= \frac{f_0 + f_1}{2} - \frac{f_1 - 2f_0 + f_{-1}}{8} = \frac{f_0 + f_1}{2} - \Delta x^2 \frac{f_1 - 2f_0 + f_{-1}}{8\Delta x^2} \\
&= \frac{f_0 + f_1}{2} - \frac{\Delta x^2}{8} \delta_x^2 f
\end{aligned} \tag{34.87}$$

with

$$\delta_x^2 f := \frac{f_1 - 2f_0 + f_{-1}}{\Delta x^2} \tag{34.88}$$

as an approximation for the second derivative of θ in the x -direction at the center of the cell $c_i(e)$.

34.4.1.2 Two-dimensional flow

In two dimensions, the one-dimensional formulas are simply applied in every spatial direction. This is not a problem on quadrangular grids where all vectors are parallel to a global coordinate axis. On grids that do not meet this criterion, this is more complicated, which is what the next section will cover.

34.4.1.3 Special features on the hexagonal grid

On the hexagonal grid, the vectors are not aligned along coordinate lines, which complicates the calculation of the second derivatives at the cell centers. Therefore, one does the approach for θ

$$g = g(x, y) = c_1 + c_2 x + c_3 y + c_4 x^2 + c_5 xy + c_6 y^2. \tag{34.89}$$

x and y are calculated on the tangent plane to the sphere in the center of the cell under consideration. The x -axis points in the direction of the edge on which $\tilde{\theta}^{(e)}$ is to be calculated. Now define the coefficient vector

$$\mathbf{f} := \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \end{pmatrix}. \tag{34.90}$$

Only c_4 is relevant for the second derivative in the x -direction at the center of the cell, it applies

$$\frac{\partial^2 g}{\partial x^2}(\mathbf{o}, \mathbf{o}) = 2c_4. \tag{34.91}$$

The goal now is to calculate the vector $\mathbf{f}$. To do this, you first define the vector

$$\mathbf{s} := \begin{pmatrix} \theta(x_1, y_1) \\ \vdots \\ \theta(x_m, y_m) \end{pmatrix} \tag{34.92}$$

the actual values of θ in the cell centers. Here $m \geq 6$ is the number of points that are calculated to calculate $\mathbf{f}$, these are the cell in the center of which the second derivative is to be calculated and all neighboring cells. Now define an error function

$$\psi(\mathbf{f}) := \sum_i^m [g(x_i, y_i) - s_i]^2. \tag{34.93}$$

Now define the polynomial matrix

$$P := \begin{pmatrix} \mathbf{1} & x_1 & y_1 & x_1^2 & x_1 y_1 & y_1^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{1} & x_m & y_m & x_m^2 & x_m y_m & y_m^2 \end{pmatrix}. \quad (34.94)$$

This allows $\mathcal{V}$ in the form

$$\begin{aligned} \mathcal{V}(\mathbf{f}) &= (P\mathbf{f} - \mathbf{s})^2 = (P\mathbf{f}) \cdot (P\mathbf{f}) - 2(P\mathbf{f}) \cdot \mathbf{s} + \mathbf{s}^2 = \sum_{i=1}^m (P\mathbf{f})_i^2 - 2 \sum_{i=1}^m (P\mathbf{f})_i s_i + \sum_{i=1}^m s_i^2 \\ &= \sum_{i=1}^m \left(\sum_{j=1}^n P_{i,j} f_j \right)^2 - 2 \sum_{i=1}^m \left(\sum_{j=1}^n P_{i,j} f_j \right) s_i + \sum_{i=1}^m s_i^2 \end{aligned} \quad (34.95)$$

note down. From this it follows

$$\begin{aligned} \frac{\partial \mathcal{V}(\mathbf{f})}{\partial f_k} &= 2 \sum_{i=1}^m \left(\sum_{j=1}^n P_{i,j} \delta_{j,k} \right) \left(\sum_{j=1}^n P_{i,j} f_j \right) - 2 \sum_{i=1}^m \left(\sum_{j=1}^n P_{i,j} \delta_{j,k} \right) s_i = 0 \\ \Leftrightarrow \frac{\partial \mathcal{V}(\mathbf{f})}{\partial f_k} &= \sum_{i=1}^m \left(\sum_{j=1}^n P_{i,j} \delta_{j,k} \right) \left(\sum_{j=1}^n P_{i,j} f_j \right) - \sum_{i=1}^m \left(\sum_{j=1}^n P_{i,j} \delta_{j,k} \right) s_i = 0 \\ \Leftrightarrow \frac{\partial \mathcal{V}(\mathbf{f})}{\partial f_k} &= \sum_{i=1}^m P_{i,k} \left(\sum_{j=1}^n P_{i,j} f_j \right) - \sum_{i=1}^m P_{i,k} s_i = \sum_{i=1}^m \sum_{j=1}^n P_{i,k} P_{i,j} f_j - \sum_{i=1}^m P_{i,k} s_i = 0 \\ \Leftrightarrow \frac{\partial \mathcal{V}(\mathbf{f})}{\partial f_k} &= \sum_{j=1}^n \sum_{i=1}^m P_{k,i}^T P_{i,j} f_j - \sum_{i=1}^m P_{k,i}^T s_i = \sum_{j=1}^n (P^T P)_{k,j} f_j - \sum_{i=1}^m P_{k,i}^T s_i = 0 \\ \Leftrightarrow \frac{\partial \mathcal{V}(\mathbf{f})}{\partial f_k} &= [(P^T P) \cdot \mathbf{f}]_k - (P^T \cdot \mathbf{s})_k = 0. \end{aligned} \quad (34.96)$$

So the equivalence applies

$$\nabla_k \mathcal{V} = 0 \Leftrightarrow (P^T P) \cdot \mathbf{f} = P^T \cdot \mathbf{s}, \quad (34.97)$$

what to do

$$\mathbf{f} = \left[(P^T P)^{-1} P^T \right] \cdot \mathbf{s} = B \cdot \mathbf{s} \quad (34.98)$$

with

$$B := \left[(P^T P)^{-1} P^T \right] \quad (34.99)$$

can transform. From this we can use Eq. (34.91) calculate the second derivatives in the cell centers in the x-direction.

34.5 HEVI procedure

There is the following conflict between explicit and implicit method:

- Explicit methods are easy to implement and fast. However, the time step resulting from the CFL criterion is usually significantly smaller than the physically necessary one. This significantly reduces the performance of explicit methods. Explicit multi-step procedures also require filters, which can destroy mimetic properties.
- Implicit methods are more complex to implement. Your speed depends on the complexity of the problem. They are more stable than explicit methods and allow a large time step, which contributes positively to their performance.

It follows that a fast implicit method would be ideal for a dynamic core. However, since the equations to be solved

are nonlinear, a three-dimensional implicit method is only possible via an iterative approach. In this section, the compromise chosen is the *HEVI concept*, which stands for *horizontally explicit, vertically implicit*.

34.5.1 Split-explicit techniques

A significant limitation with regard to the time step and thus also with regard to the efficiency of a model is the CFL criterion associated with sound waves. Therefore, the system of equations is often divided into so-called *fast modes* or *divergent modes* on the one hand and the *slow modes*, *advective modes* or *non-divergent modes* on the other hand. The fast modes include all terms associated with sound waves, while the slow modes include the remaining terms. With split-explicit techniques, the fast modes are now integrated with a time step that is approximately three times smaller. In the case of the equation system Equations (34.4) - (34.7), only the advection of the momentum for the larger time step would come into question. The advections of density and entropy, on the other hand, should be counted among the fast modes in order not to have to break down the divergences of the flow density into advection and compression components. However, if one places high demands on the energetic self-consistency of a time step method, splitting off momentum advection does not make sense.

In order to see this, one must first realize that the advection of kinetic energy is connected to the continuity equation and is therefore one of the fast modes. This has already been seen in Section 34.2.4. Therefore, both terms or equations must be integrated with the same time step. In order to preserve the discretized analogue of the Lamb transformation $-(\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla k - (\nabla \times \mathbf{v}) \times \mathbf{v}$, the generalized Coriolis term and thus the complete system of equations must then also be integrated with the smaller time step.

Due to the disadvantages discussed here, no split-explicit option is built into the dynamic core being developed.

34.5.2 Modifications for stabilization

34.5.2.1 Treatment of vertically propagating waves

Vertically propagating waves are treated implicitly for reasons of stability. To do this, you first make a note

$$\theta'' \stackrel{\theta=\tilde{\theta}/\varrho}{=} \frac{\partial \theta}{\partial \varrho} \varrho' + \frac{\partial \theta}{\partial \tilde{\theta}} \tilde{\theta}' = -\frac{\tilde{\theta}}{\varrho^2} \varrho' + \frac{1}{\varrho} \tilde{\theta}', \quad (34.100)$$

$$\Pi'' \stackrel{\text{Glg. (9.71)}}{=} \frac{R_s}{c^{(V)} \tilde{\theta}} \left(\frac{R_s \tilde{\theta}}{p_o} \right)^{R_s/c^{(V)}} \tilde{\theta}'. \quad (34.101)$$

The two lines represent linear developments compared to the previous time step and not differences to the hydrostatic background state, which are denoted by θ' , Π' . The derivatives are abbreviated

$$\alpha := -\frac{\tilde{\theta}}{\varrho^2}, \beta := \frac{1}{\varrho}, \quad (34.102)$$

$$\gamma := \frac{R_s}{c^{(V)} \tilde{\theta}} \Pi \quad (34.103)$$

away. These are calculated in the cell centers, using the old time step (time step n) for the predictor step and the arithmetic mean of the steps n and $n+1$ for the corrector step. The vertical momentum equation is written down in the form

$$\begin{aligned} w_{k+1/2}^{(n+1)} &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left[\left(\frac{\overline{\theta}^{-(k+1/2)}}{\tilde{\theta}_k} + \frac{\overline{\theta}^{(n+1)*}(k+1/2)}{\tilde{\theta}_k'^{(n+1)*}} \right) \frac{\Pi_k'^{(n+1)} - \Pi_{k+1}'^{(n+1)}}{z_k - z_{k+1}} + \frac{\overline{\theta}^{(n+1)}(k+1/2)}{\tilde{\theta}_k'^{(n+1)}} \frac{\overline{\Pi}_k - \overline{\Pi}_{k+1}}{z_k - z_{k+1}} \right] \\ &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta}^{(n+1)*}(k+1/2)}{\tilde{\theta}_k'^{(n+1)*}} \frac{\Pi_k'^{(n+1)} - \Pi_{k+1}'^{(n+1)}}{z_k - z_{k+1}} + \frac{\overline{\theta}^{(n+1)}(k+1/2)}{\tilde{\theta}_k'^{(n+1)}} \frac{\overline{\Pi}_k - \overline{\Pi}_{k+1}}{z_k - z_{k+1}} \right) \\ &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta}^{(n+1)*}(k+1/2)}{\tilde{\theta}_k'^{(n+1)*}} \frac{\Pi_k'^{(n+1)} - \Pi_{k+1}'^{(n+1)}}{z_k - z_{k+1}} + \frac{\overline{\theta}^{(n+1)}(k+1/2)}{\tilde{\theta}_k'^{(n+1)}} \frac{d\overline{\Pi}}{dz} \Big|_{k+1/2} \right). \end{aligned} \quad (34.104)$$

Here ε is the implicit weight, for which $\frac{c^{(r)}}{c^{(p)}}$ is usually used based on the findings in Section 25.5.1.3. $(n+1)^*$ is a preliminary value for the new time step. Now write down the implicit quantities

$$\theta'_k{}^{(n+1)} = \theta'_k{}^{(\text{expl.})} + \theta''_k = \theta'_k{}^{(\text{expl.})} + a_k \rho'_k + \beta_k \tilde{\theta}'_k, \quad (34.105)$$

$$\Pi'_k{}^{(n+1)} = \Pi'_k{}^{(\text{expl.})} + \Pi''_k = \Pi'_k{}^{(\text{expl.})} + \gamma_k \tilde{\theta}'_k. \quad (34.106)$$

The deleted sizes are the deviations from the explicit components, i.e

$$\psi'_k := \psi_k^{(n+1)} - \psi_k^{(\text{expl.})} \quad (34.107)$$

for $\psi = \rho, \tilde{\theta}$. This applies

$$\rho'_k = -\Delta t \frac{M_{k-1/2} - M_{k+1/2}}{V_k}, \quad (34.108)$$

$$\tilde{\theta}'_k = -\Delta t \frac{\overline{\theta_k^{(n+1)*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2}}{V_k}. \quad (34.109)$$

Defined here

$$M_{k+1/2} := A_{k+1/2} \frac{\overline{\rho_k^{(n)}}^{(k+1/2)} w_{k+1/2}^{(n+1)} + \overline{\rho_k^{(n+1)}}^{(k+1/2)} w_{k+1/2}^{(n)}}{2} \quad (34.110)$$

for $1 \leq k \leq N_L - 1$ the vertical covariant mass flow density multiplied by the boundary surfaces $A_{k+1/2}$ of the grid boxes, this is the unknown vector. Putting this into Eq. (34.104), you get

$$\begin{aligned} w_{k+1/2}^{(n+1)} &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} + \Pi''_k - \Pi'_k{}^{(\text{expl.})} - \Pi''_{k+1}}{z_k - z_{k+1}} + \overline{\theta_k^{(n+1)*}}^{(k+1/2)} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \right) \\ \Leftrightarrow w_{k+1/2}^{(n+1)} &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} + \Pi''_k - \Pi'_k{}^{(\text{expl.})} - \Pi''_{k+1}}{z_k - z_{k+1}} + \frac{\theta'_k{}^{(n+1)} + \theta'_{k+1}{}^{(n+1)}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \right) \\ \Leftrightarrow w_{k+1/2}^{(n+1)} &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} + \gamma_k \tilde{\theta}'_k - \Pi'_k{}^{(\text{expl.})} - \gamma_{k+1} \tilde{\theta}'_{k+1}}{z_k - z_{k+1}} + \frac{\theta'_k{}^{(n+1)} + \theta'_{k+1}{}^{(n+1)}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \right) \\ \Leftrightarrow w_{k+1/2}^{(n+1)} &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} + \gamma_k \tilde{\theta}'_k - \Pi'_k{}^{(\text{expl.})} - \gamma_{k+1} \tilde{\theta}'_{k+1}}{z_k - z_{k+1}} + \frac{\theta'_k{}^{(\text{expl.})} + \theta''_k + \theta'_{k+1}{}^{(\text{expl.})} + \theta''_{k+1}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \right) \end{aligned} \quad (34.111)$$

$$\begin{aligned} \Leftrightarrow w_{k+1/2}^{(n+1)} &= w_{k+1/2}^{(\text{expl.})} - \varepsilon \Delta t c^{(p)} \cdot \left(\frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} + \gamma_k \tilde{\theta}'_k - \Pi'_k{}^{(\text{expl.})} - \gamma_{k+1} \tilde{\theta}'_{k+1}}{z_k - z_{k+1}} \right. \\ &\quad \left. + \frac{\theta'_k{}^{(\text{expl.})} + a_k \rho'_k + \beta_k \tilde{\theta}'_k + \theta'_{k+1}{}^{(\text{expl.})} + a_{k+1} \rho'_{k+1} + \beta_{k+1} \tilde{\theta}'_{k+1}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \right). \end{aligned} \quad (34.112)$$

The deleted quantities contain the unknown vector, so put them on the left side:

$$\begin{aligned}
& \varepsilon \Delta t c^{(p)} \left(\frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \gamma_k \tilde{\theta}'_k - \gamma_{k+1} \tilde{\theta}'_{k+1}}{z_k - z_{k+1}} + \frac{a_k \phi'_k + \beta_k \tilde{\theta}'_k + a_{k+1} \phi'_{k+1} + \beta_{k+1} \tilde{\theta}'_{k+1}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \right) \\
&= w_{k+1/2}^{(\text{expl.})} - w_{k+1/2}^{(n+1)} - \varepsilon \Delta t c^{(p)} \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} - \Pi'_{k+1}{}^{(\text{expl.})}}{z_k - z_{k+1}} - \varepsilon \Delta t c^{(p)} \frac{\theta_k'^{(\text{expl.})} + \theta_{k+1}'^{(\text{expl.})}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \\
&\Leftrightarrow \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \gamma_k \tilde{\theta}'_k - \gamma_{k+1} \tilde{\theta}'_{k+1}}{z_k - z_{k+1}} + \frac{a_k \phi'_k + \beta_k \tilde{\theta}'_k + a_{k+1} \phi'_{k+1} + \beta_{k+1} \tilde{\theta}'_{k+1}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \\
&= \frac{w_{k+1/2}^{(\text{expl.})} - w_{k+1/2}^{(n+1)}}{\varepsilon \Delta t c^{(p)}} - \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} - \Pi'_{k+1}{}^{(\text{expl.})}}{z_k - z_{k+1}} - \frac{\theta_k'^{(\text{expl.})} + \theta_{k+1}'^{(\text{expl.})}}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \\
&\Leftrightarrow \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)}}{\varepsilon \Delta t c^{(p)}} \left(\gamma_k \tilde{\theta}'_k - \gamma_{k+1} \tilde{\theta}'_{k+1} \right) + \frac{d\bar{\Pi}}{2 dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left(a_k \phi'_k + \beta_k \tilde{\theta}'_k + a_{k+1} \phi'_{k+1} + \beta_{k+1} \tilde{\theta}'_{k+1} \right) \\
&= \frac{\left(w_{k+1/2}^{(\text{expl.})} - w_{k+1/2}^{(n+1)} \right) (z_k - z_{k+1})}{\varepsilon \Delta t c^{(p)}} - \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \left(\Pi'_k{}^{(\text{expl.})} - \Pi'_{k+1}{}^{(\text{expl.})} \right) - (z_k - z_{k+1}) \left(\theta_k'^{(\text{expl.})} + \theta_{k+1}'^{(\text{expl.})} \right)}{2} \frac{d\bar{\Pi}}{dz} \Big|_{k+1/2} \\
&\Leftrightarrow \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)}}{\varepsilon \Delta t c^{(p)}} \left(- \gamma_k \frac{\overline{\theta_k^{(n+1)*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2}}{V_k} \right. \\
&\quad \left. + \gamma_{k+1} \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)*}}^{(k+3/2)} M_{k+3/2}}{V_{k+1}} \right) \\
&\quad + \frac{d\bar{\Pi}}{2 dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left(- a_k \frac{M_{k-1/2} - M_{k+1/2}}{V_k} - \beta_k \frac{\overline{\theta_k^{(n+1)*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2}}{V_k} \right. \\
&\quad \left. - a_{k+1} \frac{M_{k+1/2} - M_{k+3/2}}{V_{k+1}} - \beta_{k+1} \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)*}}^{(k+3/2)} M_{k+3/2}}{V_{k+1}} \right) \\
&= \frac{\left(w_{k+1/2}^{(\text{expl.})} - w_{k+1/2}^{(n+1)} \right) (z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} - \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \Pi'_k{}^{(\text{expl.})} - \Pi'_{k+1}{}^{(\text{expl.})}}{\Delta t} - \frac{z_k - z_{k+1}}{\Delta t} \left(\theta_k'^{(\text{expl.})} + \theta_{k+1}'^{(\text{expl.})} \right) \frac{d\bar{\Pi}}{2 dz} \Big|_{k+1/2}.
\end{aligned} \tag{34.113}$$

Now take the replacements

$$a_k \rightarrow \frac{a_k}{V_k}, \beta_k \rightarrow \frac{\beta_k}{V_k}, \gamma_k \rightarrow \frac{\gamma_k}{V_k} \tag{34.114}$$

before. It follows

$$\begin{aligned}
& \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} \left[-\gamma_k \left(\overline{\theta_k^{(n+1)^*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
& \left. + \gamma_{k+1} \left(\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
& + \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left[-a_k (M_{k-1/2} - M_{k+1/2}) - \beta_k \left(\overline{\theta_k^{(n+1)^*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
& \left. - a_{k+1} (M_{k+1/2} - M_{k+3/2}) - \beta_{k+1} \left(\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
& = \frac{(w_{k+1/2}^{(\text{expl.})} - w_{k+1/2}^{(n+1)}) (z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} - \frac{\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} \Pi_k^{(\text{expl.})} - \Pi_{k+1}^{(\text{expl.})}}{\Delta t} - \frac{z_k - z_{k+1}}{\Delta t} \left(\theta_k^{(\text{expl.})} + \theta_{k+1}^{(\text{expl.})} \right) \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} \\
& \Leftrightarrow \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} \left[\gamma_k \left(\overline{\theta_k^{(n+1)^*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
& \left. - \gamma_{k+1} \left(\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
& + \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left[a_k (M_{k-1/2} - M_{k+1/2}) + \beta_k \left(\overline{\theta_k^{(n+1)^*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
& \left. + a_{k+1} (M_{k+1/2} - M_{k+3/2}) + \beta_{k+1} \left(\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+3/2)} M_{k+3/2} \right) \right] - \frac{w_{k+1/2}^{(n+1)} (z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} \\
& = -\frac{w_{k+1/2}^{(\text{expl.})} (z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} + \frac{\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} \Pi_k^{(\text{expl.})} - \Pi_{k+1}^{(\text{expl.})}}{\Delta t} + \frac{z_k - z_{k+1}}{\Delta t} \left(\theta_k^{(\text{expl.})} + \theta_{k+1}^{(\text{expl.})} \right) \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2}. \quad (34.115)
\end{aligned}$$

$w_{k+1/2}^{(n+1)}$ also depends on $M_{k+1/2}$. From Eq. (34.110) follows

$$w_{k+1/2}^{(n+1)} = \frac{\frac{2M_{k+1/2}}{A_{k+1/2}} - \overline{\rho_k^{(n+1)}}^{(k+1/2)} w_{k+1/2}^{(n)}}{\overline{\rho_k^{(n)}}^{(k+1/2)}}. \quad (34.116)$$

Putting this into Eq. (34.115), you get

$$\begin{aligned}
& \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} \left[\gamma_k \left(\overline{\theta_k^{(n+1)^*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
& \left. - \gamma_{k+1} \left(\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
& + \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left[a_k (M_{k-1/2} - M_{k+1/2}) + \beta_k \left(\overline{\theta_k^{(n+1)^*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
& \left. + a_{k+1} (M_{k+1/2} - M_{k+3/2}) + \beta_{k+1} \left(\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)^*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
& - \frac{\frac{2M_{k+1/2}}{A_{k+1/2}} - \overline{\rho_k^{(n+1)}}^{(k+1/2)} w_{k+1/2}^{(n)}}{\overline{\rho_k^{(n)}}^{(k+1/2)}} \frac{(z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} \\
& = -\frac{w_{k+1/2}^{(\text{expl.})} (z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} + \frac{\overline{\theta_k^{(n+1)^*}}^{(k+1/2)} \Pi_k^{(\text{expl.})} - \Pi_{k+1}^{(\text{expl.})}}{\Delta t} + \frac{z_k - z_{k+1}}{\Delta t} \left(\theta_k^{(\text{expl.})} + \theta_{k+1}^{(\text{expl.})} \right) \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2}. \quad (34.117)
\end{aligned}$$

For the density $\overline{\rho_k^{(n+1)}}^{(k+1/2)}$ applies

$$\begin{aligned}
 \overline{\rho_k^{(n+1)}}^{(k+1/2)} &= \frac{\mathbf{I}}{2} \rho_k^{(n+1)} + \frac{\mathbf{I}}{2} \rho_{k+1}^{(n+1)} \\
 &= \frac{\mathbf{I}}{2} \rho_k^{(\text{expl.})} - \Delta t \frac{M_{k-1/2} - M_{k+1/2}}{2V_k} + \frac{\mathbf{I}}{2} \rho_{k+1}^{(\text{expl.})} - \Delta t \frac{M_{k+1/2} - M_{k+3/2}}{2V_{k+1}} \\
 &= \overline{\rho_k^{(\text{expl.})}}^{(k+1/2)} - \Delta t \frac{M_{k-1/2} - M_{k+1/2}}{2V_k} - \Delta t \frac{M_{k+1/2} - M_{k+3/2}}{2V_{k+1}}.
 \end{aligned} \tag{34.118}$$

From this it follows

$$\begin{aligned}
 &\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \left[\gamma_k \left(\overline{\theta_k^{(n+1)*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
 &\quad \left. - \gamma_{k+1} \left(\overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
 &+ \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left[a_k (M_{k-1/2} - M_{k+1/2}) + \beta_k \left(\overline{\theta_k^{(n+1)*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2} \right) \right. \\
 &\quad \left. + a_{k+1} (M_{k+1/2} - M_{k+3/2}) + \beta_{k+1} \left(\overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2} - \overline{\theta_k^{(n+1)*}}^{(k+3/2)} M_{k+3/2} \right) \right] \\
 &- \frac{(z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} \frac{\frac{2M_{k+1/2}}{A_{k+1/2}} - w_{k+1/2}^{(n)} \overline{\rho_k^{(\text{expl.})}}^{(k+1/2)} + w_{k+1/2}^{(n)} \Delta t \frac{M_{k-1/2} - M_{k+1/2}}{2V_k} + w_{k+1/2}^{(n)} \Delta t \frac{M_{k+1/2} - M_{k+3/2}}{2V_{k+1}}}{\overline{\rho_k^{(n)}}^{(k+1/2)}} \\
 &= - \frac{w_{k+1/2}^{(\text{expl.})} (z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} + \overline{\theta_k^{(n+1)*}}^{(k+1/2)} \frac{\Pi_k^{(\text{expl.})} - \Pi_{k+1}^{(\text{expl.})}}{\Delta t} + \frac{z_k - z_{k+1}}{\Delta t} \left(\theta_k^{(\text{expl.})} + \theta_{k+1}^{(\text{expl.})} \right) \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2}.
 \end{aligned} \tag{34.119}$$

This is the equation to solve. This is of the form

$$c_{k-1/2} M_{k-1/2} + d_{k+1/2} M_{k+1/2} + e_{k+3/2} M_{k+3/2} = r_{k+1/2}. \tag{34.120}$$

applies to the coefficients

$$\begin{aligned}
 c_{k-1/2} &= \overline{\theta_k^{(n+1)*}}^{(k+1/2)} \gamma_k \overline{\theta_k^{(n+1)*}}^{(k-1/2)} + \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left(a_k + \beta_k \overline{\theta_k^{(n+1)*}}^{(k-1/2)} \right) \\
 &- \frac{(z_k - z_{k+1})}{\varepsilon \Delta t c^{(p)}} \frac{w_{k+1/2}^{(n)}}{2V_k \overline{\rho_k^{(n)}}^{(k+1/2)}},
 \end{aligned} \tag{34.121}$$

$$\begin{aligned}
 d_{k+1/2} &= - \left(\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \right)^2 (\gamma_k + \gamma_{k+1}) + \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left[a_{k+1} - a_k + \overline{\theta_k^{(n+1)*}}^{(k+1/2)} (\beta_{k+1} - \beta_k) \right] \\
 &- \frac{(z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)} \overline{\rho_k^{(n)}}^{(k+1/2)}} \left[\frac{2}{A_{k+1/2}} + \frac{\Delta t w_{k+1/2}^{(n)}}{2} \left(-\frac{\mathbf{I}}{V_k} + \frac{\mathbf{I}}{V_{k+1}} \right) \right],
 \end{aligned} \tag{34.122}$$

$$\begin{aligned}
 e_{k+3/2} &= \overline{\theta_k^{(n+1)*}}^{(k+1/2)} \gamma_{k+1} \overline{\theta_k^{(n+1)*}}^{(k+3/2)} - \frac{d\overline{\Pi}}{2dz} \Big|_{k+1/2} (z_k - z_{k+1}) \left(a_{k+1} + \beta_{k+1} \overline{\theta_k^{(n+1)*}}^{(k+3/2)} \right) \\
 &+ \frac{(z_k - z_{k+1})}{\varepsilon \Delta t c^{(p)}} \frac{w_{k+1/2}^{(n)}}{2V_{k+1} \overline{\rho_k^{(n)}}^{(k+1/2)}},
 \end{aligned} \tag{34.123}$$

$$\begin{aligned}
 r_{k+1/2} = & -\frac{w_{k+1/2}^{(\text{expl.})}(z_k - z_{k+1})}{\varepsilon \Delta t^2 c^{(p)}} + \frac{\overline{\theta_k^{(n+1)*}}^{(k+1/2)} \frac{\Pi_k^{(\text{expl.})} - \Pi_{k+1}^{(\text{expl.})}}{\Delta t}}{\Delta t} + \frac{z_k - z_{k+1}}{\Delta t} \left(\theta_k^{(\text{expl.})} + \theta_{k+1}^{(\text{expl.})} \right) \frac{d\bar{\Pi}}{2dz} \Big|_{k+1/2} \\
 & - \frac{(z_k - z_{k+1}) w_{k+1/2}^{(n)} \overline{\rho_k^{(\text{expl.})}}^{(k+1/2)}}{\varepsilon \Delta t^2 c^{(p)} \overline{\rho_k^{(n)}}^{(k+1/2)}}.
 \end{aligned} \tag{34.124}$$

Linear systems of equations with three-band matrices can be solved using the Thomas algorithm. From the result for $M_{k+1/2}$ the other unknowns can be determined as follows:

$$\rho_k^{(n+1)} = \rho_k^{(\text{expl.})} - \Delta t \frac{M_{k-1/2} - M_{k+1/2}}{V_k}, \tag{34.125}$$

$$\tilde{\theta}_k^{(n+1)} = \tilde{\theta}_k^{(\text{expl.})} - \Delta t \frac{\overline{\theta_k^{(n+1)*}}^{(k-1/2)} M_{k-1/2} - \overline{\theta_k^{(n+1)*}}^{(k+1/2)} M_{k+1/2}}{V_k}, \tag{34.126}$$

$$\Pi_k^{(n+1)} = \Pi_k^{(\text{expl.})} + \gamma_k V_k \left(\tilde{\theta}_k^{(n+1)} - \tilde{\theta}_k^{(\text{expl.})} \right), \tag{34.127}$$

$$w_{k+1/2}^{(n+1)} \stackrel{\text{Glg. (34.116)}}{=} \frac{\frac{2M_{k+1/2}}{A_{k+1/2}} - \overline{\rho_k^{(n+1)}}^{(k+1/2)} w_{k+1/2}^{(n)}}{\overline{\rho_k^{(n)}}^{(k+1/2)}}. \tag{34.128}$$

If you don't want to use a hydrostatic background state, you just have to use the replacements

$$\bar{\theta}_k = 0, \tag{34.129}$$

$$\bar{\Pi}_k = 0, \tag{34.130}$$

$$w_{k+1/2}^{(\text{expl.})} \rightarrow w_{k+1/2}^{(\text{expl.})} - \Delta t \frac{d\bar{\varphi}}{dz} \Big|_{k+1/2} \tag{34.131}$$

make.

34.5.2.2 Horizontal forward-backward method

The forward-backward procedure was presented in Sect. 25.4.1. It does not increase the accuracy, but it does increase the stability of the model. In the dynamic kernel to be formulated here, the horizontal momentum equation is first integrated forward, then the scalar equations are solved with the new values of the velocities.

34.5.3 Performance comparison of different HEVI processes

The performance of a HEVI process with separation of horizontal fast (acute) and slow (advective) components can be generally calculated. Let τ be the acoustic time step and T be the advective time step. We have $T \geq \tau$. However, when processing a complete time step, higher-order methods calculate the corresponding terms several times. n_τ is the number of calculations of the acoustic components and n_T is the number of calculations of the advective components. This allows effective time steps

$$\tau_{\text{eff}} := \frac{\tau}{n_\tau}, \tag{34.132}$$

$$T_{\text{eff}} := \frac{T}{n_T} \tag{34.133}$$

define. The larger these time steps are, the better for the performance of the model. The speed c of the model, i.e. the integrated time t divided by the time required for it, is calculated by

$$c = \frac{t}{\frac{t}{T_{\text{eff}}} t_T + \frac{t}{\tau_{\text{eff}}} t_\tau} = \frac{1}{\frac{1}{T_{\text{eff}}} t_T + \frac{1}{\tau_{\text{eff}}} t_\tau} = \frac{\tau_{\text{eff}} T_{\text{eff}}}{\tau_{\text{eff}} t_T + T_{\text{eff}} t_\tau}. \tag{34.134}$$

Here t_T is the time required for an advective time step and t_τ is the time required for an acoustic time step. With the notation $t_T \equiv at_\tau$ this becomes

$$c = \frac{\tau_{\text{eff}} T_{\text{eff}}}{\tau_{\text{eff}} a t_{\tau} + T_{\text{eff}} t_{\tau}} = \frac{\tau_{\text{eff}}}{t_{\tau}} \frac{T_{\text{eff}}}{a \tau_{\text{eff}} + T_{\text{eff}}}. \quad (34.135)$$

34.5.4 Determination of a predictor-corrector procedure

The basic time-stepping procedure of the model should be explicit. The explicit Euler method is only first order and therefore not precise enough. A multi-step process produces unphysical modes, which is also disadvantageous. Therefore, a predictor-corrector method is used.

34.5.4.1 Keeping the horizontal pressure gradient constant

34.5.5 Summary

The basic architecture of the time step method is that of the predictor-corrector method. In addition, some modifications are made to stabilize and increase efficiency. The basic procedure for each of the three sub-steps is as follows:

1. First, the speed tendencies of the explicit part are calculated. In the second RK step, the final trend is calculated as the arithmetic mean of the two steps.
2. Now the horizontal divergences are calculated using the scalar values of the predictor step and the new values of the horizontal velocity components, diabatic effects are also taken into account. In the second RK step, the final trend is calculated as the arithmetic mean of the two steps.
3. Using the procedure described in section 34.5.2.1, the new values of the vertical velocity and the scalar fields are calculated.
4. Finally, the new values of the mass densities of the tracers are calculated using the continuity equations, see section 36.1.

34.6 Regional version

The atmosphere is global. A regional model is still practical for conducting experiments and operational runs with increased resolution. The reason for choosing the hexagonal grid for the global model developed in this book is its numerical properties, which are similar to the quadrangular grid, combined with quasi-uniformity and orthogonality. Therefore, one could also implement a local model on a hexagonal grid. The disadvantage, however, is the effort that the grid generation process entails as well as the difficulty of parallelization and the possible additional effort that is necessary to achieve satisfactory performance. Therefore, in this section, the previous findings in this chapter will be generalized to a regional longitude-latitude grid, since the pole problem does not occur in a regional model anyway.

34.6.1 Generalization to a length-latitude grid

34.6.2 Nesting

The term *nesting* describes the generation of boundary conditions for a regional model. Be

$$\psi = \psi(\mathbf{x}, z, t) \quad (34.136)$$

a model state, where $\mathbf{x}$ denotes the horizontal coordinates. A state is now generated from a model with a larger domain, which is referred to here as an edge model, for example a global model

$$\varphi = \varphi(\mathbf{x}, z, t), \quad (34.137)$$

which is obtained by spatial and temporal interpolation of the boundary model onto the grid of the target model. In this case, the time is usually linearized linearly between the time steps of the boundary model, i.e

$$\varphi(\mathbf{x}, z, t) = \frac{t_{n+1} - t}{t_{n+1} - t_n} \varphi(\mathbf{x}, z, t_n) + \frac{t - t_n}{t_{n+1} - t_n} \varphi(\mathbf{x}, z, t_{n+1}). \quad (34.138)$$

At each time step of the target model, the model state ψ is moved a little towards φ at the edges of the domain, i.e

$$\psi_{\text{neu}}(\mathbf{x}, z, t) = (1 - f(\mathbf{x})) \psi_{\text{alt}}(\mathbf{x}, z, t) + f(\mathbf{x}) \varphi(\mathbf{x}, z, t). \quad (34.139)$$

Here $f = f(\boldsymbol{x})$ is a function that describes the admixture of the boundary state. The simplest approach would be to set this function to one at the very edge of the domain and zero otherwise. However, this can create relatively sharp gradients, which can emit unphysical waves into the model area. For example, one approach makes more sense

$$f = f[d(\boldsymbol{x})] = \cos \left[\min \left(\frac{d\pi}{2n\Delta x}, \frac{\pi}{2} \right) \right]^2. \quad (34.140)$$

Here, $d(\boldsymbol{x})$ is the distance of the location $\boldsymbol{x}$ from the edge of the domain and n is the number of grid cells within which the weight of the boundary conditions drops to zero. These procedures are also known as *Nudging*.

35 IRREVERSIBLE DYNAMICS

In this chapter, the reversible discretization developed in the previous chapter is extended to include irreversible effects. It is still assumed that the air is dry. The irreversible effects in a dry atmosphere are the diffusions. There are two types of diffusion:

- Temperature Diffusion
- Impulse Diffusion

On the molecular scale, according to Eq. (5.212) also diffusion of mass, but turbulence in a dry atmosphere does not diffuse mass. This is because turbulence diffuses only the mixing ratio, which is unity in a dry atmosphere, and thus no spatial variability to diffuse.

Accordingly, the system of equations Equations (34.4) - (34.7) must be **modified** as follows:

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} &= -c^{(p)} \theta \nabla \Pi - \nabla k + \mathbf{v} \times \boldsymbol{\eta} - \nabla \varphi + \mathbf{f}_R & (35.1) \\ \frac{\partial \varphi}{\partial t} &= -\nabla \cdot (\varrho \mathbf{v}) & (35.2) \\ \frac{\partial \tilde{\theta}}{\partial t} &= -\nabla \cdot (\tilde{\theta} \mathbf{v}) + \frac{q^{(V)}}{c^{(p)} \Pi} & (35.3) \\ \Pi &= f(\tilde{\theta}) & (35.4) \end{aligned}$$

The mass diffusion is included in the continuity equation in the form of the convergence of a flux density $\nabla \cdot (\kappa_\varphi \nabla \varphi)$, where κ_φ is the associated molecular diffusion coefficient. Two effects are included in the thermal power density $q^{(V)}$:

$$q^{(V)} = q_{\text{diss}}^{(V)} + q_{\text{Tdiff}}^{(V)} = \varrho \varepsilon + \nabla \cdot (c_d^{(v)} \varrho \kappa_T \nabla T) \quad (35.5)$$

Here ε is the dissipation. The term $\nabla \cdot (c_d^{(v)} \varrho \kappa_T \nabla T)$ describes the convergence of the heat flux density resulting from the temperature diffusion.

The temperature equation Eq. (35.4) is the same as Eq. (34.7), the diffusive effects also enter into the temperature via $\Delta \varphi$ and $\Delta \tilde{\theta}$. In analogy to the previous chapter, the horizontal and vertical discretizations are also derived separately in this chapter, even if there is no longer any distinction of the vertical spatial direction in a non-hydrostatic model.

All terms developed in this chapter are only calculated in the Predictor step and kept constant in the Corrector step.

35.1 Basic considerations about turbulence parameterizations

The diffusive (irreversible) terms represent a coupling of the continuous world of the Navier-Stokes equations and the molecular scale. As stated in Sect. 8.2.4, momentum diffusion annihilates (dissipates) kinetic energy in favor of internal energy. The atmosphere can be conceptualized as a low pass, where wavelengths $< l_c$ are filtered, where l_c is the characteristic length according to Eq. (17.159).

So far only actual physical equations have been discretized, this is called *direct numerical simulation (DNS)*. However, this approach is problematic if the resolution is Δ

$$2\Delta \gg l_c, \quad (35.6)$$

Such a discretization is namely a low-pass with the cutoff wavelength 2Δ . Accordingly, in a numerical model, the dissipation must begin earlier. According to Eq. (17.159) applies to the kinematic viscosity ν the equation

$$r = (l_c^4 \varepsilon)^{1/3}. \quad (35.7)$$

Accordingly, one expects that

$$\frac{r_{\text{numerisch}}}{r_{\text{molekular}}} \sim \left(\frac{\min(l_m, 2\Delta r)}{l_c} \right)^{4/3} \quad (35.8)$$

is a useful estimate for the numerical viscosity, here l_m is the mixing path length. The restriction to the mixing path length in the meter makes sense because the fluid in the model must never be tougher (more viscous) than the natural medium, otherwise no realistic simulations of the dynamics can be expected. For the vertical mixing path length, Eq. (17.75) within the Ekman layer a value of approx. 20 m is estimated, with this and with the estimates $l_c = 5$ mm one obtains

$$\log_{10} \left(\frac{r_{\text{numerisch}}}{r_{\text{molekular}}} \right) = 4, 8. \quad (35.9)$$

This roughly corresponds to that in Eq. (17.74) obtained value.

Outside the planetary boundary layer, a value for the vertical mixing path length of approx. 100 m can be assumed, as larger eddies exist there. The horizontal mixing path length can be estimated to be approximately 10 km outside the planetary boundary layer (two orders of magnitude greater than the vertical mixing path length). Simulations whose resolution is less than the mixing path length are referred to as *large eddy simulations (LES)*. As the resolution is further increased, the numerical and molecular diffusion coefficients converge.

35.2 Momentum diffusion

The classical Smagorinsky model is used as an approach for momentum diffusion. For this, Eq. (17.172) must now be discretized on the hexagonal grid. To do this, you first average the discretized terms:

$$K_{\Delta} = \rho c_S^2 \Delta^2 \sqrt{\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2} = \rho c_S^2 \Delta^2 \sqrt{\left(\overline{\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}} \right)^2 + \left(\overline{\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}} \right)^2} \quad (35.10)$$

To determine the averaged terms, first take the term $\frac{\partial u}{\partial x}$ as an example and calculate

$$\overline{\frac{\partial u}{\partial x}} = \frac{1}{A_c} \int_{A_c} \frac{\partial u}{\partial x} d^2 r. \quad (35.11)$$

This integral is now evaluated in Cartesian coordinates on the tangential plane:

$$\overline{\frac{\partial u}{\partial x}} = \frac{1}{A_c} \int_{y_1}^{y_2} \int_{x_1(y)}^{x_2(y)} \frac{\partial u}{\partial x} dx dy = \frac{1}{A_c} \int_{y_1}^{y_2} u(x_2, y) - u(x_1, y) dy. \quad (35.12)$$

This can be reformulated as a line integral:

$$\overline{\frac{\partial u}{\partial x}} = \frac{1}{A_c} \int_{\partial A_c} u(x, y) \mathbf{e}_y \cdot d\mathbf{r} = \frac{1}{A_c} \int_{\partial A_c} u(x, y) \cos(\varphi) ds, \quad (35.13)$$

here φ is the angle between $d\mathbf{r}$ and $\mathbf{e}_y$.

35.2.1 Hyperdiffusion

From physical derivations one usually obtains diffusive terms proportional to the second derivative of the field to be diffused. However, for numerical reasons, so-called *Hyperdiffusion* is often used in models, which is proportional to a higher power of the Nabla operator. In the one-dimensional case, the approach for diffusion is 4th order

$$\frac{\partial \psi}{\partial t} = -a \frac{\partial^4 \psi}{\partial x^4}, \quad (35.14)$$

here like a often referred to as *hyperviscosity*. If you do the approach $\psi = \psi_0 \exp(-ikx - \frac{t}{\tau})$, it follows

$$\begin{aligned}
-\frac{\mathbf{I}}{\tau} \psi &= -ak^4 \psi \\
\Leftrightarrow \frac{\mathbf{I}}{\tau} &= ak^4.
\end{aligned} \tag{35.15}$$

The shortest resolved wave has the length $2\Delta x$, from which $k = \frac{2\pi}{2\Delta x} = \frac{\pi}{\Delta x}$. If you put this in, you get

$$\begin{aligned}
\frac{\mathbf{I}}{\tau} &= a \frac{\pi^4}{\Delta x^4} \\
\Leftrightarrow a &= \frac{A^2}{\pi^4 \tau}
\end{aligned} \tag{35.16}$$

for the relationship between the diffusion coefficient and the decay time of the shortest resolved wave, where $A = \Delta x^2$ is the area of the grid cells. Expressing τ as a multiple of the model time step Δt , one obtains

$$a = \frac{A^2}{c\Delta t\pi^4}. \tag{35.17}$$

35.3 TKE as a prognostic variable

The subscale viscosity describes the influence of the TKE on the resolved scales. One can use the volumetric TKE

$$K_s := \rho k_s \tag{35.18}$$

introduce as an additional prognostic variable. For this size, Eq. (17.189):

$$\frac{\partial K_s}{\partial t} = -\nabla \cdot (K_s \mathbf{v}) - \rho \overline{u'w'} \frac{\partial \bar{u}}{\partial z} - \rho \overline{v'w'} \frac{\partial \bar{v}}{\partial z} + \rho g \overline{\frac{\theta'}{\bar{\theta}}} w' - \rho \bar{\epsilon} \tag{35.19}$$

To calculate the covariance terms of the velocity components, the K-theory approach is used:

$$\overline{u'w'} = -K \frac{\partial \bar{u}}{\partial z}, \tag{35.20}$$

$$\overline{v'w'} = -K \frac{\partial \bar{v}}{\partial z}, \tag{35.21}$$

$$\overline{g \frac{\theta'}{\bar{\theta}} w'} = -K g \frac{\partial \bar{\theta}}{\partial z} = -KN^2. \tag{35.22}$$

Putting this into Eq. (35.19), you get

$$\boxed{\boxed{\frac{\partial K_s}{\partial t} = -\nabla \cdot (K_s \mathbf{v}) + \rho K \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 \right] - \rho KN^2 - \rho \bar{\epsilon}.}} \tag{35.23}$$

To determine $\bar{\epsilon}$, one starts from Eq. (17.159) from:

$$l_c = \left(\frac{r^3}{\bar{\epsilon}} \right)^{1/4} \Leftrightarrow l_c^4 = \frac{r^3}{\bar{\epsilon}} \Leftrightarrow \bar{\epsilon} = \frac{r^3}{l_c^4}. \tag{35.24}$$

With the substitutions $r \rightarrow K$ and $l_c \rightarrow L$ one obtains

$$\bar{\epsilon} = \frac{K^3}{L^4}. \tag{35.25}$$

The viscosity coefficients can be used as functions

$$K = K[\mathbf{v}(\mathbf{r}), K_s] \quad (35.26)$$

of the current wind field and K_s can be expressed. About Eq. (35.23), this approach also contains information about the past wind field.

From Eq. (35.23), neglecting advection, one obtains an approximate diagnostic relation for the dissipation of the TKE:

$$\bar{\varepsilon} = K \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 - N^2 \right] \quad (35.27)$$

35.3.1 1.5th order closure

The TKE approach is ultimately about calculating the vertical diffusion coefficient. There are basically three approaches to this:

- In *first-order closure*, the vertical diffusion coefficient is calculated using the vertical wind shear multiplied by a length scale.
- In the *second-order closure*, prognostic variables are solved for both the TKE and the dissipation of the TKE. The vertical diffusion coefficient can be derived from this.
- With the *1.5th order closure* a prognostic equation is solved for the TKE, but not for the dissipation. The vertical diffusion coefficient is derived algebraically from the TKE.

Only the 1.5th order closure is pursued here. To determine the vertical diffusion coefficient, the kinetic gas model according to Sect. 5.4.0.2 is used as a model. In this case, particles fly a mean free path between two collisions, which is here called *mixing path length* L_m , their average speed is $\bar{v}$. The resulting diffusion coefficient is calculated according to Eq. (5.215) to

$$K_v = L_m \bar{v}. \quad (35.28)$$

The factor $\frac{1}{3}$ from Eq. (5.215) does not occur here because only vertical movements are considered here. It is now further assumed that the fluid particles move vertically with the angular frequency N according to Eq. (16.256) oscillate and have a maximum amplitude $\hat{z}$. Your trajectory is then:

$$z(t) = \hat{z} \exp(iNt). \quad (35.29)$$

From this it follows

$$\bar{v} = \frac{4\hat{z}}{T} = \frac{4\hat{z}}{2\pi} \frac{2\pi}{T} = \frac{2\hat{z}N}{\pi}, \quad (35.30)$$

since the particle covers the distance $\hat{z}$ four times during each period. For the maximum speed applies

$$v_{\max} = N\hat{z} = \frac{\pi}{2} \bar{v}. \quad (35.31)$$

The mean free path L_m here is $2\hat{z}$. Now $\hat{z}$ must be expressed by the TKE k_s . According to Eq., the total specific energy E of the harmonic oscillator is: (2.89) the relation

$$E = \frac{1}{2} N^2 \hat{z}^2. \quad (35.32)$$

On average, half of this is stored in kinetic energy, which is

$$k_s = \frac{1}{4} N^2 \hat{z}^2 \Rightarrow \hat{z} = \frac{2}{N} \sqrt{k_s} \Rightarrow L_m = \frac{4}{N} \sqrt{k_s} = \frac{C_l}{N} \sqrt{k_s} \quad (35.33)$$

leads. According to the derivation, $C_l = 4$, but empirically we find that $C_l = 1$. Putting this into Eq. (35.30), you get

$$\bar{v} = \frac{2\hat{z}N}{\pi} = \frac{4}{\pi} \sqrt{k_s}. \quad (35.34)$$

Assuming that a third of the particles fly along the direction of one of the coordinate axes, it follows for the diffusion coefficient with Eq. (35.28)

$$K_v = \frac{L_m}{3} \bar{v} = \frac{4}{3\pi} L_m \sqrt{k_s} \approx 0.424 L_m \sqrt{k_s}. \quad (35.35)$$

Empirically, one finds that the prefactor $C := \frac{4}{3\pi}$ is not the same size for all diffused quantities. This is because the correlations between the fluctuations of different sizes are different. At this point it will

$$C_m = 0.126, \quad (35.36)$$

$$C_e = 0.34, \quad (35.37)$$

$$C_h = 0.142 \quad (35.38)$$

selected [4]. Here, C_m is the prefactor for the vertical diffusion of momentum, C_e is the prefactor for the vertical diffusion of TKE and C_h is the prefactor for the vertical diffusion of humidity and potential temperature (passive tracers).

From Eq. (35.35) can be derived using Eq. (35.25) derive a formula for the dissipation of the TKE

$$\bar{\varepsilon} = \frac{(C_m L_m \sqrt{k_s})^3}{L_m^4} = C_m^3 \frac{k_s^{3/2}}{L_m} = C_\varepsilon \frac{k_s^{3/2}}{L_m}. \quad (35.39)$$

with $C_\varepsilon := C_m^3$. Putting this into Eq. (35.27), you get

$$\begin{aligned} C_\varepsilon \frac{k_s^{3/2}}{L_m} &= K \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 - N^2 \right] \\ \Leftrightarrow C_\varepsilon \frac{k_s^{3/2}}{L_m} &= L_m C_m \sqrt{k_s} \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 - N^2 \right] \\ \Leftrightarrow k_s &= \frac{C_m L_m^2}{C_\varepsilon} \left[\left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 - N^2 \right]. \end{aligned} \quad (35.40)$$

35.3.2 Convection parameterization

The basic problem of *convection parameterizations* has already been outlined in Sect. 17.9.4. The approach to bringing these considerations into the model is that the convection has to be represented in two parts:

- The resolved fraction is that seen by a non-hydrostatic model in the prognostic variables „This proportion does not need to be treated further, but is explicitly simulated.
- The unresolved portion consists of unstable sub-regions (area $0 \leq c \leq 1$), which are smaller than the grid cells. This proportion is not taken into account by the model without further action.

Convection is vertical mixing. An attempt is therefore made to represent the unresolved portion by modifying the mixing path length:

$$L_m \rightarrow c L_{\text{conv}} + (c - 1) L_m, \quad (35.41)$$

here L_{conv} is a convective mixing path length. c is the proportion of the base area of the grid cell in which thermal instability prevails:

$$c = \frac{1}{A_c} \int_{A_c} \Theta (\Gamma - \Gamma_d) dA \quad (35.42)$$

Let $\bar{\Gamma}$ be the mean negative vertical temperature gradient, i.e. the one calculated from the averaged (i.e. resolved) variables. If we further assume that Γ is normally distributed, it follows from Eq. (35.42)

$$\begin{aligned}
 c &= \int_{\Gamma_d}^{\infty} f_{\sigma}(\Gamma - \bar{\Gamma}) d\Gamma = \int_{\Gamma_d - \bar{\Gamma}}^{\infty} f_{\sigma}(\Gamma) d\Gamma = \int_{\frac{\Gamma_d - \bar{\Gamma}}{\sigma}}^{\infty} f_1(\Gamma) d\Gamma = \int_{\frac{\Gamma_d - \bar{\Gamma}}{\sigma}}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\Gamma^2}{2}\right) d\Gamma \\
 &= \frac{1}{\sqrt{\pi}} \int_{\frac{\Gamma_d - \bar{\Gamma}}{\sqrt{2}\sigma}}^{\infty} \exp(-\Gamma^2) d\Gamma = \frac{1}{\sqrt{\pi}} \left(\int_0^{\infty} \exp(-\Gamma^2) d\Gamma - \int_0^{\frac{\Gamma_d - \bar{\Gamma}}{\sqrt{2}\sigma}} \exp(-\Gamma^2) d\Gamma \right) \\
 &= \frac{1}{\sqrt{\pi}} \left(\frac{\sqrt{\pi}}{2} - \int_0^{\frac{\Gamma_d - \bar{\Gamma}}{\sqrt{2}\sigma}} \exp(-\Gamma^2) d\Gamma \right) = \frac{1}{2} - \frac{1}{\sqrt{\pi}} \int_0^{\frac{\Gamma_d - \bar{\Gamma}}{\sqrt{2}\sigma}} \exp(-\Gamma^2) d\Gamma = \frac{1}{2} \left[1 - \operatorname{erf}\left(\frac{\Gamma_d - \bar{\Gamma}}{\sqrt{2}\sigma}\right) \right]. \quad (35.43)
 \end{aligned}$$

The standard deviation of the stratification σ now needs to be determined. In a random walk, the expected value of the distance from the origin is proportional to the square root of the number of steps. Now go radially from the center of a grid cell towards the edge in steps of Δr . For the standard deviation σ_r of the probability distribution of the stratification Γ_r at a point with the distance r from the center, one therefore makes the approach

$$\sigma_r = k\sqrt{r}. \quad (35.44)$$

The standard deviation averaged over the base area of a circular cell is $\bar{\sigma}$

$$\bar{\sigma} = \frac{\int_A \sigma dA}{\int_A \sigma dA} = \frac{\int_0^R 2\pi r \sigma_r dr}{\pi R^2} = \frac{\int_0^R 2\pi r k \sqrt{r} dr}{\pi R^2} = \frac{2\pi k \int_0^R r^{3/2} dr}{\pi R^2} = 2\pi k \frac{2R^{5/2}}{5\pi R^2} = 2\pi k \frac{2R^{1/2}}{5\pi} = \frac{4k}{5\pi^{1/4}} A_c^{1/4}. \quad (35.45)$$

For k one makes a heuristic approach

$$k = \frac{\delta\Gamma}{\sqrt{d}}. \quad (35.46)$$

Here $\delta\Gamma$ is a typical fluctuation range, for which $\delta\Gamma = \frac{\Gamma_d}{3}$ is assumed. d is the typical length scale associated with this variation, which is assumed to be 1000 km.

So far, in Eq. (35.42) assumed the dry adiabatic temperature gradient Γ_d . In reality, however, a subset of a grid box is saturated; the moist adiabatic temperature gradient Γ_h must be used there. In order to take this into account approximately, from Eq. (35.42) the replacement

$$\Gamma_d \rightarrow c_f \Gamma_h + (1 - c_f) \Gamma_d \quad (35.47)$$

made. Here c_f is the cloud-filled (i.e. supersaturated) volume fraction according to App. 36.4.

35.4 Dissipation

35.5 Upper boundary condition

If you introduce $N \geq \mathbf{1}$ tracers (i.e. parts of the air that do not belong to dry air), of which $\mathbf{1} \leq N_C \leq N - \mathbf{1}$ are condensed, you need N additional continuity equations. If we make the assumption of local thermodynamic equilibrium (all condensates have the same temperature as the gas phase), there is no need to introduce additional first laws. The basic approach for the dynamic and thermodynamic coupling of the gaseous and condensed tracers to the equation system for dry air was defined in Section 10.3.

36.1 Vertical advection of a mass density

Let ρ be a mass density. In preparation, the Crank-Nicolson method is noted with n as the current time step:

$$\rho^{(n+1)} = \rho^{(n)} + \Delta t \frac{\mathbf{1}}{2} \left(\frac{\partial \rho^{(n)}}{\partial t} + \frac{\partial \rho^{(n+1)}}{\partial t} \right) \quad (36.1)$$

At this point we are only concerned with vertical convergence; the other terms are calculated explicitly:

$$\rho^{(n+1)} = \rho^{(n)} + \Delta t \dot{\rho}_{\text{expl}}^{(n)} - \Delta t \frac{\mathbf{1}}{2} \left(\frac{\partial (\rho^{(n)} w^{(n+1)})}{\partial z} + \frac{\partial (\rho^{(n+1)} w^{(n+1)})}{\partial z} \right) \quad (36.2)$$

Only the generalized density is treated in the form of the Crank-Nicolson method; the speed is taken from the new time step for reasons of stability. The share

$$-\frac{\mathbf{1}}{2} \frac{\partial (\rho^{(n)} w^{(n+1)})}{\partial z} \quad (36.3)$$

is absorbed into the explicit tendency, i.e. defined

$$\dot{\rho}_{\text{expl}}^{(n)} \rightarrow \dot{\rho}_{\text{expl}}^{(n)} - \frac{\mathbf{1}}{2} \frac{\partial (\rho^{(n)} w^{(n+1)})}{\partial z} \quad (36.4)$$

around. Vertical discretization requires a layer index $\mathbf{1} \leq i \leq N_L$:

$$\rho_i^{(n+1)} = \rho_i^{(n)} + \Delta t \dot{\rho}_{i\text{expl}}^{(n)} - \frac{\Delta t}{2} \frac{\overline{(\rho^{(n+1)})}^{(i-1/2)} w_{i-1/2}^{(n+1)} - A_{i+1/2} \overline{(\rho^{(n+1)})}^{(i+1/2)} w_{i+1/2}^{(n+1)}}{V_i} \quad (36.5)$$

The vertical averages of the density are generally noted

$$\overline{\rho}_k^{(i+1/2)} = a_{i+\frac{1}{2},i} \rho_i + a_{i+\frac{1}{2},i+1} \rho_{i+1} \quad (36.6)$$

with

$$a_{i+\frac{1}{2},i} + a_{i+\frac{1}{2},i+1} = \mathbf{1}. \quad (36.7)$$

Putting this into Eq. (36.5), you get

$$\begin{aligned} \rho_i^{(n+1)} &= \rho_i^{(n)} + \Delta t \dot{\rho}_{i\text{expl}}^{(n)} \\ &- \frac{\Delta t}{2} \left(a_{i-\frac{1}{2},i-1} \rho_{i-1}^{(n+1)} + a_{i-\frac{1}{2},i} \rho_i^{(n+1)} \right) \frac{A_{i-1/2} w_{i-1/2}^{(n+1)}}{V_i} + \frac{\Delta t}{2} \left(a_{i+\frac{1}{2},i} \rho_i^{(n+1)} + a_{i+\frac{1}{2},i+1} \rho_{i+1}^{(n+1)} \right) \frac{A_{i+1/2} w_{i+1/2}^{(n+1)}}{V_i}. \end{aligned} \quad (36.8)$$

You now define

$$W_{i+1/2} := A_{i+1/2} w_{i+1/2}^{(n+1)}, \quad (36.9)$$

thus you get

$$\begin{aligned} \rho_i^{(n+1)} &= \rho_i^{(n)} + \Delta t \dot{\rho}_{i,\text{expl}}^{(n)} \\ &- \frac{\Delta t}{2} \left(a_{i-\frac{1}{2}, i-1} \rho_{i-1}^{(n+1)} + a_{i-\frac{1}{2}, i} \rho_i^{(n+1)} \right) \frac{W_{i-1/2}^{(n+1)}}{V_i} + \frac{\Delta t}{2} \left(a_{i+\frac{1}{2}, i} \rho_i^{(n+1)} + a_{i+\frac{1}{2}, i+1} \rho_{i+1}^{(n+1)} \right) \frac{W_{i+1/2}^{(n+1)}}{V_i}. \end{aligned} \quad (36.10)$$

At $i = 1$, $w_{i-1/2} = 0$:

$$\rho_1^{(n+1)} = \rho_1^{(n)} + \Delta t \dot{\rho}_{1,\text{expl}}^{(n)} + \frac{\Delta t}{2} \left(a_{\frac{3}{2}, 1} \rho_1^{(n+1)} + a_{\frac{3}{2}, 2} \rho_2^{(n+1)} \right) \frac{W_{3/2}^{(n+1)}}{V_1} \quad (36.11)$$

If $i = N_L$ then $w_{i+1/2} = 0$:

$$\rho_{N_L}^{(n+1)} = \rho_{N_L}^{(n)} + \Delta t \dot{\rho}_{N_L,\text{expl}}^{(n)} - \frac{\Delta t}{2} \left(a_{N_L-\frac{1}{2}, N_L-1} \rho_{N_L-1}^{(n+1)} + a_{N_L-\frac{1}{2}, N_L} \rho_{N_L}^{(n+1)} \right) \frac{W_{N_L-1/2}^{(n+1)}}{V_{N_L}}. \quad (36.12)$$

The vector $\mathbf{x}$ of the unknowns is defined by

$$\mathbf{x} = \begin{pmatrix} \rho_1^{(n+1)} \\ \rho_2^{(n+1)} \\ \vdots \\ \rho_{N_L}^{(n+1)} \end{pmatrix}, \quad (36.13)$$

for this a linear system of equations applies

$$A \cdot \mathbf{x} = \mathbf{r} \quad (36.14)$$

with a matrix A and a right-hand side $\mathbf{r}$. For this right side applies

$$\mathbf{r} = \begin{pmatrix} \rho_1^{(n)} + \Delta t \dot{\rho}_{1,\text{expl}}^{(n)} \\ \rho_2^{(n)} + \Delta t \dot{\rho}_{2,\text{expl}}^{(n)} \\ \rho_3^{(n)} + \Delta t \dot{\rho}_{3,\text{expl}}^{(n)} \\ \vdots \\ \rho_{N_L-1}^{(n)} + \Delta t \dot{\rho}_{N_L-1,\text{expl}}^{(n)} \\ \rho_{N_L}^{(n)} + \Delta t \dot{\rho}_{N_L,\text{expl}}^{(n)} \end{pmatrix}. \quad (36.15)$$

For the matrix A one obtains

$$A = \begin{pmatrix} d_1 & e_1 & & \cdots & \cdots & 0 \\ b_1 & d_2 & e_2 & \cdots & \cdots & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & \cdots & & b_{N_L-1} & & d_{N_L} \end{pmatrix} \quad (36.16)$$

with vectors $\mathbf{c}, \mathbf{e} \in \mathbb{R}^{N_L-1}$, $\mathbf{e} \in \mathbb{R}^{N_L}$. For this you get

$$c_i = \frac{\Delta t}{2} \frac{a_{i+\frac{1}{2},i} W_{i+1/2}^{(n+1)}}{V_{i+1}}, \quad (36.17)$$

$$d_1 = 1 - \frac{\Delta t}{2} a_{\frac{3}{2},1} \frac{W_{3/2}^{(n+1)}}{V_1}, \quad (36.18)$$

$$d_i = 1 + \frac{\Delta t}{2} \frac{a_{i-\frac{1}{2},i} W_{i-1/2}^{(n+1)} - a_{i+\frac{1}{2},i} W_{i+1/2}^{(n+1)}}{V_i}, \quad (36.19)$$

$$d_{N_L} = 1 + \frac{\Delta t}{2} \frac{a_{N_L-\frac{1}{2},N_L} W_{N_L-1/2}^{(n+1)}}{V_{N_L}}, \quad (36.20)$$

$$e_i = -\frac{\Delta t}{2} a_{i+\frac{1}{2},i+1} \frac{W_{i+1/2}^{(n+1)}}{V_i}. \quad (36.21)$$

36.2 Limiters

Limiters serve the purpose of maintaining upper bounds for flows. These upper bounds usually refer to the fact that mass densities resulting from the flows cannot be negative, as this would be unphysical. For tracers with very variable densities, this can occur purely through advection. Since limiters are numerical interventions that cannot be derived purely from physical laws, the numerics must be constructed in such a way that they have to be called as rarely as possible and, if they do, the interventions are as small as possible.

After advection, diffusion and phase transitions, it is possible for negative densities to arise despite the limiter. These must be set to zero at the end of the time step. Although this violates conservation of mass, there is no alternative.

36.3 Discretization of condensation and resublimation

If the air is supersaturated at time t , a phase transition from gaseous to liquid or from gaseous to solid occurs until the air is saturated. If the air is undersaturated and cloud water or cloud ice is still present, the phase transition takes place in the other direction. For modeling it is assumed that after a time step of length Δt the air is saturated, i.e.

$$p_v(t + \Delta t) = p_S(t + \Delta t), \quad (36.22)$$

Here p_v is the vapor pressure and p_S is, as usual, the saturation vapor pressure. From this the density $\Delta \rho_v$ of water vapor should be determined, which must condense or resublimate to reach this state. This is not simply $\rho_S(t) - \rho_v(t)$, where ρ_S is the saturation density, as this would leave the phase transition heat unaccounted for. From Eq. (36.22) follows

$$\begin{aligned} \rho_v(t + \Delta t) R_v T(t + \Delta t) &= p_S[T(t + \Delta t)] \\ \Leftrightarrow (\rho_v + \Delta \rho_v) R_v T(t + \Delta t) &= p_S[T(t + \Delta t)], \end{aligned} \quad (36.23)$$

Here quantities without explicitly stated time dependence denote quantities at time t , i.e. $\rho_v := \rho_v(t)$. From this it follows that ρ_t is the total density

$$(\rho_v + \Delta \rho_v) R_v \left(T - \Delta \rho_v \frac{L_v}{\rho_t c_p} \right) = p_S \left(T - \Delta \rho_v \frac{L_v}{\rho_t c_p} \right). \quad (36.24)$$

If you multiply out the left side and do a first order Taylor expansion on the right side, you get

$$\begin{aligned}
p_v + \Delta_{\varrho_v} R_v T - R_v \Delta_{\varrho_v} \varrho_v \frac{L_v}{\varrho_t c_p} - (\Delta_{\varrho_v})^2 R_v \frac{L_v}{\varrho_t c_p} &= p_S - p'_S \Delta_{\varrho_v} \frac{L_v}{\varrho_t c_p} \\
\Leftrightarrow -(\Delta_{\varrho_v})^2 R_v \frac{L_v}{\varrho_t c_p} + \Delta_{\varrho_v} \left(R_v T - R_v \varrho_v \frac{L_v}{\varrho_t c_p} + p'_S \frac{L_v}{\varrho_t c_p} \right) + p_v - p_S &= 0 \\
\Leftrightarrow a (\Delta_{\varrho_v})^2 + b \Delta_{\varrho_v} + c &= 0 \\
\Leftrightarrow (\Delta_{\varrho_v})^2 + p \Delta_{\varrho_v} + q &= 0
\end{aligned} \tag{36.25}$$

with

$$a := -R_v \frac{L_v}{\varrho_t c_p} < 0, \tag{36.26}$$

$$b := R_v T - R_v \varrho_v \frac{L_v}{\varrho_t c_p} + p'_S \frac{L_v}{\varrho_t c_p}, \tag{36.27}$$

$$c := p_v - p_S, \tag{36.28}$$

$$p := \frac{b}{a}, \tag{36.29}$$

$$q := \frac{c}{a}. \tag{36.30}$$

This implies two solutions

$$(\Delta_{\varrho_v})_{1,2} = -\frac{p}{2} \pm \sqrt{\frac{p^2}{4} - q}. \tag{36.31}$$

Now it remains to be determined which of the two signs is the physically correct one. In the case of undersaturation, $p_v < p_S$, which implies $c < 0$, so $q > 0$. Furthermore, $(\Delta_{\varrho_v})^2 > 0$ and $\Delta_{\varrho_v} > 0$, which is because $p \Delta_{\varrho_v} = -q - (\Delta_{\varrho_v})^2 < 0$ is the relation $p < 0$ implied. In order for $\Delta_{\varrho_v} > 0$, the negative sign must be chosen in this case. In the case of supersaturation, $p < 0$ also applies, since the saturation vapor pressure does not appear in the expression for p , but $q < 0$, which also implies the negative sign, since otherwise $\Delta_{\varrho_v} \rightarrow 0$ does not follow for $q \rightarrow 0$. So it is in any case

$$\Delta_{\varrho_v} = -\frac{p}{2} - \sqrt{\frac{p^2}{4} - q}. \tag{36.32}$$

36.4 Parameterizations of phase transitions

If phase transitions are calculated using the averaged thermodynamic variables, the subscale variability considered in Section 17.9.3 is neglected. Here the fundamental considerations made in Section 17.9.3 are to be made usable for a model. Let $T = T(\boldsymbol{r})$ be the temperature field valid at a fixed time t in a grid box $V \subseteq \mathbb{R}^3$. Let $T_{\min}$ and $T_{\max}$ be the minimum and maximum temperatures within this set. Then, due to the strict monotonicity of $p_S(T)$, the minimum and maximum saturation vapor pressure is derived:

$$p_{S,\min} = p_S(T_{\min}), \tag{36.33}$$

$$p_{S,\max} = p_S(T_{\max}). \tag{36.34}$$

Let p_v be the average vapor pressure within the grid box under consideration. Now one makes the assumption that the vapor pressure p_v is homogeneous within V . The basic idea is that condensation begins at $p_v > p_{S,\min}$, but initially in a very small volume fraction, the cloud-filled volume fraction of the grid box c_f . For c_f you do the following approach

$$c_f(p_v \leq p_{S,\min}) = 0, \tag{36.35}$$

$$c_f(p_v \geq p_{S,\max}) = 1. \tag{36.36}$$

This is correct in any case. The simplest way to fulfill this for $p_{S,\min} \leq p_v \leq p_{S,\max}$ is a linear interpolation:

$$c_f(p_v) = \frac{p_v - p_{S,\min}}{p_{S,\max} - p_{S,\min}}. \quad (36.37)$$

This would be the case, for example, if the temperature were equally distributed between $T_{\min}$ and $T_{\max}$ and the saturation vapor pressure in this interval depended linearly on the temperature, which is true to the first order. The idea is now to use one approach to calculate the vapor pressure with which to calculate the phase transition rates in the case $p_v > p_{S,\min}$ (in which only cloud formation can take place).

$$p_v^{(\text{eff})} = p_{S,\min} + \xi(p_v - p_{S,\min}) \quad (36.38)$$

to express. We now have to determine ξ . ξ calculates over

$$\xi = \frac{p_v^{(\text{eff})} - p_{S,\min}}{p_v - p_{S,\min}} = \frac{\int_V \max(p_v - p_S(\mathbf{r}), 0) d^3r}{V(p_v - p_{S,\min})}. \quad (36.39)$$

Under the assumption already made above that T and p_S are equally distributed within V , in the case $p_{S,\min} \leq p_v \leq p_{S,\max}$ it follows

$$\begin{aligned} \xi &= \frac{\int_{p_{S,\min}}^{p_v} p_v - p'_S dp'_S}{(p_{S,\max} - p_{S,\min})(p_v - p_{S,\min})} = \frac{p_v(p_v - p_{S,\min}) - \frac{1}{2}(p_v^2 - p_{S,\min}^2)}{(p_{S,\max} - p_{S,\min})(p_v - p_{S,\min})} \\ &= \frac{p_v(p_v - p_{S,\min}) - \frac{1}{2}(p_v + p_{S,\min})(p_v - p_{S,\min})}{(p_{S,\max} - p_{S,\min})(p_v - p_{S,\min})} = \frac{p_v - \frac{1}{2}(p_v + p_{S,\min})}{p_{S,\max} - p_{S,\min}} = \frac{p_v - p_{S,\min}}{2(p_{S,\max} - p_{S,\min})} = \frac{c_f}{2}. \end{aligned} \quad (36.40)$$

In the case $p_v > p_{S,\max}$ applies

$$c_f = 1, \quad (36.41)$$

the grid box is 100 percent covered with clouds. In this case it follows for ξ

$$\begin{aligned} \xi &= \frac{\int_{p_{S,\min}}^{p_{S,\max}} p_v - p'_S dp'_S}{(p_{S,\max} - p_{S,\min})(p_v - p_{S,\min})} = \frac{p_v(p_{S,\max} - p_{S,\min}) - \frac{1}{2}(p_{S,\max}^2 - p_{S,\min}^2)}{(p_{S,\max} - p_{S,\min})(p_v - p_{S,\min})} \\ &= \frac{p_v(p_{S,\max} - p_{S,\min}) - \frac{1}{2}(p_{S,\max} + p_{S,\min})(p_{S,\max} - p_{S,\min})}{(p_{S,\max} - p_{S,\min})(p_v - p_{S,\min})} = \frac{p_v - \frac{1}{2}(p_{S,\max} + p_{S,\min})}{p_v - p_{S,\min}}. \end{aligned} \quad (36.42)$$

The previous derivation in this section refers to the formation of clouds (dealing with supersaturation, also known as saturation adjustment). The fact that only a certain proportion c_f of the grid boxes is filled with clouds also has consequences for the interactions and evaporation of condensates. The approach is this:

1. Divide all condensate densities by c_f . If $c_f < 0.1$, use 0.1 for stability. This is done because cloud physics only takes place within the cloud-filled area of the grid box and the densities there are higher by a factor of $1/c_f$.
2. Calculate the cloud physics with the rescaled densities.
3. Multiply the resulting source densities by $\max(c_f, 0, 1)$ to obtain the trends for the averaged densities (which are the prognostic variables).

The approach is used for the portion c_p of the grid box filled with precipitation.

$$c_p = \begin{cases} \frac{1}{3}, & c_f = 0 \wedge \rho_s + \rho_r + \rho_g > 0, \\ c_f, & \text{sonst.} \end{cases} \quad (36.43)$$

It is therefore assumed that the proportion filled with precipitation is equal to the proportion filled with clouds, unless there is only precipitation but no clouds in the grid box. This is typically the case under clouds from which precipitation falls.

36.5 Four-condensates scheme

This scheme takes the following four classes of condensate into account:

- liquid cloud water (index l)
- Cloud ice (index i)
- liquid precipitation (index r)
- solid precipitation (index s)

This scheme is adequate for global models. It is assumed that at and below -35°C the cloud water is completely ice-shaped and at and above -10°C the cloud water is completely liquid and there is a linear transition in between. This can be justified by observations [35].

36.5.1 Size spectra

The size distributions of the condensates are relevant to calculate the falling velocities, the interactions with the radiation field and the interactions with each other. Therefore, a formula for the effective radius must be specified for each condensate class.

- An effective radius of 12 micrometers is assumed for cloud droplets.
- For the effective radius of cloud ice, the formula developed in [36] is one of the most common approximations. This is:

$$d_{\text{eff},i} = (1,2351 + 0,0105 \cdot (t - t_o)) \cdot (45,8966 \cdot w^{0,2214} + 0,7957 \cdot w^{0,2535} \cdot (t - 83,15)). \quad (36.44)$$

Here, $t := T/\text{K}$ is the measure of the temperature in Kelvin, $t_o := 273.15$, $w := 1000 (\rho_i + \rho_s) / (\text{kg}/\text{m}^3)$ is the measure of the cloud ice density (including snow) in g/m^3 and d_{eff} the measure of the effective diameter in micrometers. The result of Eq. (36.44) is restricted in the following way:

$$d_{\text{eff}} \rightarrow \max(\min(d_{\text{eff},155}), 20 + 40 \cdot \cos(\varphi)) \quad (36.45)$$

with φ as the geographical latitude. For the effective radius r_{eff} in (36.44)

$$r_{\text{eff},i} = \frac{3\sqrt{3}}{8} d_{\text{eff},i} \cdot 10^{-6} \text{m} \quad (36.46)$$

derived. The fact that the factor is not simply 1/2 is because ice crystals i. A. are not spherical.

- It is assumed that the size distribution of raindrops is a Marshall-Palmer distribution Eq. (23.95) corresponds.
- It is assumed that the size distribution of the snowflakes is a Marshall-Palmer distribution Eq. (23.95) according to section 23.3.1.1.

The assumption of Marshall-Palmer distributions implies that the process of breaking up condensates, which limits the spectrum upwards, does not have to be explicitly simulated, but is already parameterized via the distribution.

36.5.2 Falling speeds

To determine the falling speeds of the condensates, one should refer to Section 23.2.3, but with some simplifications:

- A falling speed of zero is assumed for cloud droplets.
- A falling speed is assumed for cloud ice.
- For snow the empirical formula becomes

$$v_S = a \cdot r^b = 9,356 \frac{\text{m}^{0,7}}{\text{s}} \cdot (2 \cdot r_{\text{eff}})^{0,3} = 11,519 \frac{\text{m}^{0,7}}{\text{s}} \cdot (r_{\text{eff}})^{0,3} \quad (36.47)$$

[7] angenommen.

- Raindrops flow turbulently around them, for them Eq. (23.90) with $c_w = 0.8$ used.

36.5.2.1 Mass-weighted fall velocities

If the falling speed of a precipitation class is $v_{D,P}(D)$, it has a volume mixing ratio r_P and a size spectrum $n(D)$, a mass-weighted falling speed can be calculated

$$v_P(D) = \frac{1}{r_P} \int_0^\infty \frac{\pi D^3}{6} v_{D,P}(D) n(D) dD \quad (36.48)$$

calculate. Assume that $v_{D,P}$ has the form

$$v_{D,P}(D) = aD^b \quad (36.49)$$

as well as the Marshall-Palmer distribution Eq. (23.95) applies, follows

$$\begin{aligned} v_P(D) &= \frac{1}{r_P} \int_0^\infty \frac{\pi D^3}{6} aD^b n_0 e^{-\lambda D} dD = \frac{an_0\pi}{6r_P} \int_0^\infty D^{b+3} e^{-\lambda D} dD = \frac{an_0\pi}{6r_P\lambda^{b+4}} \int_0^\infty D^{b+3} e^{-D} dD \\ &= \frac{an_0\pi\Gamma(b+4)}{6r_P\lambda^{b+4}}. \end{aligned} \quad (36.50)$$

From Eq. (23.99) is obtained

$$\frac{1}{\lambda^4} = \frac{r_P}{\pi n_0}. \quad (36.51)$$

From this it follows

$$v_P(D) = \frac{a\Gamma(b+4)}{6\lambda^b} \stackrel{\text{Glg. (23.100)}}{=} \frac{\Gamma(b+4)}{6} aD^b. \quad (36.52)$$

36.5.3 Formation of precipitation

36.5.3.1 Warm rain

The simplest understanding of how rain occurs is to assume that it occurs when cloud water ρ_w exceeds a critical mixing ratio $q_{w,krit}$. A simple mathematical approach based on this for the source density of rainwater is:

$$Q_r = \frac{\max(\rho_w - q_{w,krit} \cdot \rho_h, 0)}{\tau}. \quad (36.53)$$

This is the so-called Kessler approach [15]. Typical values are $q_{w,krit} = 0.2 \cdot 10^{-3} \text{ kg/m}^3$, $\tau = 1000 \text{ s}$.

36.5.3.2 Snow

The Kessler approach presented in Sect. 36.5.3.1 can also be applied to the formation of snow, typical values are $q_{i,krit} = 1.0 \cdot 10^{-3} \text{ kg/m}^3$, $\tau = 1000 \text{ s}$.

36.5.3.3 Sleet

The Kessler approach presented in Sect. 36.5.3.1 can also be applied to the formation of sleet, typical values are $q_{s,krit} = 0.6 \cdot 10^{-3} \text{ kg/m}^3$, $\tau = 1000 \text{ s}$.

36.6 Five-condensate scheme

In this scheme, a fifth condensate class is added to the four-condensate scheme, namely graupel. The five condensate classes used here are:

- liquid cloud water (index l),
- cloud ice (index i),

- liquid precipitation (index r),
- snow (index s),
- Graupel (index g).

This scheme is adequate for regional models. It corresponds to the scheme presented in Sect. 36.5 with the following modifications:

- An effective radius of 0.5 millimeters is assumed for sleet particles.
- Graupel particles are turbulently flowed around, for them Eq. (23.90) with $c_w = 0.8$ and the replacement $\rho'_l \rightarrow \rho'_i$ is used.

36.7 Advanced cloud microphysics schemes

In the schemes considered so far, each condensate class is described by a prognostic variable, namely the mass density or the specific density. This would only be a complete description if all condensates of the respective class had the same radius and temperature as the gas phase. However, neither is generally the case. Two extensions are available:

- Each condensate class can be assigned its own temperature.
- The size distribution within the condensate classes can be taken into account. This happens with the so-called *multi-moment schemes*, in which the higher moments of the size distributions (or comparable sizes describing the shape of the distributions) are introduced as additional prognostic variables.

Within the planetary boundary layer, particularly within the Prandtl layer, the vertical gradients of meteorological variables are relatively large. They can only be sampled sufficiently well by a model at vertical grid point distances of one meter. Therefore, the approaches valid in the free atmosphere for the vertical turbulent flows at the bottom of the lowest model layer are no longer applicable. Therefore, in this area, the knowledge about the planetary boundary layer, which was developed in Sect. 17.2.1, is used to determine the vertical turbulent flows.

37.1 Calculation of the Monin-Obukhov length

According to Eq. (17.80) is the Monin-Obukhov length

$$L := -\frac{T_A u_\star^3}{kg(\overline{w'\theta'})}. \quad (37.1)$$

What is problematic here is the determination of $\overline{(w'\theta')_{\text{sfc}}}$. If you put Eq. one, you get

$$L = -\frac{T_A u_\star^3}{kg \frac{Q_H}{\rho c_p}} = -\frac{T_A u_\star^3}{kg \frac{T_G - T_A}{r_H}} = -\frac{T_A u_\star^3}{kg (T_G - T_A)} r_H. \quad (37.2)$$

The friction speed $u_\star$ and the flow resistance of the sensible heat r_H depend in turn on L :

$$L = -\frac{T_A u_\star^3(L)}{kg (T_G - T_A)} r_H(L). \quad (37.3)$$

If you put Eq. one, you get

$$L = -\frac{T_A u_\star^3}{g (T_G - T_A)} \frac{1}{u_\star k^2} \left[\ln \left(\frac{z}{z_o} \right) - \psi_h \left(\frac{z}{L} \right) + \ln(\gamma) \right] = \frac{T_A u_\star^2}{k^2 g (T_A - T_G)} \left[\ln \left(\frac{z}{z_o} \right) - \psi_h \left(\frac{z}{L} \right) + \ln(\gamma) \right]. \quad (37.4)$$

If you continue using Eq. (17.49), follows

$$L = \frac{T_A U^2}{g (T_A' - T_G)} \frac{\ln \left(\frac{z}{z_o} \right) - \psi_h \left(\frac{z}{L} \right) + \ln(\gamma)}{\left[\ln \left(\frac{z}{z_o} \right) - \psi_m \left(\frac{z}{L} \right) \right]^2}. \quad (37.5)$$

This is about the determination L , but all other quantities are known. The size

$$R_{i,b} := \frac{zg (T_A' - T_G)}{T_A U^2}. \quad (37.6)$$

is called *Bulk Richardson number*. With the help function

$$s(L) := \frac{\ln \left(\frac{z}{z_o} \right) - \psi_h \left(\frac{z}{L} \right) + \ln(\gamma)}{\left[\ln \left(\frac{z}{z_o} \right) - \psi_m \left(\frac{z}{L} \right) \right]^2} \quad (37.7)$$

and

$$a := \frac{R_{i,b}}{z} \quad (37.8)$$

you can do this in the form

$$L = \frac{z}{R_{i,b}} s(L) = \frac{s(L)}{a} \Leftrightarrow aL - s(L) = 0 \quad (37.9)$$

note down.

The sign of L can already be determined in advance from Eq. (37.3) can be determined. In the case $T_G < T_A$, which corresponds to stable conditions, $L > 0$. In this case apply

$$\psi_m\left(\frac{z}{L}\right) = \psi_h\left(\frac{z}{L}\right) = -4,7 \cdot \frac{z}{L}. \quad (37.10)$$

Now define

$$h(L) := \ln\left(\frac{z}{z_0}\right) + 4,7 \cdot \frac{z}{L}, \quad (37.11)$$

then it follows from Eq. (37.9)

$$\begin{aligned} aL - s(L) &= aL - \frac{h(L) + \ln(7)}{h^2(L)} = 0 \\ \Leftrightarrow f_1(L) &:= aLh^2(L) - h(L) - \ln(7) = 0. \end{aligned} \quad (37.12)$$

Eq. (37.12) cannot be solved analytically and must therefore be solved numerically. This corresponds to determining the zero of f_1 . For this you use a Newton iteration with

$$f_1(L_i) + f'_1(L_i) \cdot (L_{i+1} - L_i) = 0, \quad (37.13)$$

here i is the iteration step. It applies

$$f'_1(L) = ah^2(L) + 2aLh(L)h'(L) - h'(L). \quad (37.14)$$

Assuming $f'_1 \neq 0$ this can be done

$$\begin{aligned} \frac{f_1(L_i)}{f'_1(L_i)} + L_{i+1} - L_i &= 0 \\ \Leftrightarrow L_{i+1} &= L_i - \frac{f_1(L_i)}{f'_1(L_i)} \end{aligned} \quad (37.15)$$

rephrase.

In the case $T_G > T_A$, which corresponds to unstable conditions, $L < 0$. In this case applies

$$f_2(L) := aL - s(L) = aL - \frac{\ln\left(\frac{z}{z_0}\right) - \psi_h\left(\frac{z}{L}\right) + \ln(7)}{\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]^2} = 0. \quad (37.16)$$

From this it follows

$$\begin{aligned} f'_2(L) &= a - g'(L) = a - \frac{\frac{z}{L^2}\psi'_h\left(\frac{z}{L}\right)\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]^2 - \left[\ln\left(\frac{z}{z_0}\right) - \psi_h\left(\frac{z}{L}\right) + \ln(7)\right]2\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]\frac{z}{L^2}\psi'_m\left(\frac{z}{L}\right)}{\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]^4} \\ &= a - \frac{\frac{z}{L^2}\psi'_h\left(\frac{z}{L}\right)}{\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]^2} + \frac{2\left[\ln\left(\frac{z}{z_0}\right) - \psi_h\left(\frac{z}{L}\right) + \ln(7)\right]\frac{z}{L^2}\psi'_m\left(\frac{z}{L}\right)}{\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]^3}. \end{aligned} \quad (37.17)$$

38.1 Heat conduction

Let T be the temperature of the solid earth. In preparation, the Crank-Nicolson method is noted with n as the current time step:

$$T^{(n+1)} = T^{(n)} + \Delta t \frac{1}{2} \left(\frac{\partial T^{(n)}}{\partial t} + \frac{\partial T^{(n+1)}}{\partial t} \right) \quad (38.1)$$

At this point we are only concerned with the vertical heat conduction; the other terms are calculated explicitly:

$$T^{(n+1)} = T^{(n)} + \Delta t \dot{T}_{\text{expl}}^{(n)} + \Delta t \frac{\lambda}{2\rho c} \frac{\partial}{\partial z} \left(\frac{\partial T^{(n)}}{\partial z} + \frac{\partial T^{(n+1)}}{\partial z} \right) \quad (38.2)$$

Here λ is the thermal conductivity, ρ is the mass density and c is the specific heat capacity. These quantities are assumed to be known and constant. Furthermore, the vertical expansion of the grid boxes is neglected due to the small thickness, so one makes use of the shallow atmosphere approximation according to Eq. (33.25) use. The share

$$\frac{\lambda}{2\rho c} \frac{\partial}{\partial z} \frac{\partial T^{(n)}}{\partial z} \quad (38.3)$$

is absorbed into the explicit tendency, i.e. defined

$$\dot{T}_{\text{expl}}^{(n)} \rightarrow \dot{T}_{\text{expl}}^{(n)} - \frac{1}{2\rho c} \frac{\partial}{\partial z} \frac{\lambda \partial T^{(n)}}{\partial z} \quad (38.4)$$

around. The vertical discretization requires a layer index $1 \leq i \leq N_S$ with N_S as the number of soil layers:

$$T_i^{(n+1)} = T_i^{(n)} + \Delta t \dot{T}_{i\text{expl}}^{(n)} + \frac{\Delta t}{2\rho_i c_i \Delta z_i} \left(\lambda'_{i-1} \frac{T_{i-1}^{(n+1)} - T_i^{(n+1)}}{\Delta z'_{i-1}} - \lambda'_i \frac{T_i^{(n+1)} - T_{i+1}^{(n+1)}}{\Delta z'_i} \right) \quad (38.5)$$

The deleted sizes refer to the layer boundaries, i.e

$$\lambda'_i := \frac{\lambda'_i + \lambda'_{i+1}}{2} \quad (38.6)$$

and

$$\Delta z'_i := z_i - z_{i+1}. \quad (38.7)$$

At $i = 1$ there is no overlying soil layer, the interaction with the air is in the explicit tendency:

$$T_1^{(n+1)} = T_1^{(n)} + \Delta t \dot{T}_{1\text{expl}}^{(n)} + \frac{\Delta t}{2\rho_1 c_1 \Delta z_1} \lambda'_1 \frac{T_1^{(n+1)} - T_2^{(n+1)}}{\Delta z'_1} \quad (38.8)$$

At $i = N_S$, T_{N_S+1} is the lower boundary condition assumed to be known and constant:

$$T_{N_S}^{(n+1)} = T_{N_S}^{(n)} + \Delta t \dot{T}_{N_S\text{expl}}^{(n)} + \frac{\Delta t}{2\rho_{N_S} c_{N_S} \Delta z_{N_S}} \left(\lambda'_{N_S-1} \frac{T_{N_S-1}^{(n+1)} - T_{N_S}^{(n+1)}}{\Delta z'_{N_S-1}} - \lambda'_{N_S} \frac{T_{N_S}^{(n+1)} - T_{N_S+1}}{\Delta z'_{N_S}} \right) \quad (38.9)$$

The term with T_{N_S+1} can be absorbed into the explicit tendency, which results in

$$T_{N_S}^{(n+1)} = T_{N_S}^{(n)} + \Delta t \dot{T}_{N_S \text{expl}}^{(n)} + \frac{\Delta t}{2\rho_{N_S} c_{N_S} \Delta z_{N_S}} \left(\mathcal{J}'_{N_S-1} \frac{T_{N_S-1}^{(n+1)} - T_{N_S}^{(n+1)}}{\Delta z'_{N_S-1}} - \mathcal{J}'_{N_S} \frac{T_{N_S}^{(n+1)}}{\Delta z'_{N_S}} \right) \quad (38.10)$$

leads.

The vector $\mathbf{x}$ of the unknowns is defined by

$$\mathbf{x} = \begin{pmatrix} T_1^{(n+1)} \\ T_2^{(n+1)} \\ \vdots \\ T_{N_S}^{(n+1)} \end{pmatrix}, \quad (38.11)$$

for this a linear system of equations applies

$$A \cdot \mathbf{x} = \mathbf{r} \quad (38.12)$$

with a matrix A and a right-hand side $\mathbf{r}$. For this right side applies

$$\mathbf{r} = \begin{pmatrix} T_1^{(n)} + \Delta t \dot{T}_{1,\text{expl}}^{(n)} \\ T_2^{(n)} + \Delta t \dot{T}_{2,\text{expl}}^{(n)} \\ T_3^{(n)} + \Delta t \dot{T}_{3,\text{expl}}^{(n)} \\ \vdots \\ T_{N_S-1}^{(n)} + \Delta t \dot{T}_{N_S-1,\text{expl}}^{(n)} \\ T_{N_S}^{(n)} + \Delta t \dot{T}_{N_S,\text{expl}}^{(n)} \end{pmatrix}. \quad (38.13)$$

For the matrix A one obtains

$$A = \begin{pmatrix} d_1 & e_1 & & \cdots & \cdots & 0 \\ c_1 & d_2 & e_2 & \cdots & \cdots & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & \cdots & & c_{N_L-1} & & d_{N_L} \end{pmatrix} \quad (38.14)$$

with vectors $\mathbf{c}, \mathbf{e} \in \mathbb{R}^{N_S-1}$, $\mathbf{d} \in \mathbb{R}^{N_S}$. For this you get

$$c_i = -\frac{\Delta t}{2\rho_{i+1} c_{i+1} \Delta z_{i+1}} \frac{\mathcal{J}'_i}{\Delta z'_i}, \quad (38.15)$$

$$d_1 = 1 + \frac{\Delta t}{2\rho_1 c_1 \Delta z_1} \frac{\mathcal{J}'_1}{\Delta z'_1}, \quad (38.16)$$

$$d_i = 1 + \frac{\Delta t}{2\rho_i c_i \Delta z_i} \left(\frac{\mathcal{J}'_{i-1}}{\Delta z'_{i-1}} + \frac{\mathcal{J}'_i}{\Delta z'_i} \right), \quad (38.17)$$

$$e_i = -\frac{\Delta t}{2\rho_i c_i \Delta z_i} \frac{\mathcal{J}'_i}{\Delta z'_i}. \quad (38.18)$$

39.1 Coupling to a radiation transfer model

39.2 Remaining approximations

After these generalizations, it makes sense to consider which basic approximations are still made in the dynamic core developed here:

- The continuum hypothesis is used.
- Gases are considered ideal gases.
- It is assumed that all condensates have the same temperature as the gas phase (local thermodynamic equilibrium).
- Velocities of condensed tracers are considered diagnostic quantities.

39.3 Post processing

This section is about determining variables that are not direct model variables but are expected by weather models as standard.

39.3.1 2m temperature

The so-called *2-m-temperature* is the air temperature 2 m above the earth's surface. According to the WMO standard, the temperature near the ground is measured there and must therefore also be written out by models. To calculate it, one starts from the heat conduction equation Eq. (5.221)

$$\frac{\partial \psi}{\partial t} = \kappa \frac{\partial^2 \psi}{\partial z^2} \quad (39.1)$$

in one-dimensional form with $\kappa > 0$ as the diffusion coefficient. This can now be solved for $z > 0$ under the boundary condition

$$\psi(0, t) = \psi_0 \exp(-i\omega t). \quad (39.2)$$

You now make the approach

$$\psi(z, t) = A \exp(ikz - i\omega t), \quad (39.3)$$

this implies

$$-i\omega = -k^2 \kappa \Rightarrow k = \pm \sqrt{i} \sqrt{\frac{\omega}{\kappa}} = \pm \sqrt{\frac{\omega}{2\kappa}} (1 + i). \quad (39.4)$$

The solution with a negative sign can be physically excluded because it leads to an exponentially increasing amplitude. So the solution is

$$\begin{aligned} \psi(z, t) &= \psi_0 \exp(-i\omega t) \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z\right) \exp\left(i\sqrt{\frac{\omega}{2\kappa}} z\right) \\ &= \psi_0 \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z\right) \exp\left(i\sqrt{\frac{\omega}{2\kappa}} z\right). \end{aligned} \quad (39.5)$$

Now apply this solution to the problem of determining the 2 m temperature, i.e. $\psi \rightarrow T$. For ω you use $\omega = \frac{2\pi}{24 \text{ h}}$, i.e. the angular frequency of the daily temperature cycle. The phase component can be neglected as a first approximation. For κ one uses the vertical turbulent diffusion coefficient. The solution thus becomes

$$T(z) = T_1 + T_2 \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z\right), \quad (39.6)$$

where o. b. d. A. an offset T_1 was added and ψ_o was renamed to T_2 . The boundary conditions apply to this in the atmosphere

$$T(o) = T_1 + T_2, \quad (39.7)$$

$$T(z_l) = T_1 + T_2 \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right), \quad (39.8)$$

Here $T(o) =: T_l$ is the temperature of the earth's surface and $T(z_l) =: T_l$ is the temperature of the lowest model layer above ground. From this you get

$$T_1 = T_s - T_2, \quad (39.9)$$

$$T_l = T_s - T_2 + T_2 \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right) = T_s - T_2 \left[1 - \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right)\right] \Rightarrow T_2 = \frac{T_s - T_l}{1 - \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right)}. \quad (39.10)$$

It follows

$$\begin{aligned} T(z) &= T_s - \frac{T_s - T_l}{1 - \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right)} + \frac{T_s - T_l}{1 - \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right)} \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z\right) \\ &= T_s + (T_l - T_s) \frac{1 - \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z\right)}{1 - \exp\left(-\sqrt{\frac{\omega}{2\kappa}} z_l\right)}. \end{aligned} \quad (39.11)$$

From this the 2 m temperature can be determined with $z = 2$ m.

39.3.2 10m wind

The wind is measured by default ten meters above ground, where the vectors of a model layer are usually not located. For this purpose, the logarithmic wind profile Eq. (17.43), so

$$v_h(z_{10}) = \frac{u_*}{k} \ln\left(\frac{z_{10}}{z_o}\right), \quad (39.12)$$

$$v_h(z_l) = \frac{u_*}{k} \ln\left(\frac{z_l}{z_o}\right). \quad (39.13)$$

Here $v_h \geq 0$ is the horizontal wind speed, z_l is the height of the lowest model layer above ground and $z_{10} := 10$ m. From this it follows

$$v_h(z_{10}) = v_h(z_l) \frac{\ln\left(\frac{z_{10}}{z_o}\right)}{\ln\left(\frac{z_l}{z_o}\right)}. \quad (39.14)$$

This only applies over water. Over land, the convention is that the wind must be measured over grass in order to establish comparability. The equations are used for this

$$v_h(z_{10}) = \frac{u_*}{k} \ln\left(\frac{z_{10}}{z_g}\right), \quad (39.15)$$

$$v_h(z_l) = \frac{u_*}{k} \ln\left(\frac{z_l}{z_o}\right), \quad (39.16)$$

where z_g is the roughness length of grass (0.02 m) and the friction velocity u_* was assumed to be the same in both cases. This leads to

$$v_h(z_{10}) = v_h(z_l) \frac{\ln\left(\frac{z_{10}}{z_g}\right)}{\ln\left(\frac{z_l}{z_o}\right)}. \quad (39.17)$$

39.3.3 Total coverage

The *total cloud cover* (English *total cloud cover (TCC)*) is the proportion of the sky covered by clouds. The correct way to calculate the TCC is therefore to form an integral over the half-space and relate the cloud-covered portion to the total portion (2π). However, a simplified approach is usually chosen in models. Let N_L be the number of layers and $c_{f,i}$ be the cloud-filled portion of the i -th layer.

The first step is to calculate from $c_{f,i}$ the non-cloud-covered vertical area fraction f_i of the grid box. Assuming that the clouds consist of a single layer of thickness d_i , one obtains

$$f_i = \max \left(1 - \frac{c_{d,i}}{\min(d_i/\Delta z_i, 1)}, 0 \right), \quad (39.18)$$

where Δz_i is the layer thickness. This means that complete coverage $f_i = 0$ is already achieved at $c_{d,i} = \frac{d_i}{\Delta z_i}$. Assuming random overlap between the layers, one obtains

$$\text{TCC} = 1 - \prod_{i=1}^{N_L} f_i. \quad (39.19)$$

In reality, however, it can be assumed that the overlap between the layers is not random, but rather that clouds move e.g. B. extend vertically over several layers. This is expressed using a *coherence length* l_c and generalizes Eq. (39.19) to

$$\text{TCC} = 1 - f_1 \prod_{i=2}^{N_L} f_i + (1 - f_1) \exp \left(-\frac{|z_i - z_{i-1}|}{l_{c,i}} \right). \quad (39.20)$$

In the case of short coherence lengths $l_{c,i} \rightarrow 0$, Eq. (39.20) to Eq. (39.19) over, in the case of infinite coherence lengths $l_{c,i} \rightarrow \infty$ follows from (39.20) $\text{TCC} = 1 - f_1$, because then the clouds in all layers overlap perfectly. The cloud height d_i and the coherence length $l_{c,i}$ now need to be determined. The following approach is chosen here:

$$d_i = 10 \cdot L_{m,i}, \quad (39.21)$$

$$l_{c,i} = d_i, \quad (39.22)$$

here $L_{m,i}$ is the vertical mixing path length.

39.4 Tuning

Not all variables used in the model can be derived from theory ab initio, for example the diffusion coefficients used in the turbulence parameterizations. They usually do not have exactly the right value and are therefore also called *semi-empirical coefficients*. They should not be called constants because they are not. Of course, in order to make the model as accurate as possible, you should use the correct value for it. There are two methods available to determine this:

- You can derive them from measurements.
- You can derive them from DNS runs (*direct numerical simulation*), these are very high-resolution runs, up to *computational fluid dynamics (CFD)*.

From the literature, this results in a reasonable interval within which one can freely choose the coefficient to be determined. Within this interval you simply choose it so that the model is as accurate as possible. Since one can tune multiple parameters in an atmospheric model, this becomes a multidimensional optimization problem that requires multiple iterations.

The following coefficients in the model can be tuned:

- horizontal diffusion coefficients
- vertical diffusion coefficients
- maximum specific cloud water

The remainder of this section discusses the tuning of the individual coefficients.

- 39.4.1 Horizontal diffusion coefficients
- 39.4.2 Vertical diffusion coefficient
- 39.4.3 Maximum specific cloud water

Part VIII
Attachment

A DERIVATIONS OF SOME MATHEMATICAL FORMULAS

A.1 Square complement

The so-called *quadratic complement* is a method for solving quadratic equations of the form

$$ax^2 + bx + c = 0 \quad (\text{A.1})$$

with $a \neq 0$. With the definitions

$$p := \frac{b}{a}, \quad q := \frac{c}{a} \quad (\text{A.2})$$

you can do this in the form

$$x^2 + px + q = 0 \quad (\text{A.3})$$

note down. The quadratic addition gets its name from the fact that a quadratic term is now added to this equation and then subtracted again:

$$\begin{aligned} x^2 + px + \left(\frac{p}{2}\right)^2 - \left(\frac{p}{2}\right)^2 + q &= 0 \\ \Leftrightarrow \left(x + \frac{p}{2}\right)^2 - \left(\frac{p}{2}\right)^2 + q &= 0 \\ \Leftrightarrow \left(x + \frac{p}{2}\right)^2 &= \left(\frac{p}{2}\right)^2 - q \end{aligned} \quad (\text{A.4})$$

From this it follows

$$x_{1,2} = -\frac{p}{2} \pm \sqrt{\frac{p^2}{4} - q}. \quad (\text{A.5})$$

This formula is called *pq formula*.

A.2 Totals and series

First, the *Gaussian empirical formula* is viewed. It reads

$$\sum_{i=0}^n i = \frac{n(n+1)}{2}. \quad (\text{A.6})$$

This is proven by complete induction. For $n = 0$, $\sum_{i=0}^{n=0} i = 0 = \frac{1}{2}n(n+1)$. The statement already applies to $n \in \mathbb{N}$. Then follows

$$\sum_{i=0}^{n+1} i = \frac{n(n+1)}{2} + n+1 = \frac{n^2 + 3n + 2}{2} = \frac{(n+1)(n+2)}{2}. \quad (\text{A.7})$$

This proves the statement.

The *Theorem about the geometric series* is

$$\sum_{n=0}^{\infty} q^n = \frac{1}{1-q} \quad (\text{A.8})$$

for $q \in \mathbb{C}$ with $|q| < 1$.

First of all, for $N \in \mathbb{N}$

$$\sum_{n=0}^N q^n = \frac{1 - q^{N+1}}{1 - q}. \quad (\text{A.9})$$

This can be shown by *complete induction*. For $N = 0$ this is clear, the statement applies to N . Then applies

$$\sum_{n=0}^{N+1} q^n = \frac{1 - q^{N+1}}{1 - q} + q^{N+1} = \frac{1 - q^{N+1}}{1 - q} + \frac{q^{N+1} - q^{N+2}}{1 - q} = \frac{1 - q^{N+2}}{1 - q}. \quad (\text{A.10})$$

With the calculation rules for consequence limits and

$$\sum_{n=0}^{\infty} q^n = \lim_{N \rightarrow \infty} \sum_{n=0}^N q^n \quad (\text{A.11})$$

follows the statement. Furthermore, according to [1]

$$\sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90}. \quad (\text{A.12})$$

A.3 Combinatorics

One defines the binomial coefficient

$$\binom{n}{k} := \frac{n!}{k!(n-k)!} \quad (\text{A.13})$$

with the *Faculty*

$$n! := 1 \cdot 2 \cdot \dots \cdot n \quad (\text{A.14})$$

with $n, k \in \mathbb{N}$ and $n \geq k$. The number of ways to arrange $n \in \mathbb{N}$ elements is $n!$. For the first element you have n possibilities. For the second only $n - 1$, etc., for the last element you only have exactly one way to arrange it. A *Permutation* is a bijection on the set $\{1, 2, \dots, N\}$ with $1 \leq N \in \mathbb{N}$. The set of all these mappings is denoted by S_N . Based on the statement just proven, the number of all permutations is $|S_N|$

$$|S_N| = N!. \quad (\text{A.15})$$

One further defines the *sign of a permutation* $\pi \in S_N$ by $\text{sign}(\pi) := (-1)^M$ with M as the number of all pairwise swaps that have to be made in order to convert $\text{id} \rightarrow \pi$. If M is even, π is called *even permutation*, otherwise as *odd*.

$\binom{n}{k}$ ist die Anzahl der k -elementigen Teilmengen einer n -elementigen Menge. Dies kann man sich leicht überlegen. Seien also eine n -elementige Menge M gegeben sowie ein $k \in \mathbb{N}$ mit $k \leq n$. Für den Fall $k = 0$ ist $\binom{n}{k} = 1$, hier stimmt die Aussage also, weil die einzige in Frage kommende Menge die leere Menge $\emptyset$ ist, und diese ist Teilmenge jeder anderen Menge, auch von sich selbst. Im Fall $n, k > 0$ hat man n Möglichkeiten, das erste Element der Teilmenge auszuwählen. Für das zweite Element bleiben $n - 1$ Möglichkeiten und so weiter. Dies führt auf die Zahl $n \cdot (n - 1) \cdot \dots \cdot (n - k + 1) = \frac{n!}{(n-k)!}$. Hierbei wurden jedoch Mengen doppelt gezählt. Weil die Anzahl der Möglichkeiten, k Elemente anzuordnen, $k!$ beträgt, ist die Anzahl der k -elementigen Teilmengen einer n -elementigen Menge gleich $\frac{n!}{k!(n-k)!} = \binom{n}{k}$.

Let $n, n_1, \dots, n_k \in \mathbb{N}$ with $\sum_{i=1}^k n_i = n$. One defines the *multinomial coefficient* by

$$\binom{n}{n_1, \dots, n_k} := \frac{n!}{n_1! \dots n_k!}. \quad (\text{A.16})$$

Sei eine Menge mit k Elementen gegeben. Aus diesen wählt man n -mal ein zufälliges aus, dabei kann $n \geq k$ oder

$n \leq k$ sein. Als Ergebnis hält man die Zahlen $n_1, \dots, n_k$ fest, die angeben, wie oft die Elemente gezogen wurden, das Ergebnis ist also das Tupel $(n_1, \dots, n_k)$. Der Multinomialkoeffizient $\binom{n}{n_1, \dots, n_k}$ ist die Anzahl der Ziehungen mit Ergebnis $(n_1, \dots, n_k)$. $n!$ ist die Anzahl aller Möglichkeiten, die n gezogenen Elemente anzuordnen. Für jede solche Anordnung kann man aber die gleichartigen Elemente untereinander vertauschen, ohne das Ergebnis zu verändern. Die Anzahl der Vertauschungen beträgt $n_1! \dots n_k!$.

The *binomial theorem*, also known as the general binomial formula, is

$$(a + b)^n = \sum_{k=0}^n \binom{n}{k} a^k b^{n-k}. \quad (\text{A.17})$$

For $n = 0$ this is clear. Further applies

$$\begin{aligned} (a + b)^{n+1} &= (a + b)^n (a + b) = (a + b) \sum_{k=0}^n \binom{n}{k} a^k b^{n-k} \\ &= \sum_{k=0}^n \frac{n!}{k! (n-k)!} a^{k+1} b^{n-k} + \sum_{k=0}^n \frac{n!}{k! (n-k)!} a^k b^{n-k+1} \\ &= \sum_{k=1}^{n+1} \frac{n!}{(k-1)! (n+1-k)!} a^k b^{n-k+1} + \sum_{k=0}^n \frac{n!}{k! (n-k)!} a^k b^{n-k+1} \\ &= \sum_{k=1}^{n+1} \frac{(n+1)!}{k! (n+1-k)!} \frac{k}{n+1} a^k b^{n-k+1} \\ &\quad + \sum_{k=0}^n \frac{(n+1)!}{k! (n+1-k)!} \frac{n+1-k}{n+1} a^k b^{n-k+1} \\ &= \sum_{k=0}^{n+1} \frac{(n+1)!}{k! (n+1-k)!} a^k b^{n-k+1} \left(\frac{k + n + 1 - k}{n+1} \right) \\ &= \sum_{k=0}^{n+1} \frac{(n+1)!}{k! (n+1-k)!} a^k b^{n+1-k} = \sum_{k=0}^{n+1} \binom{n+1}{k} a^k b^{n+1-k}. \end{aligned} \quad (\text{A.18})$$

Let (x_1, x_2, x_3) be three Cartesian coordinates and (e_1, e_2, e_3) be the corresponding basis. One defines the *Levi-Civita symbol* $\varepsilon_{i,j,k}$ by

$$\varepsilon_{i,j,k} := \begin{cases} 1, & (i, j, k) \text{ gerade Permutation von } (1, 2, 3), \\ -1, & (i, j, k) \text{ ungerade Permutation von } (1, 2, 3), \\ 0, & \text{sonst.} \end{cases} \quad (\text{A.19})$$

This means in particular

$$\varepsilon_{i,j,k} = \varepsilon_{k,i,j} = \varepsilon_{j,k,i} = -\varepsilon_{j,i,k} = -\varepsilon_{k,j,i} = -\varepsilon_{i,k,j}, \quad (\text{A.20})$$

$$\varepsilon_{i,i,j} = \varepsilon_{i,j,i} = \varepsilon_{j,i,i} = 0. \quad (\text{A.21})$$

It applies

$$\begin{aligned} \sum_{n=1}^3 \varepsilon_{l,n,k} \varepsilon_{n,o,j} - \varepsilon_{l,n,j} \varepsilon_{n,o,k} &= \sum_{n=1}^3 \varepsilon_{l,n,k} \varepsilon_{j,n,o} + \varepsilon_{l,n,j} \varepsilon_{k,o,n} = \sum_{n=1}^3 \varepsilon_{j,o,n} \varepsilon_{l,k,n} + \varepsilon_{j,l,n} \varepsilon_{k,o,n} \\ &= \sum_{n=1}^3 \varepsilon_{j,o,n} \varepsilon_{l,k,n} - \varepsilon_{j,l,n} \varepsilon_{o,k,n}. \end{aligned} \quad (\text{A.22})$$

Here you have to make a case distinction. For the left expression to be nonzero, either $j = l$ and $o = k$ or $j = k$ and $o = l$ must hold. For the left expression you can write $\delta_{j,l} \delta_{o,k} - \delta_{j,k} \delta_{o,l}$. For the right expression to be nonzero, either $j = o$ and $l = k$ or $j = k$ and $l = o$ must hold. For the right expression you can write $-\delta_{j,o} \delta_{l,k} + \delta_{j,k} \delta_{o,l}$. So you can continue

$$\sum_{n=\mathbf{1}}^3 \varepsilon_{j,o,n} \varepsilon_{l,k,n} - \varepsilon_{j,l,n} \varepsilon_{o,k,n} = \delta_{j,l} \delta_{o,k} - \delta_{j,o} \delta_{l,k} = \sum_{n=\mathbf{1}}^3 \varepsilon_{j,k,n} \varepsilon_{l,o,n}, \quad (\text{A.23})$$

which is easy to understand.

A.4 Determinants

Let a square matrix $A \in \mathbb{C}^{N \times N}$ be given with $\mathbf{1} \leq N \in \mathbb{N}$. The *determinant* $\det(A)$ is defined by

$$\det(A) := \sum_{\pi \in S_N} \text{sign}(\pi) A_{\mathbf{1},\pi(\mathbf{1})} \cdots A_{N,\pi(N)}. \quad (\text{A.24})$$

Occasionally the spelling is also used

$$\begin{vmatrix} A_{\mathbf{1},\mathbf{1}} & \cdots & A_{\mathbf{1},N} \\ \vdots & \ddots & \vdots \\ A_{N,\mathbf{1}} & \cdots & A_{N,N} \end{vmatrix} := \det(A). \quad (\text{A.25})$$

First of all

$$\det(A^T) = \sum_{\pi \in S_N} \text{sign}(\pi) A_{\mathbf{1},\pi(\mathbf{1})}^T \cdots A_{N,\pi(N)}^T = \sum_{\pi \in S_N} \text{sign}(\pi) A_{\pi(\mathbf{1}),\mathbf{1}} \cdots A_{\pi(N),N}. \quad (\text{A.26})$$

By sorting each individual summand by ascending row indices, one obtains

$$\det(A^T) = \sum_{\pi \in S_N} \text{sign}(\pi) A_{\pi(\mathbf{1}),\mathbf{1}} \cdots A_{\pi(N),N} = \sum_{\pi \in S_N} \text{sign}(\pi) A_{\mathbf{1},\pi(\mathbf{1})} \cdots A_{N,\pi(N)} = \det(A). \quad (\text{A.27})$$

All following statements are therefore only proven for rows; the statement for columns then follows analogously. If two lines $\mathbf{1} \leq i, j \leq N$ of A are equal, then it is already

$$\det(A) = 0. \quad (\text{A.28})$$

To do this, sort the elements $\pi \in S_N$ into $N!/2$ pairs (π, π') such that π' emerges from π by swapping $\pi(i)$ and $\pi(j)$. In this case, $\text{sign}(\pi) = -\text{sign}(\pi')$, which shows the statement. If the j -th row emerges from the i -th row by multiplication with a complex constant $C \in \mathbb{C}$, then $A_{j,k} = CA_{i,k}$ for all $\mathbf{1} \leq k \leq N$, it also follows

$$\det(A) = 0, \quad (\text{A.29})$$

by simply dragging C in front of the sum defining the determinant. If the j -th row is a linear combination of the other $N - \mathbf{1}$ rows, there exist constants $C_l \in \mathbb{C}$ for $\mathbf{1} \leq l \leq N$ with $l \neq j$ with $A_{j,k} = \sum_{\substack{l=\mathbf{1}, \\ l \neq j}}^N C_l A_{l,k}$ for all $\mathbf{1} \leq k \leq N$, also applies in this case

$$\det(A) = 0. \quad (\text{A.30})$$

To do this you simply have to apply the previously proven statement $N - \mathbf{1}$ times.

A.5 Basic functions

The concept of function is assumed. Let $K \in \{\mathbb{R}, \mathbb{C}\}$ and $a_n \in K$ for all $n \in \mathbb{N}$. A power series p at the development point $x_o \in K$ is a series of the form

$$p(x) = \sum_{n=0}^{\infty} a_n (x - x_o)^n. \quad (\text{A.31})$$

For their derivatives the following applies (remember the sum rule)

$$p'(x) = \sum_{n=0}^{\infty} a_n n (x - x_o)^{n-1} = \sum_{n=1}^{\infty} a_n n (x - x_o)^{n-1} \sum_{n=0}^{\infty} a_{n+1} (n+1) (x - x_o)^n, \quad (\text{A.32})$$

$$\frac{d^2}{dx^2} \sum_{n=0}^N a_n x^n = \sum_{n=0}^{\infty} (n+2)(n+1) a_{n+2} (x - x_o)^n, \quad (\text{A.33})$$

$$\frac{d^m}{dx^m} \sum_{n=0}^N a_n x^n = \sum_{n=0}^{\infty} \frac{(n+m)!}{n!} a_{n+m} (x - x_o)^n \quad (\text{A.34})$$

These formulas can also be used for terminating power series, so-called *polynomials*.

Let $K \in \{\mathbb{R}, \mathbb{C}\}$ and $f: K \rightarrow K$ be a function. The function f is called locally analytic at a point $x_o \in K$ if there is a neighborhood M of x_o and a power series p at the development point x_o such that for all $x \in M$ holds

$$f(x) = p(x). \quad (\text{A.35})$$

A function is called analytic if it is locally analytic at every point. There are some standard power series called the *basic functions*:

- *Polynomials*.
- *Rational functions* (fractions of polynomials).
- The *exponential function*

$$\exp(x) := \sum_{n=0}^{\infty} \frac{x^n}{n!}. \quad (\text{A.36})$$

- The *natural logarithm function*

$$\ln := \exp^{-1}. \quad (\text{A.37})$$

- The *hyperbolic functions*

$$\sinh(x) := \frac{\exp(x) - \exp(-x)}{2} \quad \cosh(x) := \frac{\exp(x) + \exp(-x)}{2} \quad \tanh := \frac{\sinh}{\cosh}. \quad (\text{A.38})$$

- The correspondingly restricted inverse functions of the hyperbolic functions, the so-called *area functions*

$$\operatorname{arsinh} := \sinh^{-1}, \quad \operatorname{arcosh} := \cosh^{-1}, \quad \operatorname{artanh} := \tanh^{-1}. \quad (\text{A.39})$$

- The *trigonometric functions*

$$\sin(x) := -i \sinh(ix), \quad \cos(x) := \cosh(ix), \quad \tan := \frac{\sin}{\cos}. \quad (\text{A.40})$$

- The correspondingly restricted inverse functions of the trigonometric functions, the so-called *arcus functions*

$$\arcsin := \sin^{-1}, \quad \arccos := \cos^{-1}, \quad \arctan := \tan^{-1} \quad (\text{A.41})$$

The exponential function fulfills the calculation rule

$$\begin{aligned}
\exp(x+y) &\stackrel{\text{Glg. (A.17)}}{=} \sum_{k=\mathfrak{o}}^{\infty} \frac{\mathfrak{I}}{k!} \sum_{l=\mathfrak{o}}^k \binom{k}{l} x^l y^{k-l} = \sum_{k=\mathfrak{o}}^{\infty} \frac{\mathfrak{I}}{k!} \sum_{l=\mathfrak{o}}^k \frac{k!}{l!(k-l)!} x^l y^{k-l} = \sum_{k=\mathfrak{o}}^{\infty} \sum_{l=\mathfrak{o}}^k \frac{\mathfrak{I}}{l!(k-l)!} x^l y^{k-l} \\
&= \sum_{l=\mathfrak{o}}^{\infty} \sum_{k=l}^{\infty} \frac{\mathfrak{I}}{l!(k-l)!} x^l y^{k-l} = \sum_{l=\mathfrak{o}}^{\infty} \frac{x^l}{l!} \sum_{k=\mathfrak{o}}^{\infty} \frac{y^k}{k!} = \exp(x) \exp(y).
\end{aligned} \tag{A.42}$$

From this it follows

$$\mathfrak{I} = \exp(x-x) = \exp(x) \exp(-x) \Rightarrow \exp(-x) = \frac{\mathfrak{I}}{\exp(x)}. \tag{A.43}$$

It is

$$\exp(x) > \mathfrak{o} \tag{A.44}$$

for all $x \in \mathbb{R}$. For $x \geq \mathfrak{o}$ this is clear. For $x < \mathfrak{o}$ applies

$$\exp(x) = \frac{\mathfrak{I}}{\exp(-x)} > \mathfrak{o}. \tag{A.45}$$

Therefore apply

$$\cosh^2(x) = \frac{\mathfrak{I}}{4} (e^{2x} + e^{-2x} + \mathfrak{2}) = \frac{\mathfrak{I}}{4} (e^{2x} + e^{-2x} - \mathfrak{2}) + \mathfrak{I} = \sinh^2(x) + \mathfrak{I}, \tag{A.46}$$

$$\sin^2(x) + \cos^2(x) = -\sinh^2(ix) + \cosh^2(ix) = \mathfrak{I}, \tag{A.47}$$

$$\tanh' = \frac{\cosh^2 - \sinh^2}{\cosh^2} = \mathfrak{I} - \tanh^2 = \frac{\mathfrak{I}}{\cosh^2}, \tag{A.48}$$

$$\tan' = \frac{\cos^2 + \sin^2}{\cos^2} = \mathfrak{I} + \tan^2 = \frac{\mathfrak{I}}{\cos^2}. \tag{A.49}$$

The basic functions fulfill the following symmetry properties:

$$\sinh(-x) = \frac{e^{-x} - e^x}{\mathfrak{2}} = -\frac{e^x - e^{-x}}{\mathfrak{2}} = -\sinh(x) \tag{A.50}$$

$$\cosh(-x) = \frac{e^{-x} + e^x}{\mathfrak{2}} = \frac{e^x + e^{-x}}{\mathfrak{2}} = \cosh(x) \tag{A.51}$$

$$\Rightarrow \tanh(-x) = -\tanh(x) \tag{A.52}$$

$$\sin(-x) = -i \sinh(-ix) = i \sinh(ix) = -(-i \sinh(ix)) = -\sin(x) \tag{A.53}$$

$$\cos(-x) = \cosh(-ix) = \cosh(ix) = \cos(x) \tag{A.54}$$

$$\Rightarrow \tan(-x) = -\tan(x) \tag{A.55}$$

The so-called *addition theorems* apply.

$$\begin{aligned}
\sinh(x+y) &= \frac{e^x e^y - e^{-x} e^{-y}}{\mathfrak{2}} = \frac{\mathfrak{I}}{4} (\mathfrak{2} e^x e^y - \mathfrak{2} e^{-x} e^{-y}) = \frac{\mathfrak{I}}{4} ((e^x - e^{-x})(e^y + e^{-y}) + (e^y - e^{-y})(e^x + e^{-x})) \\
&= \sinh(x) \cosh(y) + \cosh(x) \sinh(y),
\end{aligned} \tag{A.56}$$

$$\begin{aligned}
\cosh(x+y) &= \frac{e^x e^y + e^{-x} e^{-y}}{\mathfrak{2}} = \frac{\mathfrak{I}}{4} (\mathfrak{2} e^x e^y + \mathfrak{2} e^{-x} e^{-y}) = \frac{\mathfrak{I}}{4} ((e^x + e^{-x})(e^y + e^{-y}) + (e^y - e^{-y})(e^x - e^{-x})) \\
&= \cosh(x) \cosh(y) + \sinh(x) \sinh(y),
\end{aligned} \tag{A.57}$$

$$\begin{aligned}
\tanh(x+y) &= \frac{\sinh(x+y)}{\cosh(x+y)} = \frac{\sinh(x) \cosh(y) + \cosh(x) \sinh(y)}{\cosh(x) \cosh(y) + \sinh(x) \sinh(y)} = \frac{\tanh(x) \cosh(y) + \sinh(y)}{\cosh(y) + \tanh(x) \sinh(y)} \\
&= \frac{\tanh(x) + \tanh(y)}{\mathfrak{I} + \tanh(x) \tanh(y)}.
\end{aligned} \tag{A.58}$$

Applying this to the trigonometric functions gives

$$\begin{aligned}\sin(x+y) &= -i\sinh(ix+iy) = -i\sinh(ix)\cosh(iy) - i\cosh(ix)\sinh(iy) \\ &= \sin(x)\cos(y) + \cos(x)\sin(y),\end{aligned}\tag{A.59}$$

$$\begin{aligned}\cos(x+y) &= \cosh(ix+iy) = \cosh(ix)\cosh(iy) + \sinh(ix)\sinh(iy) \\ &= \cos(x)\cos(y) - \sin(x)\sin(y).\end{aligned}\tag{A.60}$$

From this it follows

$$\cos(a) = \cos^2\left(\frac{a}{2}\right) - \sin^2\left(\frac{a}{2}\right) = 1 - 2\sin^2\left(\frac{a}{2}\right) = 2\cos^2\left(\frac{a}{2}\right) - 1.\tag{A.61}$$

The so-called *Euler identity* also applies

$$\exp(ix) = \frac{\exp(ix) + \exp(-ix) + \exp(ix) - \exp(-ix)}{2} = \cosh(ix) + \sinh(ix) = \cos(x) + i\sin(x).\tag{A.62}$$

The following applies to the derivations of the basic functions

$$\exp'(x) \stackrel{\text{Glg. (A.32)}}{=} \sum_{n=0}^{\infty} \frac{n+1}{(n+1)!} x^n = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \exp(x),\tag{A.63}$$

$$\sinh'(x) = \cosh(x),\tag{A.64}$$

$$\cosh'(x) = \sinh(x),\tag{A.65}$$

$$\sin'(x) = \cosh(ix) = \cos(x),\tag{A.66}$$

$$\cos'(x) = -\sin(x).\tag{A.67}$$

Because of Eq. (A.44) is $\exp$ strictly monotonically increasing on $\mathbb{R}$. Because $\cosh(x) > 0$ for all real x , $\sinh$ is strictly monotonically increasing, and we also have

$$\lim_{x \rightarrow \infty} \sinh(x) = \infty, \quad \lim_{x \rightarrow -\infty} \sinh(x) = -\infty.\tag{A.68}$$

So is

$$\operatorname{arsinh} : \mathbb{R} \rightarrow \mathbb{R}\tag{A.69}$$

defined, still applies

$$\operatorname{arsinh}'(x) = \frac{1}{\cosh(\operatorname{arsinh}'(x))} = \frac{1}{\sqrt{1+x^2}}.\tag{A.70}$$

They still apply

$$\lim_{x \rightarrow \infty} \cosh(x) = \infty, \quad \lim_{x \rightarrow -\infty} \cosh(x) = \infty,\tag{A.71}$$

the minimum is at $x = 0$, there $\cosh(0) = 1$, so define

$$\operatorname{arcosh} [1, \infty) \rightarrow [0, \infty).\tag{A.72}$$

For the derivation applies

$$\operatorname{arcosh}'(x) = \frac{1}{\sinh(\operatorname{arcosh}(x))} = \frac{1}{\sqrt{x^2-1}}.\tag{A.73}$$

The arc functions have the definition and image sets

$$\arcsin : [-1, 1] \rightarrow \left[-\frac{\pi}{2}, \frac{\pi}{2}\right], \quad (\text{A.74})$$

$$\arccos : [-1, 1] \rightarrow [0, \pi], \quad (\text{A.75})$$

$$\arctan : (-\infty, \infty) \rightarrow \left(-\frac{\pi}{2}, \frac{\pi}{2}\right). \quad (\text{A.76})$$

Their derivatives are calculated as:

$$\arcsin'(x) = \frac{1}{\cos(\arcsin(x))} = \frac{1}{\sqrt{1-x^2}}, \quad (\text{A.77})$$

$$\arccos'(x) = -\frac{1}{\sin(\arccos(x))} = \frac{1}{\sqrt{1-x^2}}, \quad (\text{A.78})$$

$$\arctan'(x) = \frac{1}{\tan'(\arctan(x))} = \frac{1}{1+x^2}. \quad (\text{A.79})$$

For the first order Taylor expansions of the basic functions to the expansion point zero follows

$$\exp(x) \approx 1 + x, \quad \sinh(x) \approx x, \quad \cosh(x) \approx 1, \quad \tanh(x) \approx x, \quad (\text{A.80})$$

$$\sin(x) \approx x, \quad \cos(x) \approx 1, \quad \tan(x) \approx x. \quad (\text{A.81})$$

Let $p(x) = \sum_{n=0}^{\infty} a_n x^n$ be a power series $\mathbb{C} \rightarrow \mathbb{C}$ with $p(x) = 0$ for all $x \in \mathbb{C}$, then $a_n = 0$ already holds for all $n \in \mathbb{N}$. This should first be seen by proving by contradiction for a polynomial, i.e. for a terminating power series. So assume that $a_n = 0$ for all $N < n \in \mathbb{N}$ and further assume that $a_N \neq 0$. For $|x| \rightarrow \infty$ every polynomial diverges, since polynomials are continuous there is in particular a $b \in \mathbb{R}$ with $b > 0$ and $|p(x)| > 0$ for all $x \in \mathbb{C}$ with $|x| > b$ contradicts the assumption. Thus the statement for polynomials is shown.

At this point a note should be made about complex numbers. The obvious hurdle with complex numbers is to recognize the existence of the imaginary unit $i = \sqrt{-1}$. One cannot imagine a number i that satisfies this equation. Nevertheless, it can be expected, so it is a theoretical aid. Before comparing with measurements, however, the result must be projected onto the real axis. Even with real numbers, one can ask oneself what one should do with a number that never ends, i.e. an irrational number like e . The clear limits have basically already been exceeded here.

A.6 Delta distribution

The *Delta distribution* $\delta(x)$ is defined by the fact that for every continuous function $f = f(x)$

$$\int_{a < 0}^{b > 0} \delta(x) f(x) dx = f(0) \quad (\text{A.82})$$

applies. It is according to [11]

$$\lim_{t \rightarrow \infty} \frac{4 \sin^2\left(\frac{\Omega t}{2}\right)}{\Omega^2 t} = 2\pi \delta(\Omega). \quad (\text{A.83})$$

According to [9] the following applies

$$\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ik(x - x_0)) dk. \quad (\text{A.84})$$

A.7 Integral formulas

A.7.1 Partial integration

Let $f, g : \mathbb{R} \rightarrow \mathbb{R}$ be Riemann integrable. Then the product rule applies

$$(fg)' = f'g + fg' \Leftrightarrow fg = \int f'g dx + \int fg' dx \Leftrightarrow \int f'g dx = fg - \int fg' dx. \quad (\text{A.85})$$

This is called *partial integration*.

A.7.2 Substitution rule

Let $a, b \in \mathbb{R}$ with $a < b$, $f : [a, b] \rightarrow \mathbb{R}$ be Riemann integrable, $I \subseteq \mathbb{R}$ an interval, $\varphi : I \rightarrow [a, b]$ continuous-differentiable and bijective and F an antiderivative of f . Then applies

$$\int_a^b f(x) dx = [F(x)]_a^b = [F(\varphi(x))]_{\varphi^{-1}(a)}^{\varphi^{-1}(b)} = \int_{\varphi^{-1}(a)}^{\varphi^{-1}(b)} \frac{d}{dx} (F(\varphi(x))) dx = \int_{\varphi^{-1}(a)}^{\varphi^{-1}(b)} f(\varphi(x)) \varphi'(x) dx. \quad (\text{A.86})$$

This is called *substitution rule*.

A.7.3 Separation of variables

The method of *separation of variables* is derived. Let $a, b \in \mathbb{R}$ with $a < b$ be given, let $h : [a, b] \rightarrow \mathbb{R}$ be Riemann integrable, $f : [a, b] \rightarrow \mathbb{R}$ be continuous-differentiable and bijective and $g : f([a, b]) \rightarrow \mathbb{R}$ Riemann integrable with $g(y) \neq 0$ for all $y \in f([a, b])$. You want the differential equation

$$\frac{df}{dx} = g(f) h(x) \quad (\text{A.87})$$

solve on $[a, b]$. You do the math

$$\frac{1}{g(f)} \frac{df}{dx} = h(x). \quad (\text{A.88})$$

This is now integrated from a to a desired $x \in [a, b]$:

$$\int_a^x \frac{1}{g(f(x'))} \frac{df}{dx'} dx' = \int_a^x h(x') dx' \Leftrightarrow \int_{f(a)}^{f(x)} \frac{1}{g(f)} df = \int_a^x h(x') dx' \quad (\text{A.89})$$

The substitution rule was used here. If these two integrals are solvable, one obtains an algebraic expression for $f(x)$.

A.7.4 Leibniz rule

Let a continuously differentiable function $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ be given. Furthermore, let two functions $a \leq b$ be given, which depend on a parameter t , $a = a(t)$, $b = b(t)$. Define the function $F = F(t)$ by

$$F(t) := \int_{a(t)}^{b(t)} f(x, t) dx. \quad (\text{A.90})$$

The *Leibniz rule* is a statement about the derivative of F . To derive this, you first define an auxiliary function

$$\tilde{F}(a, b, t) := \int_a^b f(x, t) dx. \quad (\text{A.91})$$

Then the derivative of $\tilde{F}$ holds

$$\tilde{F}'(a, b, t) = \nabla \tilde{F}(a, b, t) = \begin{pmatrix} \frac{\partial \int_a^b f(x, t) dx}{\partial a} \\ \frac{\partial \int_a^b f(x, t) dx}{\partial b} \\ \frac{\partial \int_a^b f(x, t) dx}{\partial t} \end{pmatrix}. \quad (\text{A.92})$$

This can be done using the main theorem of analysis

$$\begin{pmatrix} \frac{\partial \int_a^b f(x,t) dx}{\partial a} \\ \frac{\partial \int_a^b f(x,t) dx}{\partial b} \\ \frac{\partial \int_a^b f(x,t) dx}{\partial t} \end{pmatrix} = \begin{pmatrix} -f(a,t) \\ f(b,t) \\ \int_a^b \frac{\partial f(x,t)}{\partial t} dx \end{pmatrix} \quad (\text{A.93})$$

rephrase. With the multidimensional chain rule you get

$$\frac{dF(t)}{dt} = \begin{pmatrix} \frac{da}{dt} \\ \frac{db}{dt} \\ \frac{dt}{dt} \end{pmatrix} \cdot \nabla \tilde{F}(a, b, t) \quad (\text{A.94})$$

$$\Leftrightarrow \frac{dF(t)}{dt} = \int_{a(t)}^{b(t)} \frac{\partial f(x,t)}{\partial t} dx + f[b(t), t] \frac{db}{dt} - f[a(t), t] \frac{da}{dt}. \quad (\text{A.95})$$

This is the Leibniz rule.

A.7.5 More formulas

Now should

$$\int_0^\infty x^n e^{-\beta x} dx = \frac{n!}{\beta^{n+1}} \quad (\text{A.96})$$

with $\beta \in \mathbb{R}$, $\beta > 0$, $n \in \mathbb{N}$. This is best done via complete induction. For $n = 0$ applies

$$\int_0^\infty e^{-\beta x} dx = \frac{1}{\beta}, \quad (\text{A.97})$$

so the statement is true for $n = 0$. Now the statement already applies to n . Then follows by partial integration

$$\int_0^\infty x^{n+1} e^{-\beta x} dx = \left[-\frac{1}{\beta} x^{n+1} e^{-\beta x} \right]_0^\infty + \frac{n+1}{\beta} \int_0^\infty x^n e^{-\beta x} dx = \frac{n+1}{\beta} \frac{n!}{\beta^{n+1}} = \frac{(n+1)!}{\beta^{n+2}}. \quad (\text{A.98})$$

The statement therefore applies to all $n \in \mathbb{N}$. Still applies

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}. \quad (\text{A.99})$$

For this one first calculates with Eq. (A.8)

$$\frac{1}{e^x - 1} = \frac{e^{-x}}{1 - e^{-x}} = \frac{e^{-x} + 1 - 1}{1 - e^{-x}} = \frac{1}{1 - e^{-x}} - 1 = \sum_{n=0}^\infty e^{-nx} - 1 = \sum_{n=1}^\infty e^{-nx}. \quad (\text{A.100})$$

This means that with the equations (A.96) and (A.12)

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \sum_{n=1}^\infty \int_0^\infty x^3 e^{-nx} dx = 6 \sum_{n=1}^\infty \frac{1}{n^4} = \frac{\pi^4}{15}. \quad (\text{A.101})$$

The so-called *Gamma function* is by

$$\Gamma(n+1) := \int_0^\infty x^n e^{-x} dx \quad (\text{A.102})$$

defined. For them it follows with Eq. (A.96)

$$\Gamma(n) = (n-1)!. \quad (\text{A.103})$$

The *error function* erf is defined by

$$\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \quad (\text{A.104})$$

According to [1]

$$\lim_{x \rightarrow \infty} \operatorname{erf}(x) = 1. \quad (\text{A.105})$$

For $C > 0$ follows

$$\lim_{x \rightarrow \infty} \int_0^x e^{-Cx^2} dx = \frac{1}{\sqrt{C}} \lim_{x \rightarrow \infty} \int_0^x e^{-x^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{C}}. \quad (\text{A.106})$$

Follow it

$$\int_0^\infty e^{-Cx^2} x^2 dx = \left[x \left(-\frac{1}{2C} e^{-Cx^2} \right) \right]_0^\infty + \frac{1}{2C} \int_0^\infty e^{-Cx^2} dx = \frac{1}{4} \sqrt{\frac{\pi}{C^3}}, \quad (\text{A.107})$$

$$\begin{aligned} \int_0^\infty e^{-Cx^2} x^3 dx &= \left[x^2 \cdot \left(-\frac{1}{2C} e^{-Cx^2} \right) \right]_0^\infty + \int_0^\infty \frac{x}{C} e^{-Cx^2} dx \\ &= \int_0^\infty \frac{x}{C} e^{-Cx^2} dx = -\frac{1}{2C^2} \left[e^{-Cx^2} \right]_0^\infty = \frac{1}{2C^2}. \end{aligned} \quad (\text{A.108})$$

One defines the *gamma function* for $x > 0$ by

$$\Gamma(x) := \int_0^\infty t^{x-1} e^{-t} dt. \quad (\text{A.109})$$

For $n \in \mathbb{N}$, because of Eq. (A.96)

$$\Gamma(n+1) = \int_0^\infty t^n e^{-t} dt = n!. \quad (\text{A.110})$$

This follows in particular

$$\Gamma(n+1) = n! = n(n-1)! = n\Gamma(n). \quad (\text{A.111})$$

One can use this to derive the *Stirling formula*, which is an approximation of $n!$ for high n , which is very useful when, for example, the question is how much $(10^{23})!$ is. This is what you first calculate

$$n! = \Gamma(n+1) = \int_0^\infty t^n e^{-t} dt = \int_0^\infty e^{-t+n \ln(t)} dt = \int_0^\infty e^{-n\varphi(t)} dt \quad (\text{A.112})$$

with

$$\varphi(t) := \frac{t}{n} - \ln(t). \quad (\text{A.113})$$

They apply

$$\lim_{t \rightarrow 0} \varphi(t) = \infty, \quad \lim_{t \rightarrow \infty} \varphi(t) = \infty. \quad (\text{A.114})$$

For the first two derivatives applies

$$\varphi'(t) = \frac{1}{n} - \frac{1}{t}, \quad \varphi''(t) = \frac{1}{t^2}. \quad (\text{A.115})$$

The unique minimum is therefore $t = n$. The Taylor expansion up to the second order to the point $x = n$ is therefore

$$\varphi(t) = 1 - \ln(n) + \frac{1}{2} \frac{(t-n)^2}{n^2} + \mathcal{O}[(t-n)^3]. \quad (\text{A.116})$$

The expression $e^{-n\varphi}$ is only relevant for negative and small φ , so the Taylor expansion to the minimum is a good approximation in the integral of the gamma function:

$$n! \approx \int_0^\infty e^{-n+n\ln(n)-\frac{1}{2}\frac{(t-n)^2}{n}} dt = n^n e^{-n} \int_0^\infty e^{-\frac{t^2}{2n}} dt = n^n e^{-n} \sqrt{2\pi n} = \sqrt{2\pi} n^{n+1/2} e^{-n} \quad (\text{A.117})$$

In the last step, Eq. (A.105) is used. Eq. (A.117) is the Stirling formula.

A.7.6 Functional derivatives

Let $n \in \mathbb{N}$ with $n \geq 1$. Let $\Omega \subseteq \mathbb{R}^3$ be connected and $\psi : \Omega \rightarrow \mathbb{R}^n$ and $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be continuously differentiable. Define the functional

$$F[\psi] := \int_\Omega f(\psi(\mathbf{r})) d^3r \in \mathbb{R}. \quad (\text{A.118})$$

Now define a set of helper functions

$$D := \{h : \Omega \rightarrow \mathbb{R}^n \mid \text{stetig differenzierbar, } h(\partial\Omega) = \mathbf{0}\}. \quad (\text{A.119})$$

Based on this, a further set of difference quotients is created

$$H : D \times \mathbb{R}_{>0} : (h, \varepsilon) \mapsto \frac{F[\psi + \varepsilon h] - F[\psi]}{\varepsilon} \quad (\text{A.120})$$

defined. The functional derivative

$$\frac{\delta F}{\delta \psi} : \Omega \rightarrow \mathbb{R}^n \quad (\text{A.121})$$

is the function which

$$\frac{dH(h, \varepsilon)}{d\varepsilon} = \lim_{\varepsilon \rightarrow 0} \frac{F[\psi + \varepsilon h] - F[\psi]}{\varepsilon} = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \int_\Omega f(\psi(\mathbf{r}) + \varepsilon h(\mathbf{r})) - f(\psi(\mathbf{r})) d^3r = \int_\Omega \frac{\delta F}{\delta \psi} \cdot h(\mathbf{r}) d^3r \quad (\text{A.122})$$

satisfied for all $h \in D$. The functional derivative can be understood as the derivative of F in the direction ψ .

A.8 Vector spaces

Let $K \in \{\mathbb{R}, \mathbb{C}\}$, then one defines a vector space V over K in the following way:
There is an illustration

$$+ : V \times V \rightarrow V; (\mathbf{x}, \mathbf{y}) \mapsto \mathbf{x} + \mathbf{y} \quad (\text{A.123})$$

and another illustration

$$\cdot : K \times V \rightarrow V; (\lambda, \mathbf{x}) \mapsto \lambda \mathbf{x}. \quad (\text{A.124})$$

These two functions have the following properties:

$$(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z}), \quad \mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}, \quad \mathbf{o} + \mathbf{x} = \mathbf{x}. \quad (\text{A.125})$$

For every $\mathbf{x} \in V$ there exists a $(-\mathbf{x}) \in V$ with

$$(-\mathbf{x}) + \mathbf{x} = \mathbf{o}. \quad (\text{A.126})$$

Should continue to apply

$$\mathcal{I}_1 \cdot (\mathcal{I}_2 \mathbf{x}) = (\mathcal{I}_1 \mathcal{I}_2) \cdot \mathbf{x}, \quad \mathbf{I} \cdot \mathbf{x} = \mathbf{x}, \quad (\text{A.127})$$

$$\mathcal{I}(\mathbf{x} + \mathbf{y}) = \mathcal{I}\mathbf{x} + \mathcal{I}\mathbf{y}, \quad (\mathcal{I}_1 + \mathcal{I}_2)\mathbf{x} = \mathcal{I}_1\mathbf{x} + \mathcal{I}_2\mathbf{x}. \quad (\text{A.128})$$

Vectors that can be understood as arrows in space are noted in this book **bolditalic**.

A *matrix* A over $K\{\mathbb{R}, \mathbb{C}\}$ is a rectangular array of elements from K with $m \geq 1$ rows and $n \geq 1$ columns. Write $A_{i,j}$ for the element in the j th column of the i th row. One defines the transpose A^T of A by $A_{j,i} = A_{i,j}$ for all $1 \leq i \leq m, 1 \leq j \leq n$. The multiplication of such a matrix with a vector $\mathbf{b} = (b_1, \dots, b_n)^T$ is defined by,

$$A\mathbf{b} = \sum_{i=1}^m \sum_{j=1}^n A_{i,j} b_j \mathbf{e}_i, \quad (\text{A.129})$$

This creates an m -dimensional column vector. More generally, given a matrix B over K with n rows and $l \geq 1$ columns, then the matrix product $A \cdot B$ is defined by

$$(A \cdot B)_{i,j} := \sum_{a=1}^n A_{i,a} B_{a,j}. \quad (\text{A.130})$$

It applies

$$(A \cdot B)^T_{i,j} = (A \cdot B)_{j,i} = \sum_{a=1}^n A_{j,a} B_{a,i} = \sum_{a=1}^n B_{a,i} A_{j,a} = \sum_{a=1}^n B_{i,a}^T A_{a,j}^T = (B^T \cdot A^T)_{i,j} \quad (\text{A.131})$$

and thus is in this case

$$(A \cdot B)^T = B^T \cdot A^T. \quad (\text{A.132})$$

One further defines the dot product of two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$ by

$$\mathbf{a} \cdot \mathbf{b} = \langle \mathbf{a} | \mathbf{b} \rangle := \mathbf{a}^T \mathbf{b}. \quad (\text{A.133})$$

If A is a real matrix, then it follows

$$\langle \mathbf{a} | A\mathbf{b} \rangle = \mathbf{a}^T A\mathbf{b} = (A^T \mathbf{a})^T \mathbf{b} = \langle A^T \mathbf{a} | \mathbf{b} \rangle. \quad (\text{A.134})$$

Matrices with as many rows as columns are called *square*.

Operators are functions between functions. In meteorology only two function spaces are relevant:

$$F_1 = \{A \times \mathbb{R} \rightarrow \mathbb{R}, \text{ unendlich oft stetig-differenzierbar} \} \quad (\text{A.135})$$

$$F_2 = \{A \times \mathbb{R} \rightarrow \mathbb{R}^3, \text{ unendlich oft stetig-differenzierbar} \} \quad (\text{A.136})$$

Here A is the atmosphere. Operators are marked with an umbrella symbol. You define

$\hat{A}$ linearer Operator :

$$\Leftrightarrow \quad \hat{A}(\mathcal{I}\psi) = \mathcal{I}\hat{A}(\psi) \wedge \hat{A}(\psi_1 + \psi_2) = \hat{A}(\psi_1) + \hat{A}(\psi_2) \quad (\text{A.137})$$

for each $\mathcal{I} \in \mathbb{C}$. Let $\hat{A}$ and $\hat{B}$ be operators, then define

$$\hat{A}\hat{B} := \hat{A} \circ \hat{B} \quad (\text{A.138})$$

If $\hat{A}$ and $\hat{B}$ are linear, then the following applies

$$\hat{A} \left(\hat{B}(\lambda \psi) \right) = \hat{A} \left(\lambda \hat{B}(\psi) \right) = \lambda \hat{A} \left(\hat{B}(\psi) \right) \Leftrightarrow \hat{A}\hat{B}(\lambda \psi) = \lambda \hat{A}\hat{B}(\psi) \quad (\text{A.139})$$

Still applies

$$\hat{A}\hat{B}(\psi_1 + \psi_2) = \hat{A} \left(\hat{B}(\psi_1) + \hat{B}(\psi_2) \right) = \hat{A}\hat{B}(\psi_1) + \hat{A}\hat{B}(\psi_2). \quad (\text{A.140})$$

Successive executions of linear operators are therefore linear. Furthermore, the brackets around the argument for operators are often left out:

$$\hat{A}\psi := \hat{A}(\psi) \quad (\text{A.141})$$

Also applies

$$\begin{aligned} (\lambda_1 \hat{A} + \lambda_2 \hat{B}) \lambda \psi &= \lambda_1 \hat{A} \lambda \psi + \lambda_2 \hat{B} \lambda \psi = \lambda_1 \lambda \hat{A} \psi + \lambda_2 \lambda \hat{B} \psi = \lambda \left(\lambda_1 \hat{A} \psi + \lambda_2 \hat{B} \psi \right) \\ &= \lambda \left(\lambda_1 \hat{A} + \lambda_2 \hat{B} \right) \psi \end{aligned} \quad (\text{A.142})$$

as well as

$$\begin{aligned} (\lambda_1 \hat{A} + \lambda_2 \hat{B}) (\psi_1 + \psi_2) &= \lambda_1 \hat{A} (\psi_1 + \psi_2) + \lambda_2 \hat{B} (\psi_1 + \psi_2) \\ &= \lambda_1 \hat{A} \psi_1 + \lambda_1 \hat{A} \psi_2 + \lambda_2 \hat{B} \psi_1 + \lambda_2 \hat{B} \psi_2 \\ &= \left(\lambda_1 \hat{A} + \lambda_2 \hat{B} \right) \psi_1 + \left(\lambda_1 \hat{A} + \lambda_2 \hat{B} \right) \psi_2. \end{aligned} \quad (\text{A.143})$$

So linear combinations of linear operators are linear. Since the normal derivation rules apply to partial derivatives, we get

$$\frac{\partial}{\partial x_i} \lambda \psi = \lambda \frac{\partial}{\partial x_i} \psi \quad (\text{A.144})$$

$$\frac{\partial}{\partial x_i} (\psi_1 + \psi_2) = \frac{\partial}{\partial x_i} \psi_1 + \frac{\partial}{\partial x_i} \psi_2, \quad (\text{A.145})$$

where the time is covered by one of the x_i . Partial derivatives and linear combinations of partial derivatives (also with basis vectors) are therefore linear.

A.8.1 Vector product

Let (x_1, x_2, x_3) be three Cartesian coordinates and $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ be the corresponding basis. The vector product $\mathbf{A} \times \mathbf{B}$ of two vectors $\mathbf{A} = (A_1, A_2, A_3)^T$, $\mathbf{B} = (B_1, B_2, B_3)^T$ is defined by

$$\mathbf{A} \times \mathbf{B} := \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i B_j \mathbf{e}_k. \quad (\text{A.146})$$

This is linear because for $\lambda \in \mathbb{R}$ and $\mathbf{C} \in \mathbb{R}^3$

$$\begin{aligned} \mathbf{A} \times (\mathbf{B} + \mathbf{C}) &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i (B_j + C_j) \mathbf{e}_k = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i B_j \mathbf{e}_k + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i C_j \mathbf{e}_k \\ &= \mathbf{A} \times \mathbf{B} + \mathbf{A} \times \mathbf{C}, \end{aligned} \quad (\text{A.147})$$

$$\mathbf{A} \times (\lambda \mathbf{B}) = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i \lambda B_j \mathbf{e}_k = \lambda \mathbf{A} \times \mathbf{B}. \quad (\text{A.148})$$

Furthermore, it is anticommutative,

$$\mathbf{A} \times \mathbf{B} = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i B_j \mathbf{e}_k = \sum_{i,j,k=1}^3 -\varepsilon_{j,i,k} B_j A_i \mathbf{e}_k = -\mathbf{B} \times \mathbf{A}. \quad (\text{A.149})$$

For the l th component, $1 \leq l \leq 3$, of the vector product one finds

$$(\mathbf{A} \times \mathbf{B})_l = \left(\sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i B_j \mathbf{e}_k \right) \cdot \mathbf{e}_l = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i B_j \delta_{k,l} = \sum_{i,j=1}^3 \varepsilon_{i,j,l} A_i B_j. \quad (\text{A.150})$$

The vector product has the orthogonality properties

$$\begin{aligned} \mathbf{A} \cdot (\mathbf{A} \times \mathbf{B}) &= \sum_{i=1}^3 A_i (\mathbf{A} \times \mathbf{B})_i = \sum_{i=1}^3 A_i \sum_{j,k=1}^3 \varepsilon_{j,k,i} A_j B_k = \sum_{k=1}^3 B_k \sum_{i,j=1}^3 \varepsilon_{k,i,j} A_i A_j \\ &= \sum_{k=1}^3 B_k \sum_{i,j=1}^3 A_i A_j - A_j A_i = 0 \end{aligned} \quad (\text{A.151})$$

as well as

$$\mathbf{B} \cdot (\mathbf{A} \times \mathbf{B}) \stackrel{\text{Glg. (A.149)}}{=} -\mathbf{B} \cdot (\mathbf{B} \times \mathbf{A}) = -0 = 0. \quad (\text{A.152})$$

Furthermore, the so-called *Graßmann identity* applies:

$$\begin{aligned} \mathbf{A} \times (\mathbf{B} \times \mathbf{C}) &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i (\mathbf{B} \times \mathbf{C})_j \mathbf{e}_k = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i \left(\sum_{l,m,n=1}^3 \varepsilon_{l,m,n} B_l C_m \mathbf{e}_n \right)_j \mathbf{e}_k \\ &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i \sum_{l,m=1}^3 \varepsilon_{l,m,j} B_l C_m \mathbf{e}_k = \sum_{k=1}^3 \mathbf{e}_k \sum_{i=1}^3 A_i \sum_{j,l,m=1}^3 \varepsilon_{j,k,i} \varepsilon_{j,l,m} B_l C_m \\ &= \sum_{k=1}^3 \mathbf{e}_k \sum_{i=1}^3 A_i (B_k C_i - B_i C_k) = \mathbf{B} (\mathbf{A} \cdot \mathbf{C}) - \mathbf{C} (\mathbf{A} \cdot \mathbf{B}) \end{aligned} \quad (\text{A.153})$$

This is also known as *BAC-CAB rule*. You can still write

$$\mathbf{B} \equiv \mathbf{B}_{\parallel} + \mathbf{B}_{\perp}, \quad (\text{A.154})$$

where $\mathbf{B}_{\parallel}$ should denote the part of $\mathbf{B}$ parallel to $\mathbf{A}$ and

$$\mathbf{B}_{\perp} := \mathbf{B} - \mathbf{B}_{\parallel} \quad (\text{A.155})$$

the remaining portion of $\mathbf{B}$ that is perpendicular to $\mathbf{A}$, as will be shown. It applies

$$\mathbf{B}_{\parallel} = \left(\frac{1}{|\mathbf{A}|^2} \mathbf{A} \cdot \mathbf{B} \right) \mathbf{A}. \quad (\text{A.156})$$

From this it follows

$$\mathbf{A} \cdot \mathbf{B}_\perp = \mathbf{A} \cdot (\mathbf{B} - \mathbf{B}_\parallel) = \mathbf{A} \cdot \mathbf{B} - \mathbf{A} \cdot \left(\frac{1}{|\mathbf{A}|^2} \mathbf{A} \cdot \mathbf{B} \right) \mathbf{A} = 0, \quad (\text{A.157})$$

so $\mathbf{B}_\perp$ is indeed perpendicular to $\mathbf{A}$. With Eq. (A.153) can also be noted

$$\begin{aligned} \mathbf{A} \times (\mathbf{B} \times \mathbf{A}) &= \mathbf{B}A^2 - \mathbf{A}(\mathbf{A} \cdot \mathbf{B}) = A^2 \mathbf{B} - A^2 \mathbf{B}_\parallel = A^2 \mathbf{B}_\perp \\ \Rightarrow \mathbf{B}_\perp &= \frac{1}{A^2} \mathbf{A} \times (\mathbf{B} \times \mathbf{A}). \end{aligned} \quad (\text{A.158})$$

It applies

$$\begin{aligned} \mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) &= \sum_{i=1}^3 A_i (\mathbf{B} \times \mathbf{C})_i = \sum_{i=1}^3 A_i \sum_{j,k=1}^3 \varepsilon_{j,k,i} B_j C_k = \sum_{i,j,k=1}^3 \varepsilon_{j,k,i} A_i B_j C_k = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_i B_j C_k \\ &= \sum_{k=1}^3 C_k \sum_{i,j=1}^3 \varepsilon_{i,j,k} A_i B_j = \sum_{i=1}^3 C_k (\mathbf{A} \times \mathbf{B})_k = \mathbf{C} \cdot (\mathbf{A} \times \mathbf{B}). \end{aligned} \quad (\text{A.159})$$

B.1 Multidimensional derivatives

Directional derivatives are derivatives of a function of several variables along a specific direction, with the partial derivatives being special cases of these in which the derivative is derived in the direction of one of the coordinate axes.

Let $n, m \in \mathbb{N}$ be differentiable with $n, m \geq 1$ and $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$. Then the derivative is a function $f' : \mathbb{R}^n \rightarrow \mathbb{R}^{m \times n}$ and it holds

$$(f')_{i,j} = \left(\frac{\partial f_i}{\partial x_j} \right). \quad (\text{B.1})$$

The matrix f' is called the *Jacobi matrix* of f . In particular, the definition of the gradient of a differentiable scalar function $g: \mathbb{R}^n \rightarrow \mathbb{R}$ results as the transpose of the derivative:

$$\text{grad}(g) := (g')^T = \left(\frac{\partial g}{\partial x_i} \right) \quad (\text{B.2})$$

Define the Nabla operator ∇ by

$$\nabla := \sum_{i=1}^3 \mathbf{e}_i \frac{\partial}{\partial x_i}. \quad (\text{B.3})$$

Let $n, m \in \mathbb{N}$ with $n, m \geq 1$ and a differentiable function $T: \mathbb{R}^n \rightarrow \mathbb{R}^m$ be given and a differentiable curve $r: \mathbb{R} \rightarrow \mathbb{R}^n$ be given. One defines a function $\tau: \mathbb{R} \rightarrow \mathbb{R}^m$ by $\tau(t) := T(r(t))$. For the derivative $\frac{d\tau}{dt} = \frac{d}{dt}T(r(t))$ applies

$$\frac{d\tau}{dt} = T' \frac{dr}{dt}. \quad (\text{B.4})$$

This corresponds again to the saying *external derivative times internal derivative*. If you take e.g. For example, assuming that $T = T(x, y, z, t)$ is the temperature field and $\mathbf{r}(t) = (x(t), y(t), z(t), t)^T$ is a 4-particle trajectory, then $T(t) = T(\mathbf{r}(t)) = T(x(t), y(t), z(t), t)$ is the temperature at the location of the particle at time t . With the multidimensional chain rule applies

$$\frac{dT}{dt} = \frac{\partial T}{\partial t} + \frac{dx}{dt} \frac{\partial T}{\partial x} + \frac{dy}{dt} \frac{\partial T}{\partial y} + \frac{dz}{dt} \frac{\partial T}{\partial z}. \quad (\text{B.5})$$

This is called the *material derivative* or *total derivative*, because the property of a solid particle is considered here. One defines a differential operator

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \quad (\text{B.6})$$

with the components (u, v, w) of the wind field. If you have been given three generalized coordinates x_1, x_2, x_3 (for example spherical coordinates or pressure coordinates), this can be written as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \sum_{i=1}^3 u_i \frac{\partial}{\partial x_i} \quad (\text{B.7})$$

with the generalized velocities u_i . The *divergence* div of a vector field $\mathbf{w} = (w_1, w_2, w_3)^T$ is defined by

$$\text{div}(\mathbf{w}) := \nabla \cdot \mathbf{w} = \sum_{i=1}^3 \frac{\partial w_i}{\partial x_i}. \quad (\text{B.8})$$

The *Laplace operator* Δ of a scalar field ψ is the divergence of the gradient, i.e

$$\Delta \psi := \operatorname{div} (\operatorname{grad} (\psi)) = \nabla^2 \psi = \sum_{i=1}^3 \frac{\partial^2 \psi}{\partial x_i^2}. \quad (\text{B.9})$$

The Laplace operator applied to a vector field is defined by

$$\Delta \mathbf{w} := \sum_{i=1}^3 \mathbf{e}_i \Delta w_i. \quad (\text{B.10})$$

The rotation rot of a vector field is given by

$$\operatorname{rot} (\mathbf{w}) := \nabla \times \mathbf{w} = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \mathbf{e}_k \frac{\partial}{\partial x_i} w_j \quad (\text{B.11})$$

defined. One further defines the operator of the horizontal material derivative by

$$\frac{D_h}{Dt} := \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} = \frac{\partial}{\partial t} + \mathbf{v}_h \cdot \nabla \quad (\text{B.12})$$

Analogously, one defines the *horizontal* ∇ -operator by

$$\nabla_h := \nabla - \mathbf{k} \cdot \nabla. \quad (\text{B.13})$$

The horizontal Laplace operator Δ_h is defined by

$$\Delta_h := \frac{\mathbf{I}}{r^2} \Delta_{\theta, \varphi} = (\nabla_h)^2 \quad (\text{B.14})$$

with the angle component of the Laplace operator, see Eq. (B.96), and r as the sphere radius. Since the $\mathbf{i}$ component of the rotation is the rotation of the vector field under consideration in the x_j, k plane, one can

$$\mathbf{k} \cdot \mathbf{w} \quad (\text{B.15})$$

as the horizontal component of the rotation of the vector field $\mathbf{w}$. The operator

$$-\mathbf{v} \cdot \nabla \quad (\text{B.16})$$

is the *advection operator*, which is applicable to scalar and vector fields. The horizontal portion of this is

$$-\mathbf{v}_h \cdot \nabla. \quad (\text{B.17})$$

You have a differential balance equation of the size in the form

$$\frac{D\psi}{Dt} = \sum_i F_i \quad (\text{B.18})$$

given with physical forcings F_i , the equation follows for the local time change of ψ

$$\frac{\partial \psi}{\partial t} = -\mathbf{v} \cdot \nabla T + \sum_i F_i = -\mathbf{v}_h \cdot \nabla - w \frac{\partial L}{\partial z} + \sum_i F_i, \quad (\text{B.19})$$

The *Advection* is the proportion of the local temporal change that is caused by transport.

B.1.1 Radius of curvature

Imagine a trajectory

$$\mathbf{r} : I \subseteq \mathbb{R} \rightarrow \mathbb{R}^2; a \mapsto (x, y)^T \quad (\text{B.20})$$

before, where I is an interval. We are only looking at a small section here

$$\mathbf{r} : I' \subseteq I \rightarrow \mathbb{R}^2; \tau \mapsto (x, y)^T, \quad (\text{B.21})$$

I' sei ebenfalls ein Intervall, und definiere

$$\tau_1 := \sup(I'), \quad (\text{B.22})$$

$$\tau_2 := \sup(I'), \quad (\text{B.23})$$

$$\mathbf{r}_1 = (x_1, y_1)^T := f(\tau_1), \quad (\text{B.24})$$

$$\mathbf{r}_2 = (x_2, y_2)^T := f(\tau_2). \quad (\text{B.25})$$

$$(\text{B.26})$$

O.B.d. A. one can place the origin of the KS in $\mathbf{r}_1$. Now you look for a point $\mathbf{r}_o := (x_o, y_o)^T$, which is required to have the same distance $|r|$ from $\mathbf{r}_1$ and $\mathbf{r}_2$, i.e

$$\sqrt{(\mathbf{r}_1 - \mathbf{r}_o)^2} \stackrel{!}{=} \sqrt{(\mathbf{r}_2 - \mathbf{r}_o)^2}, \quad (\text{B.27})$$

$$\Rightarrow r_1^2 + r_o^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_o = r_2^2 + r_o^2 - 2\mathbf{r}_2 \cdot \mathbf{r}_o, \quad (\text{B.28})$$

$$\Rightarrow 0 = r_2^2 - 2\mathbf{r}_2 \cdot \mathbf{r}_o. \quad (\text{B.29})$$

Now one expands $\mathbf{r}_2$ to the second order,

$$\mathbf{r}_2 = \mathbf{r}_1 + \frac{d\mathbf{r}}{d\tau}\Delta\tau + \frac{1}{2}\frac{d^2\mathbf{r}}{d\tau^2}\Delta\tau^2 + \mathcal{O}(\Delta\tau^3) \quad (\text{B.30})$$

with

$$\Delta\tau := \tau_2 - \tau_1, \quad (\text{B.31})$$

where the higher order terms are no longer noted:

$$x_2 = x'\Delta\tau + \frac{1}{2}x''\Delta\tau^2 \quad y_2 = y'\Delta\tau + \frac{1}{2}y''\Delta\tau^2 \quad (\text{B.32})$$

The derivatives are to be calculated at the point $\tau = \tau_1$. The second order must be taken into account here, since curvature is about changing the derivative of a trajectory. Putting this into Eq. (B.29), follows

$$\begin{aligned} 0 &= x'^2\Delta\tau^2 + \frac{1}{4}x''^2\Delta\tau^4 + x'x''\Delta\tau^3 + y'^2\Delta\tau^2 + \frac{1}{4}y''^2\Delta\tau^4 + y'y''\Delta\tau^3 \\ &\quad - 2x'\Delta\tau x_o - x''\Delta\tau^2 x_o - 2y'\Delta\tau y_o - y''\Delta\tau^2 y_o. \end{aligned} \quad (\text{B.33})$$

The first order of $\Delta\tau$ implies:

$$2x'x_o + 2y'y_o = 0 \quad (\text{B.34})$$

The second order of $\Delta\tau$ implies:

$$x''x_o + y''y_o = x'^2 + y'^2 \quad (\text{B.35})$$

From Eq. (B.34) follows

$$x_o = -\frac{y'y_o}{x'}. \quad (\text{B.36})$$

In Eq. Inserting (B.35) results in this

$$-x''y' \frac{y_0}{x'} + y''y_0 = x'^2 + y'^2 \Rightarrow y_0 = \frac{x'^2 + y'^2}{y'' - x'' \frac{y'}{x'}}. \quad (\text{B.37})$$

With Eq. (B.36) follows

$$x_0 = -\frac{y'}{x'} \frac{x'^2 + y'^2}{y'' - x'' \frac{y'}{x'}}. \quad (\text{B.38})$$

This follows for the amount of the radius of curvature

$$|r| = \sqrt{\mathbf{1} + \frac{y'^2}{x'^2}} \frac{x'^2 + y'^2}{\left|y'' - x'' \frac{y'}{x'}\right|}. \quad (\text{B.39})$$

O.B.d. A. you can set $\tau = x$, it follows from this

$$x' = \mathbf{1}, \quad x'' = \mathbf{0}. \quad (\text{B.40})$$

Therefore applies

$$|r| = \sqrt{\mathbf{1} + y'^2} \frac{\mathbf{1} + y'^2}{|y''|} \Rightarrow |r| = \frac{(\mathbf{1} + y'^2)^{3/2}}{|y''|}. \quad (\text{B.41})$$

Regarding the sign of r , you specify that it should be positive if the trajectory curves to the left, i.e

$$r = \frac{(\mathbf{1} + y'^2)^{3/2}}{y''}. \quad (\text{B.42})$$

If you need a linear expression for $\mathbf{1}/r$, you usually use

$$\frac{\mathbf{1}}{r} \approx y''. \quad (\text{B.43})$$

B.1.2 Calculation rules for differential operators

Let $\mathbf{u}, \mathbf{v}, \mathbf{w} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ with $\mathbf{u} = (u_1, u_2, u_3)^T$, $\mathbf{v} = (v_1, v_2, v_3)^T$ and $\mathbf{w} = (w_1, w_2, w_3)^T$ three vector fields, $\psi, \chi : \mathbb{R}^3 \rightarrow \mathbb{R}$ two scalar fields and $\lambda \in \mathbb{C}$ one scalar. It is defined

$$\Delta \mathbf{v} := \sum_{i=1}^3 \Delta v_i \mathbf{e}_i. \quad (\text{B.44})$$

They apply

$$\nabla (\psi + \chi) = \nabla \psi + \nabla \chi, \quad \nabla \times (\mathbf{v} + \mathbf{w}) = \nabla \times \mathbf{v} + \nabla \times \mathbf{w}, \quad (\text{B.45})$$

$$\nabla (\lambda \psi) = \lambda \nabla \psi, \quad \nabla \times (\lambda \mathbf{v}) = \lambda \nabla \times \mathbf{v} \quad (\text{B.46})$$

according to the findings in section A.8. Still apply

$$\nabla \times \nabla \psi = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} \frac{\partial \psi}{\partial x_j} \mathbf{e}_k = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial^2 \psi}{\partial x_i \partial x_j} \mathbf{e}_k = \mathbf{0}, \quad (\text{B.47})$$

$$\nabla \cdot \nabla \times \mathbf{v} = \left(\sum_{l=1}^3 \mathbf{e}_l \frac{\partial}{\partial x_l} \right) \cdot \left(\sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} v_j \mathbf{e}_k \right) = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial^2 v_j}{\partial x_k \partial x_i} = \mathbf{0}, \quad (\text{B.48})$$

$$\nabla \cdot (\psi \mathbf{v}) = \sum_{i=1}^3 \frac{\partial}{\partial x_i} (\psi v_i) = \sum_{i=1}^3 v_i \frac{\partial \psi}{\partial x_i} + \psi \frac{\partial v_i}{\partial x_i} = \mathbf{v} \cdot \nabla \psi + \psi \nabla \cdot \mathbf{v}, \quad (\text{B.49})$$

$$\frac{\partial}{\partial x_i} \nabla \times \mathbf{v} = \frac{\partial}{\partial x_i} \sum_{j,k,l=1}^3 \varepsilon_{j,k,l} \frac{\partial}{\partial x_j} v_k \mathbf{e}_l = \sum_{j,k,l=1}^3 \varepsilon_{j,k,l} \frac{\partial}{\partial x_j} \frac{\partial v_k}{\partial x_i} \mathbf{e}_l = \nabla \times \frac{\partial}{\partial x_i} \mathbf{v}, \quad (\text{B.50})$$

$$\begin{aligned} \nabla \times \psi \mathbf{v} &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} (\psi v_j) \mathbf{e}_k = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \left(v_j \frac{\partial \psi}{\partial x_i} + \psi \frac{\partial v_j}{\partial x_i} \right) \mathbf{e}_k \\ &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial \psi}{\partial x_i} v_j \mathbf{e}_k + \sum_{i,j,k=1}^3 \psi \frac{\partial}{\partial x_i} v_j \mathbf{e}_k = (\nabla \psi) \times \mathbf{v} + \psi \nabla \times \mathbf{v} \\ &= -\mathbf{v} \times \nabla \psi + \psi \nabla \times \mathbf{v}, \end{aligned} \quad (\text{B.51})$$

$$\begin{aligned} \nabla (\mathbf{v} \cdot \mathbf{w}) &= \nabla \sum_{i=1}^3 v_i w_i = \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\sum_{j=1}^3 v_j w_j \right) \mathbf{e}_i = \sum_{i=1}^3 \sum_{j=1}^3 \left(\frac{\partial v_j}{\partial x_i} w_j + v_j \frac{\partial w_j}{\partial x_i} \right) \mathbf{e}_i \\ &= \sum_{i=1}^3 \sum_{j=1}^3 \left(\frac{\partial v_j}{\partial x_i} w_j + w_j \frac{\partial v_i}{\partial x_j} - w_j \frac{\partial v_i}{\partial x_j} + v_j \frac{\partial w_j}{\partial x_i} + v_j \frac{\partial w_i}{\partial x_j} - v_j \frac{\partial w_i}{\partial x_j} \right) \mathbf{e}_i \\ &= \sum_{i=1}^3 \sum_{j=1}^3 \left(w_j \left(\frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j} \right) + v_j \left(\frac{\partial w_j}{\partial x_i} - \frac{\partial w_i}{\partial x_j} \right) + w_j \frac{\partial v_i}{\partial x_j} + v_j \frac{\partial w_i}{\partial x_j} \right) \mathbf{e}_i \\ &= \sum_{i,j=1}^3 w_j \frac{\partial v_i}{\partial x_j} \mathbf{e}_i + \sum_{i,j=1}^3 v_j \frac{\partial w_i}{\partial x_j} \mathbf{e}_i + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k}^2 \left(w_j \left(\frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j} \right) + v_j \left(\frac{\partial w_j}{\partial x_i} - \frac{\partial w_i}{\partial x_j} \right) \right) \mathbf{e}_i \\ &= \sum_{j=1}^3 w_j \frac{\partial}{\partial x_j} \sum_{i=1}^3 v_i \mathbf{e}_i + \sum_{j=1}^3 v_j \frac{\partial}{\partial x_j} \sum_{i=1}^3 w_i \mathbf{e}_i + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k}^2 \left(w_j \left(\frac{\partial v_j}{\partial x_k} - \frac{\partial v_k}{\partial x_j} \right) + v_j \left(\frac{\partial w_j}{\partial x_k} - \frac{\partial w_k}{\partial x_j} \right) \right) \mathbf{e}_k \\ &= (\mathbf{w} \cdot \nabla) \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{w} + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k}^2 v_j \left(\frac{\partial w_j}{\partial x_k} - \frac{\partial w_k}{\partial x_j} \right) \mathbf{e}_k + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k}^2 w_j \left(\frac{\partial v_j}{\partial x_k} - \frac{\partial v_k}{\partial x_j} \right) \mathbf{e}_k \\ &= (\mathbf{v} \cdot \nabla) \mathbf{w} + (\mathbf{w} \cdot \nabla) \mathbf{v} + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} v_j \varepsilon_{i,j,k} \left(\frac{\partial w_j}{\partial x_k} - \frac{\partial w_k}{\partial x_j} \right) \mathbf{e}_k + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} w_j \varepsilon_{i,j,k} \left(\frac{\partial v_j}{\partial x_k} - \frac{\partial v_k}{\partial x_j} \right) \mathbf{e}_k \\ &= (\mathbf{v} \cdot \nabla) \mathbf{w} + (\mathbf{w} \cdot \nabla) \mathbf{v} + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} v_i \varepsilon_{i,j,k} \left(\frac{\partial w_i}{\partial x_k} - \frac{\partial w_k}{\partial x_i} \right) \mathbf{e}_k + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} w_i \varepsilon_{i,j,k} \left(\frac{\partial v_i}{\partial x_k} - \frac{\partial v_k}{\partial x_i} \right) \mathbf{e}_k \\ &= (\mathbf{v} \cdot \nabla) \mathbf{w} + (\mathbf{w} \cdot \nabla) \mathbf{v} + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} v_i (\nabla \times \mathbf{w})_j \mathbf{e}_k + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} w_i (\nabla \times \mathbf{v})_j \mathbf{e}_k \\ &= (\mathbf{v} \cdot \nabla) \mathbf{w} + (\mathbf{w} \cdot \nabla) \mathbf{v} + \mathbf{v} \times (\nabla \times \mathbf{w}) + \mathbf{w} \times (\nabla \times \mathbf{v}), \end{aligned} \quad (\text{B.52})$$

$$\begin{aligned}
\nabla \times (\mathbf{v} \times \mathbf{w}) &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} (\mathbf{v} \times \mathbf{w})_j \mathbf{e}_k = \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} (\varepsilon_{ikj} v_i w_k + \varepsilon_{kij} v_k w_i) \mathbf{e}_k \\
&= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k}^2 \frac{\partial}{\partial x_i} (v_k w_i - v_i w_k) \mathbf{e}_k = \sum_{i,k=1}^3 \frac{\partial}{\partial x_i} (v_k w_i - v_i w_k) \mathbf{e}_k \\
&= \sum_{i,k=1}^3 \left(\frac{\partial v_k}{\partial x_i} w_i + v_k \frac{\partial w_i}{\partial x_i} - v_i \frac{\partial w_k}{\partial x_i} - w_k \frac{\partial v_i}{\partial x_i} \right) \mathbf{e}_k = \sum_{i=1}^3 w_i \frac{\partial}{\partial x_i} \sum_{k=1}^3 v_k \mathbf{e}_k - \sum_{i=1}^3 v_i \frac{\partial}{\partial x_i} \sum_{k=1}^3 w_k \mathbf{e}_k \\
&+ \sum_{i=1}^3 \frac{\partial w_i}{\partial x_i} \sum_{k=1}^3 v_k \mathbf{e}_k - \sum_{i=1}^3 \frac{\partial v_i}{\partial x_i} \sum_{k=1}^3 w_k \mathbf{e}_k \\
&= (\mathbf{w} \cdot \nabla) \mathbf{v} - \mathbf{w} (\nabla \cdot \mathbf{v}) + \mathbf{v} (\nabla \cdot \mathbf{w}) - (\mathbf{v} \cdot \nabla) \mathbf{w},
\end{aligned} \tag{B.53}$$

$$\begin{aligned}
\nabla (\nabla \cdot \mathbf{v}) &= \nabla \sum_{i=1}^3 \frac{\partial v_i}{\partial x_i} = \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial^2 v_j}{\partial x_i \partial x_j} \mathbf{e}_i = \sum_{i=1}^3 \left(\sum_{j=1}^3 \left(\frac{\partial^2 v_j}{\partial x_i \partial x_j} \right) + \Delta v_i - \Delta v_i \right) \mathbf{e}_i \\
&= \Delta \mathbf{v} + \sum_{i=1}^3 \sum_{j=1}^3 \left(\frac{\partial^2 v_j}{\partial x_i \partial x_j} - \frac{\partial^2 v_i}{\partial x_j^2} \right) \mathbf{e}_i = \Delta \mathbf{v} + \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left(\frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j} \right) \mathbf{e}_i \\
&= \Delta \mathbf{v} + \sum_{i=1}^3 \sum_{\substack{j=1, \\ j \neq i}}^3 \frac{\partial}{\partial x_j} \left(\frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j} \right) \mathbf{e}_i = \Delta \mathbf{v} + \sum_{i=1}^3 \sum_{\substack{j=1, \\ j \neq i}}^3 \frac{\partial}{\partial x_j} \left[\sum_{k=1}^3 \varepsilon_{i,j,k}^2 \left(\frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j} \right) \right] \mathbf{e}_i \\
&= \Delta \mathbf{v} + \sum_{i=1}^3 \sum_{\substack{j=1, \\ j \neq i}}^3 \frac{\partial}{\partial x_j} \left[\sum_{k=1}^3 \varepsilon_{i,j,k} (\nabla \times \mathbf{v})_k \right] \mathbf{e}_i = \Delta \mathbf{v} + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_j} (\nabla \times \mathbf{v})_k \mathbf{e}_i \\
&= \Delta \mathbf{v} + \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} (\nabla \times \mathbf{v})_j \mathbf{e}_k \\
&= \Delta \mathbf{v} + \sum_{i,j,k=1}^3 \left(\nabla \times \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} \mathbf{v} \right)_j \mathbf{e}_k = \Delta \mathbf{v} + \nabla \times \left(\sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} \mathbf{v} \right) \mathbf{e}_k \\
&= \Delta \mathbf{v} + \nabla \times \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial}{\partial x_i} v_j \mathbf{e}_k = \Delta \mathbf{v} + \nabla \times (\nabla \times \mathbf{v}),
\end{aligned} \tag{B.54}$$

$$\begin{aligned}
\nabla \cdot (\mathbf{v} \times \mathbf{w}) &= \sum_{i=1}^3 \frac{\partial}{\partial x_i} (\mathbf{v} \times \mathbf{w})_i = \sum_{i=1}^3 \frac{\partial}{\partial x_i} (\varepsilon_{k,j,i} v_k w_j + \varepsilon_{j,k,i} v_j w_k) \\
&= \sum_{i=1}^3 \left(\varepsilon_{k,j,i} \frac{\partial v_k}{\partial x_i} w_j + \varepsilon_{k,j,i} v_k \frac{\partial w_j}{\partial x_i} + \varepsilon_{j,k,i} \frac{\partial v_j}{\partial x_i} w_k + \varepsilon_{j,k,i} v_j \frac{\partial w_k}{\partial x_i} \right) \\
&= \sum_{i=1}^3 w_i \left(\varepsilon_{k,j,i} \frac{\partial v_j}{\partial x_k} + \varepsilon_{j,k,i} \frac{\partial v_k}{\partial x_j} \right) - v_i \left(\varepsilon_{k,j,i} \frac{\partial w_j}{\partial x_k} + \varepsilon_{j,k,i} \frac{\partial w_k}{\partial x_j} \right) \\
&= \sum_{i=1}^3 w_i (\nabla \times \mathbf{v})_i - v_i (\nabla \times \mathbf{w})_i = \mathbf{w} \cdot (\nabla \times \mathbf{v}) - \mathbf{v} \cdot (\nabla \times \mathbf{w}),
\end{aligned} \tag{B.55}$$

$$\begin{aligned}
\mathbf{u} \cdot [(\mathbf{v} \cdot \nabla) \nabla \psi] &= \sum_{i=1}^3 u_i [(\mathbf{v} \cdot \nabla) \nabla \psi]_i = \sum_{i=1}^3 u_i \left[(\mathbf{v} \cdot \nabla) \frac{\partial \psi}{\partial x_i} \right] = \sum_{i=1}^3 u_i \sum_{j=1}^3 v_j \frac{\partial^2 \psi}{\partial x_j \partial x_i} \\
&= \sum_{i,j=1}^3 u_i v_j \frac{\partial^2 \psi}{\partial x_j \partial x_i} = \sum_{i,j=1}^3 v_i u_j \frac{\partial^2 \psi}{\partial x_j \partial x_i} = \sum_{i=1}^3 v_i \sum_{j=1}^3 u_j \frac{\partial}{\partial x_j} (\nabla \psi)_i \\
&= \sum_{i=1}^3 v_i [(\mathbf{u} \cdot \nabla) \nabla \psi]_i = \mathbf{v} \cdot [(\mathbf{u} \cdot \nabla) \nabla \psi].
\end{aligned} \tag{B.56}$$

Also applies

$$(\mathbf{v} \cdot \nabla) \mathbf{v} \stackrel{\text{Glg. (B.52)}}{=} \frac{1}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times (\nabla \times \mathbf{v}). \quad (\text{B.57})$$

This is called *Lamb transformation*. This also applies to the advection of a scalar product

$$\begin{aligned} (\mathbf{u} \cdot \nabla) (\mathbf{v} \cdot \mathbf{w}) &= \left(\sum_{i=1}^3 u_i \frac{\partial}{\partial x_i} \right) \left(\sum_{j=1}^3 v_j w_j \right) = \sum_{i,j=1}^3 u_i \left[\frac{\partial v_j}{\partial x_i} w_j + \frac{\partial w_j}{\partial x_i} v_j \right] \\ &= \sum_{j=1}^3 w_j \sum_{i=1}^3 u_i \frac{\partial v_j}{\partial x_i} + \sum_{j=1}^3 v_j \sum_{i=1}^3 u_i \frac{\partial w_j}{\partial x_i} = \mathbf{w} \cdot [(\mathbf{u} \cdot \nabla) \mathbf{v}] + \mathbf{v} \cdot [(\mathbf{u} \cdot \nabla) \mathbf{w}]. \end{aligned} \quad (\text{B.58})$$

Let $\mathbf{k} = (k_1, k_2, k_3)^T \in \mathbb{C}^3$, $\varphi : \mathbb{R}^3 \rightarrow \mathbb{C}$; $\varphi(\mathbf{r}) = \exp(\mathbf{k} \cdot \mathbf{r})$ and $\mathbf{A} \in \mathbb{R}^3$. Then apply

$$\begin{aligned} \nabla \varphi(\mathbf{r}) &= \sum_{i=1}^3 \frac{\partial}{\partial x_i} \varphi(\mathbf{r}) \mathbf{e}_i = \sum_{i=1}^3 \frac{\partial}{\partial x_i} \exp(\mathbf{k} \cdot \mathbf{r}) \mathbf{e}_i = \sum_{i=1}^3 \frac{\partial}{\partial x_i} \exp \left(\sum_{j=1}^3 k_j x_j \right) \mathbf{e}_i \\ &= \sum_{i=1}^3 k_i \exp(\mathbf{k} \cdot \mathbf{r}) \mathbf{e}_i = \varphi(\mathbf{r}) \mathbf{k}, \end{aligned} \quad (\text{B.59})$$

$$\begin{aligned} \nabla \times [\mathbf{A} \varphi(\mathbf{r})] &= \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} \frac{\partial [A_j \exp(i\mathbf{k} \cdot \mathbf{r})]}{\partial x_i} \mathbf{e}_k = i \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_j k_i \exp(i\mathbf{k} \cdot \mathbf{r}) \mathbf{e}_k \\ &= i \exp(i\mathbf{k} \cdot \mathbf{r}) \sum_{i,j,k=1}^3 \varepsilon_{i,j,k} A_j k_i \mathbf{e}_k = i \exp(i\mathbf{k} \cdot \mathbf{r}) \mathbf{A} \times \mathbf{k} = i [\mathbf{A} \varphi(\mathbf{r})] \times \mathbf{k}, \end{aligned} \quad (\text{B.60})$$

$$\Delta \varphi(\mathbf{r}) = \nabla \cdot \nabla \varphi(\mathbf{r}) = \nabla \cdot (\varphi(\mathbf{r}) \mathbf{k}) = \mathbf{k} \cdot \nabla \varphi = \mathbf{k}^2 \varphi(\mathbf{r}). \quad (\text{B.61})$$

B.2 Differential operators under coordinate transformations

In general, points in $\mathbb{R}^3$ are denoted by three real numbers $x = (x_1, x_2, x_3)$, which in linear combination with the standard base $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ produce a vector $\mathbf{r}$:

$$\mathbf{r} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3 \quad (\text{B.62})$$

In this context, you can imagine a vector as an arrow. In order to be able to solve things with a certain geometry more elegantly, generalized coordinates q_i are introduced (see also section 2.2). Scalar fields f can then be written as $f = f(q)$. Here q stands for the tuple $q = (q_1, q_2, q_3)$. As a note, the functions $f = f(x)$ and $f = f(q)$ are not the same, if you use the same arguments you generally get different values. Most of the time, however, there is no distinction between this in the notation because both functions express the same thing.

If you want to write down a vector field $\mathbf{v}$ in generalized coordinates, the simplest idea would be to also write down the values of $\mathbf{v}$ in generalized coordinates. If $\mathbf{v}$ is a velocity field, one could write down the values of $\mathbf{v}$ in the forms $\dot{q}$ or $\mathbf{v} \equiv \mathbf{r}(q)$. Since this is often unclear, in general coordinate systems (also called *curvilinear coordinates*) a location-dependent basis is introduced, the elements of which are defined by

$$\mathbf{e}_i := \frac{1}{|\frac{\partial \mathbf{r}}{\partial q_i}|} \frac{\partial \mathbf{r}}{\partial q_i}. \quad (\text{B.63})$$

These elements are standardized. Can

$$\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3 \quad (\text{B.64})$$

achieved by swapping the $\mathbf{e}_i$, the q is called *orthogonal*; Coordinates that violate this are not discussed in this book. One then writes for vector fields

$$\mathbf{v} = \sum_{i=1}^3 v_i \mathbf{e}_i, \quad (\text{B.65})$$

where both the v_i and the $\mathbf{e}_i$ depend on the location. Partial derivatives with respect to the local basis are defined by directional derivatives along the local coordinate axes:

$$\frac{\partial}{\partial x_i} := \mathbf{e}_i \cdot \nabla = \frac{\mathbf{1}}{|\frac{\partial \mathbf{r}}{\partial q_i}|} \left(\frac{\partial x}{\partial q_i} \frac{\partial}{\partial x} + \frac{\partial y}{\partial q_i} \frac{\partial}{\partial y} + \frac{\partial z}{\partial q_i} \frac{\partial}{\partial z} \right) = \frac{\mathbf{1}}{|\frac{\partial \mathbf{r}}{\partial q_i}|} \frac{\partial}{\partial q_i}. \quad (\text{B.66})$$

Let $\mathbf{v}, \mathbf{w}$ be two vector fields, then the dot product is

$$\mathbf{v} \cdot \mathbf{w} = v^{(m)} w^{(n)} g_{m,n}. \quad (\text{B.67})$$

For the vector product applies

$$\mathbf{v} \times \mathbf{w} = \begin{vmatrix} \mathbf{q}_2 \times \mathbf{q}_3 & \mathbf{q}_3 \times \mathbf{q}_1 & \mathbf{q}_1 \times \mathbf{q}_2 \\ v^{(1)} & v^{(2)} & v^{(3)} \\ w^{(1)} & w^{(2)} & w^{(3)} \end{vmatrix} \quad (\text{B.68})$$

Let f be a scalar field, then the gradient of f in generalized coordinates holds

$$\nabla f = \mathbf{q}^{(n)} \frac{\partial}{\partial q^{(n)}} = \mathbf{q}^{(n)} \nabla_n f. \quad (\text{B.69})$$

This therefore applies in generalized coordinates

$$\nabla \cdot \mathbf{v} = \frac{\mathbf{1}}{\sqrt{g}} \frac{\partial}{\partial q^{(n)}} \left(\mathbf{q}^{(n)} \cdot \mathbf{v} \sqrt{g} \right). \quad (\text{B.70})$$

So it applies

$$\nabla \times \mathbf{v} = \frac{\mathbf{1}}{\sqrt{g}} \begin{vmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 \\ \frac{\partial}{\partial q^{(1)}} & \frac{\partial}{\partial q^{(2)}} & \frac{\partial}{\partial q^{(3)}} \\ v_1 & v_2 & v_3 \end{vmatrix} \quad (\text{B.71})$$

B.2.1 Spherical coordinates

In this section $\mathbf{v}$ is a vector field and f is a scalar field, both are said to have all the necessary properties. In spherical coordinates applies

$$\mathbf{r} = r \begin{pmatrix} \sin(\theta) \cos(\varphi) \\ \sin(\theta) \sin(\varphi) \\ \cos(\theta) \end{pmatrix}. \quad (\text{B.72})$$

Let $\mathbf{r} = \mathbf{r}(r, \theta, \varphi)$ be the transformation from spherical to Cartesian coordinates, then the equation J applies to their derivation

$$J = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \varphi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \varphi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \varphi} \end{pmatrix} = \begin{pmatrix} \sin(\theta) \cos(\varphi) & r \cos(\theta) \cos(\varphi) & -r \sin(\theta) \sin(\varphi) \\ \sin(\theta) \sin(\varphi) & r \cos(\theta) \sin(\varphi) & r \sin(\theta) \cos(\varphi) \\ \cos(\theta) & -r \sin(\theta) & 0 \end{pmatrix}. \quad (\text{B.73})$$

The normalized columns of this are

$$\mathbf{e}_r = \mathbf{e}^{(r)} = \begin{pmatrix} \sin(\theta) \cos(\varphi) \\ \sin(\theta) \sin(\varphi) \\ \cos(\theta) \end{pmatrix}, \quad (\text{B.74})$$

$$\mathbf{e}_\theta = \mathbf{e}^{(\theta)} = \begin{pmatrix} \cos(\theta) \cos(\varphi) \\ \cos(\theta) \sin(\varphi) \\ -\sin(\theta) \end{pmatrix}, \quad (\text{B.75})$$

$$\mathbf{e}_\varphi = \mathbf{e}^{(\varphi)} = \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \\ 0 \end{pmatrix}. \quad (\text{B.76})$$

The columns of J are the covariant basis vectors

$$\mathbf{q}_r = \begin{pmatrix} \sin(\theta) \cos(\varphi) \\ \sin(\theta) \sin(\varphi) \\ \cos(\theta) \end{pmatrix}, \quad (\text{B.77})$$

$$\mathbf{q}_\theta = r \begin{pmatrix} \cos(\theta) \cos(\varphi) \\ \cos(\theta) \sin(\varphi) \\ -\sin(\theta) \end{pmatrix}, \quad (\text{B.78})$$

$$\mathbf{q}_\varphi = r \sin(\theta) \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \\ 0 \end{pmatrix}. \quad (\text{B.79})$$

This results in the determinant g of the metric tensor

$$g = \begin{vmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & r^2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & r^2 \sin^2(\theta) \end{vmatrix} = r^4 \sin^2(\theta). \quad (\text{B.80})$$

Since this matrix is diagonal, spherical coordinates are orthogonal. This therefore applies to the contravariant basis vectors

$$\mathbf{q}^{(r)} = \begin{pmatrix} \sin(\theta) \cos(\varphi) \\ \sin(\theta) \sin(\varphi) \\ \cos(\theta) \end{pmatrix}, \quad (\text{B.81})$$

$$\mathbf{q}^{(\theta)} = \frac{\mathbf{I}}{r} \begin{pmatrix} \cos(\theta) \cos(\varphi) \\ \cos(\theta) \sin(\varphi) \\ -\sin(\theta) \end{pmatrix}, \quad (\text{B.82})$$

$$\mathbf{q}^{(\varphi)} = \frac{\mathbf{I}}{r \sin(\theta)} \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \\ 0 \end{pmatrix}. \quad (\text{B.83})$$

Now you write for a vector field

$$\begin{aligned} \mathbf{v} &= v^{(r)} \mathbf{q}_r + v^{(\theta)} \mathbf{q}_\theta + v^{(\varphi)} \mathbf{q}_\varphi = v_r \mathbf{q}^{(r)} + v_\theta \mathbf{q}^{(\theta)} + v_\varphi \mathbf{q}^{(\varphi)} \\ &= \tilde{v}^{(r)} \mathbf{e}_r + \tilde{v}^{(\theta)} \mathbf{e}_\theta + \tilde{v}^{(\varphi)} \mathbf{e}_\varphi = \tilde{v}_r \mathbf{e}^{(r)} + \tilde{v}_\theta \mathbf{e}^{(\theta)} + \tilde{v}_\varphi \mathbf{e}^{(\varphi)}. \end{aligned} \quad (\text{B.84})$$

It should be clear at this point that the dimensions of the components of $\mathbf{v}$ appearing here in the first line are not uniform, since the same is true for the basis elements. Due to the orthogonality of the spherical coordinates,

$$\tilde{v}^{(r)} = \tilde{v}_r, \quad \tilde{v}^{(\theta)} = \tilde{v}_\theta, \quad \tilde{v}^{(\varphi)} = \tilde{v}_\varphi. \quad (\text{B.85})$$

The conversion of the components is:

$$v_r = \tilde{v}_r, \quad v_\theta = r \tilde{v}_\theta, \quad v_\varphi = r \sin(\theta) \tilde{v}_\varphi, \quad (\text{B.86})$$

$$v^{(r)} = \tilde{v}_r, \quad v^{(\theta)} = \frac{\mathbf{I}}{r} \tilde{v}_\theta, \quad v^{(\varphi)} = \frac{\mathbf{I}}{r \sin(\theta)} \tilde{v}_\varphi. \quad (\text{B.87})$$

First, the gradient is considered, with Eq. (B.69) is obtained

$$\nabla f = \mathbf{q}^{(r)} \frac{\partial f}{\partial r} + \mathbf{q}^{(\theta)} \frac{\partial f}{\partial \theta} + \mathbf{q}^{(\varphi)} \frac{\partial f}{\partial \varphi} = \mathbf{e}^{(r)} \frac{\partial f}{\partial r} + \frac{1}{r} \mathbf{e}^{(\theta)} \frac{\partial f}{\partial \theta} + \frac{1}{r \sin(\theta)} \mathbf{e}^{(\varphi)} \frac{\partial f}{\partial \varphi}. \quad (\text{B.88})$$

Now the divergence is considered. Vm Eq. To be able to use (B.70), you first calculate

$$\mathbf{q}^{(r)} \cdot \mathbf{v} = v^{(r)}, \quad \mathbf{q}^{(\theta)} \cdot \mathbf{v} = v^{(\theta)}, \quad \mathbf{q}^{(\varphi)} \cdot \mathbf{v} = v^{(\varphi)}. \quad (\text{B.89})$$

Therefore applies

$$\begin{aligned} \nabla \cdot \mathbf{v} &= \frac{1}{r^2 \sin(\theta)} \left(\frac{\partial (v^{(r)} r^2 \sin(\theta))}{\partial r} + \frac{\partial (v^{(\theta)} r^2 \sin(\theta))}{\partial \theta} + \frac{\partial (v^{(\varphi)} r^2 \sin(\theta))}{\partial \varphi} \right) \\ &= \frac{\partial v^{(r)}}{\partial r} + \frac{\partial v^{(\theta)}}{\partial \theta} + \frac{\partial v^{(\varphi)}}{\partial \varphi} + \frac{2v^{(r)}}{r} + \cot(\theta) v^{(\theta)} \\ &= \frac{\partial \tilde{v}^{(r)}}{\partial r} + \frac{1}{r} \frac{\partial \tilde{v}^{(\theta)}}{\partial \theta} + \frac{1}{r \sin(\theta)} \frac{\partial \tilde{v}^{(\varphi)}}{\partial \varphi} + \frac{2\tilde{v}^{(r)}}{r} + \frac{\cot(\theta)}{r} \tilde{v}^{(\theta)}. \end{aligned} \quad (\text{B.90})$$

By combining the equations (B.88) and (B.90) we get for the Laplace operator

$$\begin{aligned} \Delta f &= \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 f}{\partial \varphi^2} + \frac{2}{r} \frac{\partial f}{\partial r} + \frac{\cot(\theta)}{r^2} \frac{\partial f}{\partial \theta} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 f}{\partial \varphi^2}. \end{aligned} \quad (\text{B.91})$$

This can be reshaped a bit. Diffeomorphism is used for this

$$\theta \leftrightarrow \mu := \cos(\theta), \quad (\text{B.92})$$

then applies

$$\frac{d}{d\theta} = \frac{d\mu}{d\theta} \frac{d}{d\mu} = -\sin(\theta) \frac{d}{d\mu}. \quad (\text{B.93})$$

This means that the Laplace operator becomes

$$\begin{aligned} \Delta &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \left(-\sin(\theta) \frac{\partial}{\partial \mu} \right) \left(\sin(\theta) \left(-\sin(\theta) \frac{d}{d\mu} \right) \right) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2}{\partial \varphi^2} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{1}{r^2 (1 - \mu^2)} \frac{\partial^2}{\partial \varphi^2} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Delta_{\mu, \varphi} \end{aligned} \quad (\text{B.94})$$

with

$$\Delta_{\mu, \varphi} = \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{1}{1 - \mu^2} \frac{\partial^2}{\partial \varphi^2} \quad (\text{B.95})$$

as the angular component of the Laplace operator. This angular component is calculated in spherical coordinates by comparing with Eq. (B.91) to

$$\Delta_{\theta, \varphi} = \frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \varphi^2}. \quad (\text{B.96})$$

Now the rotation is calculated, using Eq. (B.71)

$$\nabla \times \mathbf{v} = \frac{\mathbf{I}}{r^2 \sin(\theta)} \left[\mathbf{q}_r \left(\frac{\partial v_\varphi}{\partial \theta} - \frac{\partial v_\theta}{\partial \varphi} \right) + \mathbf{q}_\theta \left(\frac{\partial v_r}{\partial \varphi} - \frac{\partial v_\varphi}{\partial r} \right) + \mathbf{q}_\varphi \left(\frac{\partial v_\theta}{\partial r} - \frac{\partial v_r}{\partial \theta} \right) \right]. \quad (\text{B.97})$$

By rescaling to standardized basic elements you get

$$\begin{aligned} \nabla \times \mathbf{v} &= \frac{\mathbf{I}}{r^2 \sin(\theta)} \left[\mathbf{e}_r \left(\frac{\partial (r \sin(\theta) \tilde{v}_\varphi)}{\partial \theta} - \frac{\partial (r \tilde{v}_\theta)}{\partial \varphi} \right) + r \mathbf{e}_\theta \left(\frac{\partial \tilde{v}_r}{\partial \varphi} - \frac{\partial (r \sin(\theta) \tilde{v}_\varphi)}{\partial r} \right) \right. \\ &\quad \left. + r \sin(\theta) \mathbf{e}_\varphi \left(\frac{\partial (r \tilde{v}_\theta)}{\partial r} - \frac{\partial \tilde{v}_r}{\partial \theta} \right) \right] \\ &= \frac{\tilde{v}_\theta}{r} \mathbf{e}_\varphi + \frac{\tilde{v}_\varphi}{r \tan(\theta)} \mathbf{e}_r - \frac{\tilde{v}_\varphi}{r} \mathbf{e}_\theta + \mathbf{e}_r \left(\frac{\mathbf{I}}{r} \frac{\partial \tilde{v}_\varphi}{\partial \theta} - \frac{\mathbf{I}}{r \sin(\theta)} \frac{\partial \tilde{v}_\theta}{\partial \varphi} \right) \\ &\quad + \mathbf{e}_\theta \left(\frac{\mathbf{I}}{r \sin(\theta)} \frac{\partial \tilde{v}_r}{\partial \varphi} - \frac{\partial \tilde{v}_\varphi}{\partial r} \right) + \mathbf{e}_\varphi \left(\frac{\partial \tilde{v}_\theta}{\partial r} - \frac{\mathbf{I}}{r} \frac{\partial \tilde{v}_r}{\partial \theta} \right) \end{aligned} \quad (\text{B.98})$$

For the velocity advection one uses the Lamb transformation Eq. (B.57)

$$(\mathbf{v} \cdot \nabla) \mathbf{v} = \frac{\mathbf{I}}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) + (\nabla \times \mathbf{v}) \times \mathbf{v}. \quad (\text{B.99})$$

In preparation, one uses Eq. (B.67):

$$\mathbf{v}^2 = \left(v^{(r)} \right)^2 + r^2 \left(v^{(\theta)} \right)^2 + r^2 \sin^2(\theta) \left(v^{(\varphi)} \right)^2 \quad (\text{B.100})$$

From this it follows

$$\begin{aligned} \frac{\mathbf{I}}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) &= \frac{\mathbf{I}}{2} \mathbf{q}^{(r)} \frac{\partial}{\partial r} \left(\left(v^{(r)} \right)^2 + r^2 \left(v^{(\theta)} \right)^2 + r^2 \sin^2(\theta) \left(v^{(\varphi)} \right)^2 \right) \\ &\quad + \frac{\mathbf{I}}{2} \mathbf{q}^{(\theta)} \frac{\partial}{\partial \theta} \left(\left(v^{(r)} \right)^2 + r^2 \left(v^{(\theta)} \right)^2 + r^2 \sin^2(\theta) \left(v^{(\varphi)} \right)^2 \right) \\ &\quad + \frac{\mathbf{I}}{2} \mathbf{q}^{(\varphi)} \frac{\partial}{\partial \varphi} \left(\left(v^{(r)} \right)^2 + r^2 \left(v^{(\theta)} \right)^2 + r^2 \sin^2(\theta) \left(v^{(\varphi)} \right)^2 \right) \\ &= \mathbf{q}^{(r)} \left(v^{(r)} \frac{\partial v^{(r)}}{\partial r} + r^2 v^{(\theta)} \frac{\partial v^{(\theta)}}{\partial r} + r \left(v^{(\theta)} \right)^2 + r \sin^2(\theta) \left(v^{(\varphi)} \right)^2 + r^2 \sin^2(\theta) v^{(\varphi)} \frac{\partial v^{(\varphi)}}{\partial r} \right) \\ &\quad + \mathbf{q}^{(\theta)} \left(v^{(r)} \frac{\partial v^{(r)}}{\partial \theta} + r^2 v^{(\theta)} \frac{\partial v^{(\theta)}}{\partial \theta} + r^2 \sin(\theta) \cos(\theta) \left(v^{(\varphi)} \right)^2 + r^2 \sin^2(\theta) v^{(\varphi)} \frac{\partial v^{(\varphi)}}{\partial \theta} \right) \\ &\quad + \mathbf{q}^{(\varphi)} \left(v^{(r)} \frac{\partial v^{(r)}}{\partial \varphi} + r^2 v^{(\theta)} \frac{\partial v^{(\theta)}}{\partial \varphi} + r^2 \sin^2(\theta) v^{(\varphi)} \frac{\partial v^{(\varphi)}}{\partial \varphi} \right). \end{aligned} \quad (\text{B.101})$$

Vm Eq. To be able to evaluate (B.68), you first calculate it

$$\mathbf{q}_r \times \mathbf{q}_\theta = \frac{\mathbf{I}}{\sin(\theta)} \mathbf{q}_\varphi = r^2 \sin(\theta) \mathbf{q}^{(\varphi)}, \quad (\text{B.102})$$

$$\mathbf{q}_\theta \times \mathbf{q}_\varphi = r^2 \sin(\theta) \mathbf{q}_r = r^2 \sin(\theta) \mathbf{q}^{(r)}, \quad (\text{B.103})$$

$$\mathbf{q}_\varphi \times \mathbf{q}_r = \sin(\theta) \mathbf{q}_\theta = r^2 \sin(\theta) \mathbf{q}^{(\theta)}. \quad (\text{B.104})$$

It follows with Eq. (B.68)

$$\begin{aligned}
& (\nabla \times \mathbf{v}) \times \mathbf{v} \\
&= \begin{vmatrix} \mathbf{q}^{(r)} & \mathbf{q}^{(\theta)} & \mathbf{q}^{(\varphi)} \\ \frac{\partial v_\varphi}{\partial \theta} - \frac{\partial v_\theta}{\partial \varphi} & \frac{\partial v_r}{\partial \varphi} - \frac{\partial v_\varphi}{\partial r} & \frac{\partial v_\theta}{\partial r} - \frac{\partial v_r}{\partial \theta} \\ v^{(r)} & v^{(\theta)} & v^{(\varphi)} \end{vmatrix} \\
&= \mathbf{q}^{(r)} \left[v^{(\varphi)} \left(\frac{\partial v_r}{\partial \varphi} - \frac{\partial v_\varphi}{\partial r} \right) - v^{(\theta)} \left(\frac{\partial v_\theta}{\partial r} - \frac{\partial v_r}{\partial \theta} \right) \right] \\
&+ \mathbf{q}^{(\theta)} \left[v^{(r)} \left(\frac{\partial v_\theta}{\partial r} - \frac{\partial v_r}{\partial \theta} \right) - v^{(\varphi)} \left(\frac{\partial v_\varphi}{\partial \theta} - \frac{\partial v_\theta}{\partial \varphi} \right) \right] \\
&+ \mathbf{q}^{(\varphi)} \left[v^{(\theta)} \left(\frac{\partial v_\varphi}{\partial \theta} - \frac{\partial v_\theta}{\partial \varphi} \right) - v^{(r)} \left(\frac{\partial v_r}{\partial \varphi} - \frac{\partial v_\varphi}{\partial r} \right) \right] \\
&= \mathbf{q}^{(r)} \left[v^{(\varphi)} \left(\frac{\partial v^{(r)}}{\partial \varphi} - \frac{\partial (r^2 \sin^2(\theta) v^{(\varphi)})}{\partial r} \right) - v^{(\theta)} \left(\frac{\partial (r^2 v^{(\theta)})}{\partial r} - \frac{\partial v^{(r)}}{\partial \theta} \right) \right] \\
&+ \mathbf{q}^{(\theta)} \left[v^{(r)} \left(\frac{\partial (r^2 v^{(\theta)})}{\partial r} - \frac{\partial v^{(r)}}{\partial \theta} \right) - v^{(\varphi)} \left(\frac{\partial (r^2 \sin^2(\theta) v^{(\varphi)})}{\partial \theta} - \frac{\partial (r^2 v^{(\theta)})}{\partial \varphi} \right) \right] \\
&+ \mathbf{q}^{(\varphi)} \left[v^{(\theta)} \left(\frac{\partial (r^2 \sin^2(\theta) v^{(\varphi)})}{\partial \theta} - \frac{\partial (r^2 v^{(\theta)})}{\partial \varphi} \right) - v^{(r)} \left(\frac{\partial v^{(r)}}{\partial \varphi} - \frac{\partial (r^2 \sin^2(\theta) v^{(\varphi)})}{\partial r} \right) \right] \\
&= \mathbf{q}^{(r)} \left[v^{(\varphi)} \left(\frac{\partial v^{(r)}}{\partial \varphi} - r^2 \sin^2(\theta) \frac{\partial v^{(\varphi)}}{\partial r} - 2r \sin^2(\theta) v^{(\varphi)} \right) - v^{(\theta)} \left(2r v^{(\theta)} + r^2 \frac{\partial v^{(\theta)}}{\partial r} - \frac{\partial v^{(r)}}{\partial \theta} \right) \right] \\
&+ \mathbf{q}^{(\theta)} \left[v^{(r)} \left(2r v^{(\theta)} + r^2 \frac{\partial v^{(\theta)}}{\partial r} - \frac{\partial v^{(r)}}{\partial \theta} \right) - v^{(\varphi)} \left(r^2 \sin^2(\theta) \frac{\partial v^{(\varphi)}}{\partial \theta} + 2r^2 \sin(\theta) \cos(\theta) v^{(\varphi)} - r^2 \frac{\partial v^{(\theta)}}{\partial \varphi} \right) \right] \\
&+ \mathbf{q}^{(\varphi)} \left[v^{(\theta)} \left(r^2 \sin^2(\theta) \frac{\partial v^{(\varphi)}}{\partial \theta} + 2r^2 \sin(\theta) \cos(\theta) v^{(\varphi)} - r^2 \frac{\partial v^{(\theta)}}{\partial \varphi} \right) \right. \\
&\quad \left. - v^{(r)} \left(\frac{\partial v^{(r)}}{\partial \varphi} - 2r \sin^2(\theta) v^{(\varphi)} - r^2 \sin^2(\theta) \frac{\partial v^{(\varphi)}}{\partial r} \right) \right]. \tag{B.105}
\end{aligned}$$

Thus follows

$$\begin{aligned}
& (\mathbf{v} \cdot \nabla) \mathbf{v} \\
&= \mathbf{q}^{(r)} \left[v^{(r)} \frac{\partial v^{(r)}}{\partial r} + v^{(\theta)} \frac{\partial v^{(r)}}{\partial \theta} + v^{(\varphi)} \frac{\partial v^{(r)}}{\partial \varphi} - r \left(v^{(\theta)} \right)^2 - r \sin^2(\theta) \left(v^{(\varphi)} \right)^2 \right] \\
&+ \mathbf{q}^{(\theta)} \left[r^2 \left(v^{(r)} \frac{\partial v^{(\theta)}}{\partial r} + v^{(\theta)} \frac{\partial v^{(\theta)}}{\partial \theta} + v^{(\varphi)} \frac{\partial v^{(\theta)}}{\partial \varphi} \right) - r^2 \sin(\theta) \cos(\theta) \left(v^{(\varphi)} \right)^2 + 2r v^{(\theta)} v^{(r)} \right] \\
&+ \mathbf{q}^{(\varphi)} \left[r^2 \sin^2(\theta) \left(v^{(r)} \frac{\partial v^{(\varphi)}}{\partial r} + v^{(\theta)} \frac{\partial v^{(\varphi)}}{\partial \theta} + v^{(\varphi)} \frac{\partial v^{(\varphi)}}{\partial \varphi} \right) \right. \\
&\quad \left. + 2r \sin(\theta) v^{(\varphi)} \left(\sin(\theta) v^{(r)} + r \cos(\theta) v^{(\theta)} \right) \right] \\
&= \mathbf{e}_r \left[\tilde{v}_r \frac{\partial \tilde{v}_r}{\partial r} + \tilde{v}_\theta \frac{\mathbf{I}}{r} \frac{\partial \tilde{v}_r}{\partial \theta} + \tilde{v}_\varphi \frac{\mathbf{I}}{r \sin(\theta)} \frac{\partial \tilde{v}_r}{\partial \varphi} - \frac{\mathbf{I}}{r} (\tilde{v}_\theta)^2 - \frac{\mathbf{I}}{r} (\tilde{v}_\varphi)^2 \right] \\
&+ \frac{\mathbf{I}}{r} \mathbf{e}_\theta \left[r^2 \left(\tilde{v}_r \frac{\mathbf{I}}{r} \frac{\partial \tilde{v}_\theta}{\partial r} - \frac{\tilde{v}_r \tilde{v}_\theta}{r^2} + \tilde{v}_\theta \frac{\mathbf{I}}{r^2} \frac{\partial \tilde{v}_\theta}{\partial \theta} + \tilde{v}_\varphi \frac{\mathbf{I}}{r^2 \sin(\theta)} \frac{\partial \tilde{v}_\theta}{\partial \varphi} \right) - \frac{\mathbf{I}}{\tan(\theta)} (\tilde{v}_\varphi)^2 + 2\tilde{v}_\theta \tilde{v}_r \right] \\
&+ \frac{\mathbf{I}}{r \sin(\theta)} \mathbf{e}_\varphi \left[r \sin(\theta) \left(\tilde{v}_r \frac{\partial \tilde{v}_\varphi}{\partial r} + \frac{\mathbf{I}}{r} \tilde{v}_\theta \frac{\partial \tilde{v}_\varphi}{\partial \theta} + \tilde{v}_\varphi \frac{\mathbf{I}}{r \sin(\theta)} \frac{\partial \tilde{v}_\varphi}{\partial \varphi} \right) - \sin(\theta) \tilde{v}_r \tilde{v}_\varphi - \cos(\theta) \tilde{v}_\theta \tilde{v}_\varphi \right. \\
&\quad \left. + 2\tilde{v}_\varphi \left(\sin(\theta) \tilde{v}_r + r \cos(\theta) \frac{\mathbf{I}}{r} \tilde{v}_\theta \right) \right]. \tag{B.106}
\end{aligned}$$

So for the material derivation applies

$$\begin{aligned} \frac{D\mathbf{v}}{Dt} = & \mathbf{e}_r \left(\frac{D\tilde{v}_r}{Dt} - \frac{\tilde{v}_\varphi^2 + \tilde{v}_\theta^2}{r} \right) + \mathbf{e}_\theta \left(\frac{D\tilde{v}_\theta}{Dt} + \frac{\tilde{v}_r\tilde{v}_\theta}{r} - \frac{\tilde{v}_\varphi^2}{r\tan(\theta)} \right) \\ & + \mathbf{e}_\varphi \left(\frac{D\tilde{v}_\varphi}{Dt} + \frac{\tilde{v}_r\tilde{v}_\varphi}{r} + \frac{\tilde{v}_\theta\tilde{v}_\varphi}{r\tan(\theta)} \right) \end{aligned} \quad (\text{B.107})$$

B.2.1.1 Transformation to geographical coordinates

In order to transform to geographical coordinates, one considers the definition of this CS in Sect. D.1.3 and Eq. (B.66):

$$\frac{\partial}{\partial x} = \frac{\mathbf{i}}{r\cos(\varphi)} \frac{\partial}{\partial \lambda} = \frac{\mathbf{i}}{r\sin(\theta)} \frac{\partial}{\partial \varphi} \quad (\text{B.108})$$

$$\frac{\partial}{\partial y} = \frac{\mathbf{i}}{r} \frac{\partial}{\partial \varphi} = -\frac{\mathbf{i}}{r} \frac{\partial}{\partial \theta} \quad (\text{B.109})$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial r} \quad (\text{B.110})$$

The final identity transforms into the ordinary spherical coordinates. This applies analogously to second derivatives. For the representation of the Laplace operator Eq. (B.91) follows

$$\begin{aligned} \Delta = & \frac{\mathbf{i}}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\mathbf{i}}{r^2 \cos^2(\varphi)} \frac{\partial^2}{\partial \lambda^2} + \frac{\mathbf{i}}{r^2 \cos(\varphi)} \frac{\partial}{\partial \varphi} \left(\cos(\varphi) \frac{\partial}{\partial \varphi} \right) \\ = & \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\mathbf{z}}{r} \frac{\partial}{\partial z} - \frac{\tan(\varphi)}{r} \frac{\partial}{\partial y}. \end{aligned} \quad (\text{B.111})$$

Eq. (B.90) becomes

$$\begin{aligned} \nabla \cdot \mathbf{v} = & \frac{\partial v_z}{\partial r} + \frac{\mathbf{i}}{r} \frac{\partial v_y}{\partial \varphi} + \frac{\mathbf{i}}{r\cos(\varphi)} \frac{\partial v_x}{\partial \lambda} + \frac{\mathbf{z}v_z}{r} - \frac{v_y \tan(\varphi)}{r} = \nabla \cdot \mathbf{v} \\ = & \frac{\partial v_z}{\partial r} + \frac{\partial v_y}{\partial y} + \frac{\partial v_x}{\partial x} + \frac{\mathbf{z}v_z}{r} - \frac{v_y \tan(\varphi)}{r}. \end{aligned} \quad (\text{B.112})$$

If $\mathbf{v} = (u, v, w)^T$ is the wind vector, it follows

$$\nabla \cdot \mathbf{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} - \frac{v \tan(\varphi)}{r} + \frac{\mathbf{z}w}{r}. \quad (\text{B.113})$$

Eq. (B.98) becomes

$$\begin{aligned} \nabla \times \mathbf{v} = & -\frac{v_y}{r} \mathbf{i} + \frac{v_x \tan(\varphi)}{r} \mathbf{k} + \frac{v_x}{r} \mathbf{j} + \mathbf{k} \left(-\frac{\mathbf{i}}{r} \frac{\partial v_x}{\partial \varphi} + \frac{\mathbf{i}}{r\cos(\varphi)} \frac{\partial v_y}{\partial \lambda} \right) \\ & - \mathbf{j} \left(\frac{\mathbf{i}}{r\cos(\varphi)} \frac{\partial v_z}{\partial \lambda} - \frac{\partial v_x}{\partial r} \right) + \mathbf{i} \left(-\frac{\partial v_y}{\partial r} + \frac{\mathbf{i}}{r} \frac{\partial v_z}{\partial \varphi} \right) \\ = & -\frac{v_y}{r} \mathbf{i} + \frac{v_x \tan(\varphi)}{r} \mathbf{k} + \frac{v_x}{r} \mathbf{j} + \mathbf{k} \left(-\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) \\ & - \mathbf{j} \left(\frac{\partial v_z}{\partial x} - \frac{\partial v_x}{\partial r} \right) + \mathbf{i} \left(-\frac{\partial v_y}{\partial r} + \frac{\partial v_z}{\partial y} \right). \end{aligned} \quad (\text{B.114})$$

If $\mathbf{v}$ is the wind vector again, it follows

$$\nabla \times \mathbf{v} = \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) \mathbf{i} + \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) \mathbf{j} + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \mathbf{k} + \frac{u \tan(\varphi)}{r} \mathbf{k} + \frac{u}{r} \mathbf{j} - \frac{v}{r} \mathbf{i}. \quad (\text{B.115})$$

Still applies

$$\zeta := \mathbf{k} \cdot (\nabla \times \mathbf{v}) = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} + \frac{u \tan(\varphi)}{r}. \quad (\text{B.116})$$

It should be noted that this applies

$$\nabla_h \times \mathbf{v}_h = \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \mathbf{k} + \frac{u \tan(\varphi)}{r} \mathbf{k} + \frac{u}{r} \mathbf{j} - \frac{v}{r} \mathbf{i} \neq \zeta \mathbf{k}. \quad (\text{B.117})$$

For the *material derivative* it follows with Eq. (B.107)

$$\begin{aligned} \frac{D\mathbf{v}}{Dt} &= \mathbf{i} \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} - \frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} \right) \\ &\quad + \mathbf{j} \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} + \frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} \right) \\ &\quad + \mathbf{k} \left(\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} - \frac{u^2 + v^2}{a+z} \right) \end{aligned} \quad (\text{B.118})$$

$$\begin{aligned} &= \mathbf{i} \left(\frac{Du}{Dt} - \frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} \right) \\ &\quad + \mathbf{j} \left(\frac{Dv}{Dt} + \frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} \right) \\ &\quad + \mathbf{k} \left(\frac{Dw}{Dt} - \frac{u^2 + v^2}{a+z} \right) \\ &=: \frac{D\mathbf{v}}{Dt} \Big|_{\text{comp}} + \frac{D\mathbf{v}}{Dt} \Big|_{\text{met}}. \end{aligned} \quad (\text{B.119})$$

The material derivative of the speed is therefore composed of the material derivatives of the components

$$\frac{D\mathbf{v}}{Dt} \Big|_{\text{comp}} := \mathbf{i} \frac{Du}{Dt} + \mathbf{j} \frac{Dv}{Dt} + \mathbf{k} \frac{Dw}{Dt}. \quad (\text{B.120})$$

and the metric terms

$$\frac{D\mathbf{v}}{Dt} \Big|_{\text{met}} := \mathbf{i} \left(-\frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} \right) + \mathbf{j} \left(\frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} \right) - \mathbf{k} \frac{u^2 + v^2}{a+z}. \quad (\text{B.121})$$

The **red** term is the centrifugal acceleration.

Another form of the advective part of Eq. (B.118) is

$$\begin{aligned} (\mathbf{v} \cdot \nabla) \mathbf{v} &= [(\mathbf{v}_h + w\mathbf{k}) \cdot \nabla] (\mathbf{v}_h + w\mathbf{k}) = (\mathbf{v}_h \cdot \nabla) \mathbf{v}_h + w \frac{\partial \mathbf{v}_h}{\partial z} + (\mathbf{v} \cdot \nabla) (w\mathbf{k}) \\ &\stackrel{\text{Glg. (B.57)}}{=} (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h + \nabla \frac{v_h^2}{2} + w \frac{\partial \mathbf{v}_h}{\partial z} + (\mathbf{v} \cdot \nabla) (w\mathbf{k}) \end{aligned}$$

$$\Leftrightarrow (\mathbf{v} \cdot \nabla) \mathbf{v} = (\nabla_h \times \mathbf{v}_h) \times \mathbf{v}_h + \nabla_h \frac{v_h^2}{2} + w \frac{\partial \mathbf{v}_h}{\partial z} + (\mathbf{v} \cdot \nabla) (w\mathbf{k}). \quad (\text{B.122})$$

In the last step

$$\left(\mathbf{k} \frac{\partial}{\partial z} \times \mathbf{v}_h \right) \times \mathbf{v}_h = \left(-\frac{\partial v}{\partial z} \right) \times \begin{pmatrix} u \\ v \\ 0 \end{pmatrix} = - \left(u \frac{\partial u}{\partial z} + v \frac{\partial v}{\partial z} \right) \mathbf{k} = -\mathbf{k} \frac{\partial v_h^2}{\partial z} \quad (\text{B.123})$$

used. Eq. (B.122) is called *2D vector invariant form of velocity advection*. Another useful form of this is

$$\begin{aligned}
(\mathbf{v} \cdot \nabla) \mathbf{v} &= (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h + \nabla \frac{\mathbf{v}_h^2}{2} + w \frac{\partial \mathbf{v}_h}{\partial z} + (\mathbf{v} \cdot \nabla) (w \mathbf{k}) \\
&= (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h + \nabla \frac{\mathbf{v}_h^2}{2} + w \frac{\partial \mathbf{v}}{\partial z} + (\mathbf{v}_h \cdot \nabla) (w \mathbf{k}).
\end{aligned} \tag{B.124}$$

Because of

$$\begin{aligned}
(\nabla \times \mathbf{v}) \times \mathbf{v}_h &= [\nabla \times (\mathbf{v}_h + w \mathbf{k})] \times \mathbf{v}_h = (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h + (\nabla \times w \mathbf{k}) \times \mathbf{v}_h \\
&\stackrel{\text{Glg. (B.115)}}{=} (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h + \left(\frac{\partial w}{\partial y} \mathbf{i} - \frac{\partial w}{\partial x} \mathbf{j} \right) \times \mathbf{v}_h = (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h + \mathbf{k} (\mathbf{v}_h \cdot \nabla w) \\
\Rightarrow (\nabla \times \mathbf{v}_h) \times \mathbf{v}_h &= (\nabla \times \mathbf{v}) \times \mathbf{v}_h - \mathbf{k} (\mathbf{v}_h \cdot \nabla w)
\end{aligned} \tag{B.125}$$

and

$$\begin{aligned}
(\mathbf{v}_h \cdot \nabla) (w \mathbf{k}) &= \mathbf{k} (\mathbf{v}_h \cdot \nabla w) + w \left(u \frac{\partial \mathbf{k}}{\partial x} + v \frac{\partial \mathbf{k}}{\partial y} \right) = \mathbf{k} (\mathbf{v}_h \cdot \nabla w) + w \left(\frac{u}{r \cos(\varphi)} \frac{\partial \mathbf{k}}{\partial \lambda} + \frac{v}{r} \frac{\partial \mathbf{k}}{\partial \varphi} \right) \\
&= \mathbf{k} (\mathbf{v}_h \cdot \nabla w) + w \left(\frac{u}{r} \mathbf{i} + \frac{v}{r} \mathbf{j} \right) = \mathbf{k} (\mathbf{v}_h \cdot \nabla w) + \frac{w}{r} \mathbf{v}_h
\end{aligned} \tag{B.126}$$

applies

$$(\mathbf{v} \cdot \nabla) \mathbf{v} = (\nabla \times \mathbf{v}) \times \mathbf{v}_h + \nabla \frac{\mathbf{v}_h^2}{2} + w \frac{\partial \mathbf{v}}{\partial z} + \frac{w}{r} \mathbf{v}_h. \tag{B.127}$$

By comparing with section 13.3 one finds that the term $\frac{w}{r} \mathbf{v}_h$ does not appear under the shallow atmosphere approximation.

The metric terms in Eq. (B.118)

$$\frac{D\mathbf{v}}{Dt} \Big|_{\text{met}} = \begin{pmatrix} -\frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} \\ \frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} \\ -\frac{u^2 + v^2}{a+z} \end{pmatrix}. \tag{B.128}$$

The metric terms in Eq. (B.115)

$$\nabla \times \mathbf{v}_{\text{met}} = \begin{pmatrix} -\frac{v}{r} \\ \frac{u}{r} \\ \frac{u \tan(\varphi)}{r} \end{pmatrix}. \tag{B.129}$$

If you multiply this vectorially by $\mathbf{v}$, you get Eq. (B.128):

$$\nabla \times \mathbf{v}_{\text{met}} \times \mathbf{v} = \begin{pmatrix} -\frac{v}{r} \\ \frac{u}{r} \\ \frac{u \tan(\varphi)}{r} \end{pmatrix} \times \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} -\frac{uv \tan(\varphi)}{a+z} + \frac{uw}{a+z} \\ \frac{u^2 \tan(\varphi)}{a+z} + \frac{vw}{a+z} \\ -\frac{u^2 + v^2}{a+z} \end{pmatrix} = \frac{D\mathbf{v}}{Dt} \Big|_{\text{met}}. \tag{B.130}$$

The metric terms in momentum advection are therefore consequences of the metric terms in rotation.

B.3 Multidimensional integral calculus

Let $M, N \subseteq \mathbb{R}^3$, $f: M \rightarrow \mathbb{R}$ be continuous, $T: N \rightarrow M$ be a diffeomorphism, then we have

$$\int_M f d^3 r = \int_N f \circ T |\det(T')| d^3 r, \tag{B.131}$$

this corresponds to the multidimensional substitution formula. The determinant $\det(T')$ is called *functional determinant*. As an example, take $M = \mathbb{R}$, $N = [0, \infty) \times [0, \pi] \times [0, 2\pi)$ and

$$T = r \begin{pmatrix} \sin(\vartheta) \cos(\varphi) \\ \sin(\vartheta) \sin(\varphi) \\ \cos(\vartheta) \end{pmatrix}, \quad (\text{B.132})$$

then applies

$$T' = \begin{pmatrix} \sin(\vartheta) \cos(\varphi) & r \cos(\vartheta) \cos(\varphi) & -r \sin(\vartheta) \sin(\varphi) \\ \sin(\vartheta) \sin(\varphi) & r \cos(\vartheta) \sin(\varphi) & r \sin(\vartheta) \cos(\varphi) \\ \cos(\vartheta) & -r \sin(\vartheta) & 0 \end{pmatrix}. \quad (\text{B.133})$$

applies to the determinant

$$\begin{aligned} \det(T') &= -r \sin(\vartheta) \cos(\varphi) (-r \sin(\vartheta)^2 \cos(\varphi) - r \cos(\vartheta)^2 \cos(\varphi)) \\ &\quad - r \sin(\vartheta) \sin(\varphi) (-r \sin(\vartheta)^2 \sin(\varphi) - r \cos(\vartheta)^2 \sin(\varphi)) \\ &= r^2 \sin(\vartheta) \cos(\varphi)^2 + r^2 \sin(\vartheta) \sin(\vartheta)^2 = r^2 \sin(\vartheta), \end{aligned} \quad (\text{B.134})$$

in the case of geographical coordinates the functional determinant is $r^2 \cos(\varphi)$.

Stokes' theorem Eq. (15.26) has already been introduced. Let $A \subseteq \mathbb{R}^3$ be connected and $\mathbf{v} : A \rightarrow \mathbb{R}^3$ be continuous-differentiable. Then applies

$$\boxed{\int_A \nabla \cdot \mathbf{v} d^3 r = \int_{\partial A} \mathbf{v} \cdot d\mathbf{n}. \quad (\text{B.135})}$$

This is the *Gaussian theorem*.

A sphere $K_N(R)$ in $\mathbb{R}^N$ with radius $R \geq 0$ can be defined by

$$K_N(R) := \left\{ \mathbf{x} = (x_1, \dots, x_N)^T \in \mathbb{R}^N \left| \sum_{i=1}^N x_i^2 \leq R^2 \right. \right\}. \quad (\text{B.136})$$

Their volume is

$$V_N(R) = \int_{K_N} dx_1 \dots dx_N. \quad (\text{B.137})$$

It applies

$$\int_{\mathbb{R}^N} \exp\left(-\sum_{i=1}^N x_i^2\right) dx_1 \dots dx_N = \int_0^\infty e^{-R^2} \frac{dV_N}{dR} dR, \quad (\text{B.138})$$

this corresponds to a transformation to spherical coordinates. You can also transform the integral $V_N(R)$ to spherical coordinates by writing

$$V_N(R) = \int_{K_N} dV_N = \int_0^R f_N(R) dR, \quad (\text{B.139})$$

here $f_N(R)$ is the functional determinant integrated across the surface. The N -dimensional spherical coordinates consist of $N - 1$ angles and a distance. Therefore $f_N(R)$ is the determinant of a real $N \times N$ -matrix in which the factor R occurs in $N - 1$ columns. $f_N(R)$ is therefore of degree $N - 1$, you can write

$$f_N(R) = NC_N R^{N-1}. \quad (\text{B.140})$$

By differentiating Eq. (B.139) to R and with Eq. (B.138) follows

$$\frac{dV_N}{dR} = NC_N R^{N-1} \Rightarrow NC_N \int_0^\infty e^{-R^2} R^{N-1} dR = \left(\int_{-\infty}^\infty e^{-x^2} dx \right)^N = \pi^{N/2}. \quad (\text{B.141})$$

The last step follows with Eq. (A.105). It applies with the substitution rule

$$\int_0^\infty e^{-R^2} R^{N-1} dR = \int_0^\infty e^{-R^2} R^{\frac{N-1}{2}} \frac{1}{2} R^{-\frac{1}{2}} dR = \frac{1}{2} \int_0^\infty e^{-R^2} R^{N/2-1} dR = \frac{1}{2} \Gamma\left(\frac{N}{2}\right). \quad (\text{B.142})$$

It follows with Eq. (A.111)

$$V_N = C_N R^N = \frac{\pi^{N/2}}{\frac{N}{2} \Gamma\left(\frac{N}{2}\right)} R^N = \frac{\pi^{N/2}}{\Gamma\left(\frac{N}{2} + 1\right)} R^N. \quad (\text{B.143})$$

B.3.1 Transport theorem

Let a time-dependent connected set $\Omega = \Omega(t) \subseteq \mathbb{R}^3$ be given, which moves with the continuously differentiable vector field $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$.

The so-called *transport theorem* is the three-dimensional generalization of the Leibniz rule Eq. (A.95).

$$\frac{dF(t)}{dt} = \int_{\Omega(t)} \frac{\partial f(x, y, z, t)}{\partial t} dx + \int_{\partial\Omega} f(x, y, z, t) (\mathbf{v} \cdot d\mathbf{n}). \quad (\text{B.144})$$

This is the transport theorem or *Reynolds transport theorem*. f can also be the component of a vector field. The derivation can thus be generalized vectorially:

$$\frac{d\mathbf{F}(t)}{dt} = \int_{\Omega(t)} \frac{\partial \mathbf{f}(x, y, z, t)}{\partial t} dx + \int_{\partial\Omega} \mathbf{f}(x, y, z, t) (\mathbf{v} \cdot d\mathbf{n}) \quad (\text{B.145})$$

C ORTHOGONAL FUNCTION SYSTEMS

When complete, orthogonal function systems are suitable for developing functions. A system of polynomials $f_n(x)$ with $n \in \mathbb{N}$ and $\mathcal{O}(f_n) = n$ is said to be orthogonal on the interval $[a, b]$ with respect to the function w if for $n, m \in \mathbb{N}$ with $n \neq m$

$$\int_a^b w(x) f_n(x) f_m(x) dx = 0. \quad (\text{C.1})$$

All orthogonal polynomial systems satisfy a *Rodrigues formula*

$$f_n(x) = \frac{1}{e_n w(x)} \frac{d^n}{dx^n} [w(x) g(x)^n] \quad (\text{C.2})$$

with a polynomial $g(x)$, which does not depend on n .

C.1 Complex exponential functions

The expansion of a function according to complex exponential functions is called *Fourier transformation* (FT). Let $f(x)$ be a complex function of a real variable, then one defines the *Fourier transform* $\tilde{F}_1\{f\} = \tilde{f}(k)$ or the *spectrum* of f by

$$\tilde{F}_1\{f\} = \tilde{f}(k) := C \int_{-\infty}^{\infty} \exp(-ikx) f(x) dx \quad (\text{C.3})$$

with a real constant $C > 0$. $\tilde{F}_1$ denotes the operator of the one-dimensional Fourier transform. Eq. (C.3) is, with the exception of a possible factor, the covariance of the function f with the *Fourier component* e^{ikx} . It applies

$$\tilde{f}(k)^* = C \int_{-\infty}^{\infty} \exp(ikx) f^*(x) dx = \tilde{f}^*(-k). \quad (\text{C.4})$$

If f is real, this becomes

$$\tilde{f}(k)^* = \tilde{f}(-k). \quad (\text{C.5})$$

The *inverse Fourier transformation* is defined by

$$\tilde{F}_1^{-1}\{f\} := \tilde{C} \int_{-\infty}^{\infty} \tilde{f}(k) \exp(ikx) dk \quad (\text{C.6})$$

with a second constant $\tilde{C} > 0$. It is a linear combination of the $\tilde{f}(k)$ with the corresponding waves. That this is actually the inverse of Eq. (C.3) should now be seen:

$$\begin{aligned} \tilde{C} \int_{-\infty}^{\infty} \tilde{f}(k) \exp(ikx) dk &= \tilde{C} C \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(-ikx') f(x') dx' \exp(ikx) dk \\ &= \tilde{C} C \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(ik(x-x')) dk f(x') dx' \\ &\stackrel{\text{Glg. (A.84)}}{=} \tilde{C} C \int_{-\infty}^{\infty} 2\pi \delta(x-x') f(x') dx' = \tilde{C} C 2\pi f(x) \end{aligned} \quad (\text{C.7})$$

$$\Leftrightarrow \tilde{C} C \stackrel{=}{=} 1/2\pi \quad f(x) \quad (\text{C.8})$$

So you have to accept the condition

$$\tilde{C} = \frac{1}{2\pi C} \quad (\text{C.9})$$

regard. From this you can immediately

$$\left[\widetilde{F}_1 \{ \delta (x - x_o) \} \right] (k) = C e^{-ikx_o}, \quad (\text{C.10})$$

$$\left[\widetilde{F}_1 \{ e^{ik'x} \} \right] (k) = \mathbf{2}\pi C \delta (k' - k), \quad (\text{C.11})$$

$$\left[\widetilde{F}_1^{-1} \{ \delta (k - k_o) \} \right] (x) = \widetilde{C} e^{ik_o x}, \quad (\text{C.12})$$

$$\left[\widetilde{F}_1^{-1} \{ e^{ikx'} \} \right] (x) = \mathbf{2}\pi \widetilde{C} \delta (x' + x) \quad (\text{C.13})$$

derive. The function

$$\arg \left(\widetilde{f}(k) \right) \quad (\text{C.14})$$

is called the *phase spectrum* of f , while one

$$\left| \widetilde{f}(k) \right| \quad (\text{C.15})$$

referred to as *amplitude spectrum*. The square of $\left| \widetilde{f}(k) \right|$ is called *power spectrum* or *power spectrum*. The FT is linear because it is defined in terms of an integral and the integration is linear. This applies to functions f, g and constants a, b

$$\widetilde{F}\{af + bg\} = a\widetilde{F}\{f\} + b\widetilde{F}\{g\}. \quad (\text{C.16})$$

Let $N(\mu, \sigma)$ be the normal distribution with expected value μ and standard deviation σ . Then holds

$$\begin{aligned} \widetilde{F}\{N(\mu, \sigma)\} &= \frac{C}{\sqrt{\mathbf{2}\pi\sigma}} \int_{-\infty}^{\infty} \exp \left[-ikx - \frac{(x - \mu)^2}{\mathbf{2}\sigma^2} \right] dx = \frac{C}{\sqrt{\mathbf{2}\pi\sigma}} \int_{-\infty}^{\infty} \exp \left[-\frac{\mathbf{1}}{\mathbf{2}\sigma^2} (x^2 + \mu^2 - \mathbf{2}x(\mu - ik\sigma^2)) \right] dx \\ &= \frac{C}{\sqrt{\mathbf{2}\pi\sigma}} \int_{-\infty}^{\infty} \exp \left[-\frac{\mathbf{1}}{\mathbf{2}\sigma^2} (x - (\mu - ik\sigma^2))^2 - \frac{\mathbf{1}}{\mathbf{2}\sigma^2} (k^2\sigma^4 + \mathbf{2}\mu i\sigma^2 k) \right] dx \\ &= \exp \left[-\frac{\mathbf{1}}{\mathbf{2}\sigma^2} (k^2\sigma^4 + \mathbf{2}\mu i\sigma^2 k) \right] \frac{C}{\sqrt{\mathbf{2}\pi\sigma}} \int_{-\infty}^{\infty} \exp \left[-\frac{\mathbf{1}}{\mathbf{2}\sigma^2} x^2 \right] dx \\ &= C \exp \left(-\frac{k^2}{\mathbf{2}/\sigma^2} \right) \exp (-\mu ik). \end{aligned} \quad (\text{C.17})$$

The FT of a normal distribution is therefore an unnormalized normal distribution with a mean value (consider the case $C = \mathbf{1}/\sqrt{\mathbf{2}\pi}$) and modified by a complex phase factor

$$\mu_k = \mathbf{0} \quad (\text{C.18})$$

and standard deviation

$$\sigma_k = \frac{\mathbf{1}}{\sigma} \quad (\text{C.19})$$

The FT therefore turns a narrow normal distribution into a wide one. In the case of a complex-valued function $f(x, y)$ of two real variables, we first consider the auxiliary function

$$f_y(x) := f(x, y). \quad (\text{C.20})$$

The FT of this is

$$\widetilde{f}_y(k_x) = C \int_{-\infty}^{\infty} e^{-ik_x x} f_y(x) dx. \quad (\text{C.21})$$

If you apply the inverse FT to this, you get $f_y(x) = f(x, y)$ again. Now define the Fourier transform $\tilde{f}(k_x, k_y)$ of the function $f(x, y)$ by the Fourier transform in the y direction of $\tilde{f}_y(k_x)$, i.e

$$\begin{aligned}\tilde{f}(k_x, k_y) &:= C \int_{-\infty}^{\infty} e^{-ik_y y} \tilde{f}_y(k_x) dy = C^2 \int_{-\infty}^{\infty} e^{-ik_y y} \int_{-\infty}^{\infty} e^{-ik_x x} f(x, y) dx dy \\ &= C^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(k_x x + k_y y)} f(x, y) dx dy.\end{aligned}\quad (\text{C.22})$$

Applying the inverse FT twice yields the function $f(x, y)$. x is not distinguished before y in the derivation, which is why the order in which the FT is applied does not matter. You take notes

$$\tilde{F}_2\{f\} = \tilde{f}(k_x, k_y) := C_2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(k_x x + k_y y)} f(x, y) dx dy, \quad (\text{C.23})$$

$$\tilde{F}_2^{-1}\{f\} := \tilde{C}_2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k_x, k_y) e^{i(k_x x + k_y y)} dk_x dk_y, \quad (\text{C.24})$$

where

$$C_2 \tilde{C}_2 = \left(C \tilde{C}\right)^2 = \frac{1}{(2\pi)^2} \quad (\text{C.25})$$

must apply. If you continue this inductively, you get the n -dimensional FT, where on

$$C_n \tilde{C}_n = \left(C \tilde{C}\right)^n = \frac{1}{(2\pi)^n} \quad (\text{C.26})$$

must be taken into account.

Eq. (C.8) is

$$f(x) = \tilde{C} \int_{-\infty}^{\infty} \tilde{f}(k) \exp(ikx) dk, \quad (\text{C.27})$$

If you transfer this to an analogously defined function g , you get

$$g(x) = \tilde{C} \int_{-\infty}^{\infty} \tilde{g}(k') \exp(ik'x) dk'. \quad (\text{C.28})$$

If you multiply the last two equations together, you get

$$f(x) g(x) = \tilde{C}^2 \int_{k=-\infty}^{\infty} \int_{k'=-\infty}^{\infty} \tilde{g}(k') \tilde{f}(k) \exp[i(k+k')x] dk' dk. \quad (\text{C.29})$$

Integrating this over x gives

$$\begin{aligned}\int_{-\infty}^{\infty} f(x) g(x) dx &= \tilde{C}^2 \int_{k=-\infty}^{\infty} \int_{k'=-\infty}^{\infty} \tilde{g}(k') \tilde{f}(k) \int_{-\infty}^{\infty} \exp[i(k+k')x] dx dk' dk \\ &\stackrel{\text{Glg. (A.84)}}{=} \tilde{C}^2 \int_{k=-\infty}^{\infty} \int_{k'=-\infty}^{\infty} \tilde{g}(k') \tilde{f}(k) 2\pi \delta(k+k') dk' dk \\ &= 2\pi \tilde{C}^2 \int_{-\infty}^{\infty} \tilde{g}(-k) \tilde{f}(k) dk\end{aligned}\quad (\text{C.30})$$

For $g = f$ you get the so-called *Parseval identity*

$$\int_{-\infty}^{\infty} f^2(x) dx = 2\pi \tilde{C}^2 \int_{-\infty}^{\infty} \tilde{f}(-k) \tilde{f}(k) dk. \quad (\text{C.31})$$

C.1.1 Convolution theorem

Let f, g be two continuously differentiable functions $\mathbb{R} \rightarrow \mathbb{R}$. The Fourier transforms of these two functions are

$$\tilde{f}(k) = C \int_{-\infty}^{\infty} \exp(-ikx) f(x) dx, \quad \tilde{g}(k) = C \int_{-\infty}^{\infty} \exp(-ikx) g(x) dx. \quad (\text{C.32})$$

Define the continuously differentiable function h by

$$h(x) = f(x) g(x). \quad (\text{C.33})$$

The so-called *convolution theorem* is about how the Fourier transform of h is related to the Fourier transform of f and g . For the spectrum of h applies

$$\tilde{h}(k) = C^2 \int_{-\infty}^{\infty} f(x) g(x) \exp(-ikx) dx. \quad (\text{C.34})$$

Expressing f and g in terms of their spectra, one obtains

$$f(x) = \tilde{C} \int_{-\infty}^{\infty} \exp(ikx) \tilde{f}(k) dk, \quad g(x) = \tilde{C} \int_{-\infty}^{\infty} \exp(ikx) \tilde{g}(k) dk. \quad (\text{C.35})$$

Putting this into Eq. (C.34), you get

$$\begin{aligned} \tilde{h}(k) &= C^2 \int_{x=-\infty}^{\infty} \tilde{C} \int_{k'=-\infty}^{\infty} \exp(ik'x) \tilde{f}(k') dk' \tilde{C} \int_{k''=-\infty}^{\infty} \exp(ik''x) \tilde{g}(k'') dk'' \exp(-ikx) dx \\ &= \frac{1}{4\pi^2} \int_{x=-\infty}^{\infty} \int_{k'=-\infty}^{\infty} \exp(ik'x) \tilde{f}(k') dk' \int_{k''=-\infty}^{\infty} \exp(ik''x) \tilde{g}(k'') dk'' \exp(-ikx) dx \\ &= \frac{1}{4\pi^2} \int_{x=-\infty}^{\infty} \int_{k'=-\infty}^{\infty} \exp(ik'x) \tilde{f}(k') dk' \int_{k''=-\infty}^{\infty} \exp(ik''x) \tilde{g}(k'') dk'' \exp(-ikx) dx \\ &= \frac{1}{4\pi^2} \int_{k'=-\infty}^{\infty} \int_{k''=-\infty}^{\infty} \tilde{f}(k') \tilde{g}(k'') \int_{x=-\infty}^{\infty} \exp(ik'x) \exp(ik''x) \exp(-ikx) dk'' dk' dx \\ &= \frac{1}{4\pi^2} \int_{k'=-\infty}^{\infty} \int_{k''=-\infty}^{\infty} \tilde{f}(k') \tilde{g}(k'') \int_{x=-\infty}^{\infty} \exp[i(k' + k'' - k)x] dk'' dk' dx \\ &\stackrel{\text{Glg. (A.84)}}{=} \frac{1}{4\pi^2} \int_{k'=-\infty}^{\infty} \int_{k''=-\infty}^{\infty} \tilde{f}(k') \tilde{g}(k'') \int_{x=-\infty}^{\infty} 2\pi \delta(k' + k'' - k) dk'' dk' \\ &\stackrel{k''=k-k'}{=} \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k') \tilde{g}(k - k') dk'. \end{aligned} \quad (\text{C.36})$$

The statement

$$\tilde{h}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(k') \tilde{g}(k - k') dk' \quad (\text{C.37})$$

is called the convolution theorem. The special case

$$g = \frac{f}{2} \quad (\text{C.38})$$

corresponds to the kinetic energy. In this case you get

$$\tilde{h}(k) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \tilde{f}(k') \tilde{f}(k - k') dk' \neq \pi \tilde{C}^2 \tilde{f}(-k) \tilde{f}(k). \quad (\text{C.39})$$

Now the question is whether one considers $\tilde{h}(k)$ or $\tilde{f}(-k) \tilde{f}(k)$ as a kinetic energy spectrum, as the Parseval

identity Eq. (C.31) suggests. The latter is chosen because $\tilde{f}(-k)\tilde{f}(k)$ depends exclusively on movements of the wave number k , which is not the case with $\tilde{h}(k)$.

C.2 Legendre polynomials

Eq. (D.50) is called *Legendre'sche differential equation*. This is:

$$\frac{d}{d\mu} (\mathbf{1} - \mu^2) P'(\mu) = -\lambda P \quad (\text{C.40})$$

One starts with $P(\mu)$

$$P(\mu) = \sum_{i=0}^{\infty} U_i \mu^i, \quad (\text{C.41})$$

so that applies

$$P'(\mu) = \sum_{i=0}^{\infty} i U_i \mu^{i-1} = \sum_{i=0}^{\infty} (i+1) U_{i+1} \mu^i, \quad (\text{C.42})$$

$$P''(\mu) = \sum_{i=0}^{\infty} i(i-1) U_i \mu^{i-2} = \sum_{i=0}^{\infty} (i+2)(i+1) U_{i+2} \mu^i. \quad (\text{C.43})$$

If you put this in

$$-2\mu P'(\mu) + (\mathbf{1} - \mu^2) P''(\mu) = -\lambda P(\mu) \quad (\text{C.44})$$

one, you get

$$\begin{aligned} -2 \sum_{i=0}^{\infty} i U_i \mu^i + \sum_{i=0}^{\infty} (i+2)(i+1) U_{i+2} \mu^i - \sum_{i=0}^{\infty} i(i-1) U_i \mu^i &= -\lambda \sum_{i=0}^{\infty} U_i \mu^i \\ \Leftrightarrow -2i U_i + (i+2)(i+1) U_{i+2} - i(i-1) U_i &= -\lambda U_i \\ \Leftrightarrow U_{i+2} &= U_i \frac{i(i+1) - \lambda}{(i+2)(i+1)}. \end{aligned} \quad (\text{C.45})$$

In general, this does not approach zero for $i \rightarrow \infty$, so P would diverge. So there must be a $n \in \mathbb{N}$ with $\lambda = n(n+1)$, this is a condition on λ . Additionally you have to set $U_{n+1} = 0$. $P(\mu)$ is therefore an n -th order polynomial in μ , where n is arbitrary, one writes $P_n(\mu)$ for this Legendre polynomial. About Eq. (C.45) and a normalization is set $P_n(\mu)$. Alternatively, one can write the Legendre polynomials as

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n, \quad (\text{C.46})$$

this is now to be shown. Define

$$\delta_k := \begin{cases} 0, & k \text{ ungerade,} \\ 1, & k \text{ gerade.} \end{cases} \quad (\text{C.47})$$

Now one can use the binomial theorem Eq. Use (A.17) to

$$(x^2 - 1)^n = \sum_{k=0}^n \binom{n}{k} x^{2k} (-1)^{n-k} = \sum_{k=0}^n \delta_k \binom{n}{k/2} x^k (-1)^{n-k/2} \quad (\text{C.48})$$

to note down, so that for the above notation the Legendre polynomials follow Eq. (C.46) with Eq. (A.34)

$$\begin{aligned}
P_n(x) &= \frac{\mathbf{I}}{2^n n!} \sum_{k=0}^n \frac{(k+n)!}{k!} \binom{n}{\frac{k+n}{2}} (-\mathbf{I})^{n-\frac{k+n}{2}} \delta_{k+n} x^k \\
&= \frac{\mathbf{I}}{2^n n!} \sum_{k=0}^n \frac{(n+k)!}{k!} \frac{n!}{\left(\frac{n+k}{2}\right)! \left(n-\frac{n+k}{2}\right)!} (-\mathbf{I})^{n-\frac{k+n}{2}} \delta_{n+k} x^k \\
&= \frac{\mathbf{I}}{2^n} \sum_{k=0}^n \frac{(n+k)!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)! \left(\frac{n-k}{2}\right)!} (-\mathbf{I})^{\frac{n-k}{2}} \delta_{n+k} x^k.
\end{aligned} \tag{C.49}$$

For the first two derivatives of the Legendre polynomials follows

$$\begin{aligned}
P'_n(x) &= \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-1} (k+\mathbf{I}) \frac{(n+k+\mathbf{I})!}{(k+\mathbf{I})!} \frac{\mathbf{I}}{\left(\frac{n+k+\mathbf{I}}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k-1}{2}\right)!} (-\mathbf{I})^{\frac{n-k-1}{2}} \delta_{n+k+\mathbf{I}} x^k \\
&= \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-1} \frac{(n+k+\mathbf{I})!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k+\mathbf{I}}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k-1}{2}\right)!} (-\mathbf{I})^{\frac{n-k-1}{2}} \delta_{n+k+\mathbf{I}} x^k,
\end{aligned} \tag{C.50}$$

$$\begin{aligned}
P''_n(x) &= \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-2} (k+\mathbf{I}) \frac{(n+k+\mathbf{2})!}{(k+\mathbf{I})!} \frac{\mathbf{I}}{\left(\frac{n+k+\mathbf{2}}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k-2}{2}\right)!} (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k+\mathbf{2}} x^k \\
&= \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-2} \frac{(n+k+\mathbf{2})!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k+\mathbf{2}}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k-2}{2}\right)!} (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k} x^k \\
&= \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-2} \frac{(n+k+\mathbf{2})!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n+k}{2}+\mathbf{I}\right)!} \frac{\left(\frac{n-k}{2}\right)}{\left(\frac{n-k}{2}\right)!} (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k} x^k \\
&= \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-2} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k}{2}\right)!} \frac{(n+k+\mathbf{I})!}{k!} (n-k) (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k} x^k.
\end{aligned} \tag{C.51}$$

Now it is shown that the Legendre polynomials according to Eq. (C.46) actually solve the Legendre differential equation (D.50):

$$\begin{aligned}
&-2xP'_n(x) + (1-x^2)P''_n(x) \stackrel{!}{=} -n(n+\mathbf{I})P_n(x) \\
&\Leftrightarrow -2x \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-1} \frac{(n+k+\mathbf{I})!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k+\mathbf{I}}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k-1}{2}\right)!} (-\mathbf{I})^{\frac{n-k-1}{2}} \delta_{n+k+\mathbf{I}} x^k \\
&+ \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-2} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k}{2}\right)!} \frac{(n+k+\mathbf{I})!}{k!} (n-k) (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k} x^k \\
&- \frac{\mathbf{I}}{2^n} \sum_{k=0}^{n-2} \frac{(n+k+\mathbf{2})!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k+\mathbf{2}}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k-2}{2}\right)!} (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k} x^{k+2} \\
&= -n(n+\mathbf{I}) \frac{\mathbf{I}}{2^n} \sum_{k=0}^n \frac{(n+k)!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k}{2}\right)!} (-\mathbf{I})^{\frac{n-k}{2}} \delta_{n+k} x^k \\
&\Leftrightarrow -2 \sum_{k=0}^n k \frac{(n+k)!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k}{2}\right)!} (-\mathbf{I})^{\frac{n-k}{2}} \delta_{n+k} x^k \\
&+ \sum_{k=0}^{n-2} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k}{2}\right)!} \frac{(n+k+\mathbf{I})!}{k!} (n-k) (-\mathbf{I})^{\frac{n-k-2}{2}} \delta_{n+k} x^k \\
&- \sum_{k=0}^n k(k-\mathbf{I}) \frac{(n+k)!}{k!} \frac{\mathbf{I}}{\left(\frac{n+k}{2}\right)!} \frac{\mathbf{I}}{\left(\frac{n-k}{2}\right)!} (-\mathbf{I})^{\frac{n-k}{2}} \delta_{n+k} x^k
\end{aligned}$$

$$\begin{aligned}
&= -n(n+1) \sum_{k=0}^n \frac{(n+k)!}{k!} \frac{1}{\left(\frac{n+k}{2}\right)!} \frac{1}{\left(\frac{n-k}{2}\right)!} (-1)^{\frac{n-k}{2}} \delta_{n+k} x^k \\
&\Leftrightarrow -2 \sum_{k=0}^n k \frac{(n+k)!}{k!} \frac{1}{\left(\frac{n+k}{2}\right)!} \frac{1}{\left(\frac{n-k}{2}\right)!} (-1)^{\frac{n-k}{2}} \delta_{n+k} x^k \\
&\quad - \sum_{k=0}^{n-2} \frac{1}{\left(\frac{n+k}{2}\right)! \left(\frac{n-k}{2}\right)!} \frac{(n+k)!}{k!} (n+k+1)(n-k) (-1)^{\frac{n-k}{2}} \delta_{n+k} x^k \\
&\quad - \sum_{k=0}^n k(k-1) \frac{(n+k)!}{k!} \frac{1}{\left(\frac{n+k}{2}\right)!} \frac{1}{\left(\frac{n-k}{2}\right)!} (-1)^{\frac{n-k}{2}} \delta_{n+k} x^k \\
&= -n(n+1) \sum_{k=0}^n \frac{(n+k)!}{k!} \frac{1}{\left(\frac{n+k}{2}\right)!} \frac{1}{\left(\frac{n-k}{2}\right)!} (-1)^{\frac{n-k}{2}} \delta_{n+k} x^k
\end{aligned} \tag{C.52}$$

The equality of the coefficients of the three polynomials is shown. From $k=0$ to $k=n-2$ this means

$$2k + n^2 - nk + kn - k^2 + n - k + k^2 - k \stackrel{!}{=} n^2 + n, \tag{C.53}$$

which is true. For $k=n-1$ applies

$$\delta_{n+k} = 0, \tag{C.54}$$

and for $k=n$ holds

$$-2n - n(n-1) \stackrel{!}{=} -n(n+1), \tag{C.55}$$

which is also true. Now the normalization of the Legendre polynomials is determined on the set $[-1, 1]$ that is relevant for this problem.

$$\begin{aligned}
\int_{-1}^1 P_n^2(x) dx &= \frac{1}{2^{2n} n!^2} \int_{-1}^1 \frac{d^n}{dx^n} (x^2-1)^n \frac{d^n}{dx^n} (x^2-1)^n dx \\
&\stackrel{n\text{-fache p.I.}}{=} \frac{1}{2^{2n} n!^2} (-1)^n \int_{-1}^1 (x^2-1)^n \frac{d^{2n}}{dx^{2n}} (x^2-1)^n dx \\
&= \frac{1}{2^{2n} n!^2} (-1)^n (2n)! \int_{-1}^1 (x^2-1)^n dx
\end{aligned} \tag{C.56}$$

It still applies

$$\begin{aligned}
\int (x^2-1)^n dx &= \int (x+1)^n (x-1)^n dx \stackrel{n\text{-fache p.I.}}{=} (-1)^n \int \frac{n! (x+1)^{2n}}{(2n)!} n! dx \\
&= (-1)^n \frac{n!^2}{(2n)!} \int (x+1)^{2n} dx = (-1)^n \frac{n!^2}{(2n)!} \left[\frac{(x+1)^{2n+1}}{2n+1} \right],
\end{aligned} \tag{C.57}$$

that follows

$$\int_{-1}^1 P_n^2(x) dx = \frac{1}{2^{2n} n!^2} (-1)^n (2n)! \frac{1}{(2n)!} (-1)^n n!^2 \frac{2^{2n+1}}{2n+1} = \frac{2}{2n+1}. \tag{C.58}$$

Now the orthogonality of the Legendre polynomials is shown, let $n, m \in \mathbb{N}$ with $n \neq m$, then it holds

$$\frac{d}{dx} \left[(1-x^2) \frac{d}{dx} \right] P_n(x) = -n(n+1) P_n(x) \tag{C.59}$$

and analogously for m . You do the math

$$\int_{-1}^1 P_m(x) \frac{d}{dx} \left[(1-x^2) \frac{d}{dx} \right] P_n(x) dx = - \int_{-1}^{(1)} P'_m(x) (1-x^2) P'_n(x) dx \quad (\text{C.60})$$

as well as

$$\int_{-1}^1 P_n(x) \frac{d}{dx} \left[(1-x^2) \frac{d}{dx} \right] P_m(x) dx = - \int_{-1}^1 P'_n(x) (1-x^2) P'_m(x) dx, \quad (\text{C.61})$$

also apply

$$\int_{-1}^1 P_m(x) \frac{d}{dx} \left[(1-x^2) \frac{d}{dx} \right] P_n(x) dx = -n(n+1) \int_{-1}^1 P_m(x) P_n(x) dx, \quad (\text{C.62})$$

$$\int_{-1}^{(1)} P_n(x) \frac{d}{dx} \left[(1-x^2) \frac{d}{dx} \right] P_m(x) dx = -m(m+1) \int_{-1}^1 P_n(x) P_m(x) dx. \quad (\text{C.63})$$

That's it

$$-n(n+1) \int_{-1}^1 P_m(x) P_n(x) dx = -m(m+1) \int_{-1}^{(1)} P_n(x) P_m(x) dx \quad (\text{C.64})$$

and because $n \neq m$

$$\int_{-1}^1 P_n(x) P_m(x) dx = 0. \quad (\text{C.65})$$

That sums it up

$$\int_{-1}^1 P_n(x) P_m(x) dx = \frac{2}{2n+1} \delta_{mn}. \quad (\text{C.66})$$

Now should

$$(2l+1) x P_l(x) = (l+1) P_{l+1}(x) + l P_{l-1}(x) \quad (\text{C.67})$$

be shown. First, it is clear that on the left and right sides of the equal sign there are polynomials of degree $l+1$, each with only even or odd powers. You write

$$P_l(x) = \frac{1}{2^l} \frac{d^l}{dx^l} \sum_{k=0}^l \frac{1}{k! (l-k)!} x^{2k} (-1)^{l-k} = \frac{1}{2^l} \sum_{k=(\frac{l}{2})_+}^l \frac{1}{k! (l-k)!} \frac{(2k)!}{(2k-l)!} x^{2k-l} (-1)^{l-k}, \quad (\text{C.68})$$

where $(\frac{l}{2})_+$ is the smallest natural number $\geq \frac{l}{2}$. Follow from this

$$(\mathfrak{z}l + \mathfrak{I}) x P_l(x) = \frac{\mathfrak{z}l + \mathfrak{I}}{\mathfrak{z}^l} \sum_{k=\left(\frac{l}{\mathfrak{z}}\right)_+}^l \frac{\mathfrak{I}}{k! (l-k)!} \frac{(\mathfrak{z}k)!}{(\mathfrak{z}k-l)!} x^{\mathfrak{z}k-l+\mathfrak{I}} (-\mathfrak{I})^{l-k}, \quad (\text{C.69})$$

$$(l + \mathfrak{I}) P_{l+\mathfrak{I}}(x) = -\frac{\mathfrak{I}}{\mathfrak{z}^l \mathfrak{z}} \sum_{k=\left(\frac{l+\mathfrak{I}}{\mathfrak{z}}\right)_+}^{l+\mathfrak{I}} \frac{l + \mathfrak{I}}{k! (l + \mathfrak{I} - k)!} \frac{(\mathfrak{z}k)!}{(\mathfrak{z}k - l - \mathfrak{I})!} x^{\mathfrak{z}k-l-\mathfrak{I}} (-\mathfrak{I})^{l-k} \quad (\text{C.70})$$

$$= \frac{l + \mathfrak{I}}{\mathfrak{z}^l} \sum_{k=\left(\frac{l-\mathfrak{I}}{\mathfrak{z}}\right)_+}^l \frac{(\mathfrak{z}k + \mathfrak{I})}{k! (l-k)!} \frac{(\mathfrak{z}k)!}{(\mathfrak{z}k - l + \mathfrak{I})!} x^{\mathfrak{z}k-l+\mathfrak{I}} (-\mathfrak{I})^{l-k} \quad (\text{C.71})$$

$$P_{l-\mathfrak{I}}(x) = -\frac{\mathfrak{z}l}{\mathfrak{z}^l} \sum_{k=\left(\frac{l-\mathfrak{I}}{\mathfrak{z}}\right)_+}^{l-\mathfrak{I}} \frac{\mathfrak{I}}{k! (l - \mathfrak{I} - k)!} \frac{(\mathfrak{z}k)!}{(\mathfrak{z}k - l + \mathfrak{I})!} x^{\mathfrak{z}k-l+\mathfrak{I}} (-\mathfrak{I})^{l-k}. \quad (\text{C.72})$$

Two polynomials are equal if and only if all their coefficients are equal.

$$\begin{aligned} \mathfrak{z}kl - \mathfrak{z}l^2 + l + \mathfrak{z}k + \mathfrak{I} &= \mathfrak{z}kl + l + \mathfrak{z}k + \mathfrak{I} - \mathfrak{z}l^2 \\ \Leftrightarrow (\mathfrak{z}l + \mathfrak{I})(\mathfrak{z}k - l + \mathfrak{I}) &= (l + \mathfrak{I})(\mathfrak{z}k + \mathfrak{I}) - (l - k)\mathfrak{z}l \end{aligned} \quad (\text{C.73})$$

$$\begin{aligned} \Leftrightarrow \frac{\mathfrak{z}l + \mathfrak{I}}{l - k} \frac{\mathfrak{z}k - l + \mathfrak{I}}{\mathfrak{z}k - l + \mathfrak{I}} &= \frac{l + \mathfrak{I}}{l - k} \frac{\mathfrak{z}k + \mathfrak{I}}{\mathfrak{z}k - l + \mathfrak{I}} - \frac{l - k}{l - k} \frac{\mathfrak{z}l}{\mathfrak{z}k - l + \mathfrak{I}} \\ \Leftrightarrow \frac{\mathfrak{z}l + \mathfrak{I}}{l - k} &= \frac{l + \mathfrak{I}}{l - k} \frac{\mathfrak{z}k + \mathfrak{I}}{\mathfrak{z}k - l + \mathfrak{I}} - \frac{\mathfrak{z}l}{\mathfrak{z}k - l + \mathfrak{I}} \end{aligned} \quad (\text{C.74})$$

Now the lower and upper limits of the sums have to be examined. For $k = l$ one obtains

$$\mathfrak{z}l + \mathfrak{I} = (l + \mathfrak{I}) \frac{\mathfrak{z}l + \mathfrak{I}}{\mathfrak{z}l - l + \mathfrak{I}}. \quad (\text{C.75})$$

When it comes to the lower limit, a distinction must be made between cases. If l is even, everything is shown. For l odd one calculates

$$(l + \mathfrak{I}) \frac{l}{l - \frac{l-\mathfrak{I}}{\mathfrak{z}}} - \mathfrak{z}l = \mathfrak{o}. \quad (\text{C.76})$$

For $l = \mathfrak{o}$ the statement also applies. This means that Eq. (C.67) shown. From this equation it follows

$$\cos(\theta) P_l(\cos(\theta)) = \frac{l + \mathfrak{I}}{\mathfrak{z}l + \mathfrak{I}} P_{l+\mathfrak{I}}(\cos(\theta)) + \frac{l}{\mathfrak{z}l + \mathfrak{I}} P_{l-\mathfrak{I}}(\cos(\theta)). \quad (\text{C.77})$$

Now the solution to Eq. (D.48) for $m \neq \mathfrak{o}$ will be discussed. This DGL was:

$$\frac{d}{d\mu} (\mathfrak{I} - \mu^2) P'(\mu) = P\left(-\mathfrak{z} + \frac{m^2}{\mathfrak{I} - \mu^2}\right). \quad (\text{C.78})$$

With the approach

$$P(\mu) = (\mathfrak{I} - \mu^2)^{m/2} T(\mu) \quad (\text{C.79})$$

you get

$$P'(\mu) = -\mu m (\mathfrak{I} - \mu^2)^{m/2-\mathfrak{I}} T(\mu) + (\mathfrak{I} - \mu^2)^{m/2} T'(\mu), \quad (\text{C.80})$$

$$(\mathfrak{I} - \mu^2) P'(\mu) = -\mu m (\mathfrak{I} - \mu^2)^{m/2} T(\mu) + (\mathfrak{I} - \mu^2)^{m/2+\mathfrak{I}} T'(\mu). \quad (\text{C.81})$$

Putting this into Eq. (C.78), you get

$$\begin{aligned}
& -m(1-\mu^2)^{m/2} T(\mu) + \mu^2 m^2 (1-\mu^2)^{m/2-1} T(\mu) - 2\mu(m+1)(1-\mu^2)^{m/2} T'(\mu) \\
& + (1-\mu^2)^{m/2+1} T''(\mu) = -\lambda(1-\mu^2)^{m/2} T(\mu) + m^2(1-\mu^2)^{m/2-1} T(\mu) \\
& \Leftrightarrow -mT(\mu) + \mu^2 m^2 (1-\mu^2)^{-1} T(\mu) - 2\mu(m+1) T'(\mu) + (1-\mu^2) T''(\mu) \\
& = -\lambda T(\mu) + m^2 (1-\mu^2)^{-1} T(\mu) \\
& \Leftrightarrow (1-\mu^2) T''(\mu) - 2\mu(m+1) T'(\mu) = \left(-\lambda + m + m^2 \frac{1-\mu^2}{1-\mu^2} \right) T(\mu) \\
& \Leftrightarrow (1-\mu^2) T''(\mu) - 2\mu(m+1) T'(\mu) = (-\lambda + m(m+1)) T(\mu). \tag{C.82}
\end{aligned}$$

It will be a power series approach again

$$T(\mu) = \sum_{i=0}^{\infty} a_i \mu^i \tag{C.83}$$

made. You need the following notations for the first two derivatives:

$$T'(\mu) = \sum_{i=1}^{\infty} i a_i \mu^{i-1} \tag{C.84}$$

$$T''(\mu) = \sum_{i=0}^{\infty} (i+2)(i+1) a_{i+2} \mu^i \tag{C.85}$$

$$T''(\mu) = \sum_{i=2}^{\infty} i(i-1) a_i \mu^{i-2} \tag{C.86}$$

Putting this into Eq. (C.82), you get a recursion formula again:

$$\begin{aligned}
& (i+2)(i+1) a_{i+2} - i(i-1) a_i - 2(m+1) i a_i = (-\lambda + m(m+1)) a_i \\
& \Leftrightarrow a_{i+2} = a_i \frac{-\lambda + (m+2i)(m+1) + i(i-1)}{(i+2)(i+1)} = a_i \frac{-\lambda + (i+m+1)(i+m)}{(i+2)(i+1)} \tag{C.87}
\end{aligned}$$

Since this doesn't approach zero for high i , this has to stop somewhere. So there must be a $I \in \mathbb{N}$ with

$$\lambda = (I+m+1)(I+m). \tag{C.88}$$

As a product of two integers, λ is also an integer, and λ is not negative because the two factors cannot have different signs. So there is a $l \in \mathbb{N}$ with

$$\lambda = l(l+1). \tag{C.89}$$

That's it

$$l = I + m. \tag{C.90}$$

Since $l, I \geq 0$, $m \leq l$. Since $m < -l$ leads to the same DGL as $-m > l$ and there are no solutions for this, there are no solutions for $m < -l$ either. So you have

$$\lambda = l(l+1), \quad l = 0, 1, 2, 3, \dots, \quad m = 0, \pm 1, \pm 2, \pm 3, \dots, \pm l. \tag{C.91}$$

By comparing with Eq. (C.79) you can see that $m+I=l$ is also the degree of $P(\mu)$. The solutions $T = T_{l,m}$ are therefore determined by two natural numbers l, m .

Now we want to derive a closed form for the $T_{l,m}$. The $T_{l,m}$ satisfy the DGL

$$\frac{d}{d\mu} (1-\mu^2) T'_{l,m}(\mu) = 2\mu m T'_{l,m}(\mu) + (m(m+1) - \lambda) T_{l,m}(\mu). \tag{C.92}$$

For $m = 0$ the solutions are the well-known Legendre polynomials $P_l(\mu)$ Eq. (C.46). If the solution $T_{l,m}(\mu)$ is known and $m < l$, then the solution follows $T_{l,m+1}(\mu)$

$$T_{l,m+1}(\mu) = \frac{d}{d\mu} T_{l,m}(\mu). \quad (\text{C.93})$$

To show this, one first derives Eq. (C.92) from:

$$\begin{aligned} -2T'_{l,m}(\mu) - 4\mu T''_{l,m}(\mu) + (1-\mu^2) T'''_{l,m}(\mu) &= 2mT'_{l,m}(\mu) + 2\mu m T''_{l,m}(\mu) + (m(m+1) - l) T'_{l,m}(\mu) \\ \Leftrightarrow -2\mu T''_{l,m}(\mu) + (1-\mu^2) T'''_{l,m}(\mu) \\ &= 2(1+m) T'_{l,m}(\mu) + (m(m+1) - l) T'_{l,m}(\mu) + 2\mu(1+m) T''_{l,m}(\mu) \end{aligned} \quad (\text{C.94})$$

Substituting $T_{l,m+1} = T'_{l,m}$, it follows

$$\begin{aligned} \frac{d}{d\mu} (1-\mu^2) T'_{l,m+1}(\mu) &= \frac{d}{d\mu} (1-\mu^2) \frac{d}{d\mu} T'_{l,m}(\mu) \\ &= -2\mu T''_{l,m}(\mu) + (1-\mu^2) T'''_{l,m}(\mu) = 2(1+m) T'_{l,m}(\mu) + (m(m+1) - l) T'_{l,m}(\mu) + 2\mu(1+m) T''_{l,m}(\mu) \\ &= 2\mu(m+1) T'_{l,m+1}(\mu) + ((m+1)(m+2) - l) T_{l,m+1}(\mu). \end{aligned} \quad (\text{C.95})$$

The solution $T_{l,m}(\mu)$ is therefore the m th derivative of the l th Legendre polynomial

$$T_{l,m}(\mu) = \frac{d^m}{d\mu^m} P_l(\mu). \quad (\text{C.96})$$

The complete solutions $P_{l,m}$ of Eq. (C.78) are called *associated Legendre function*:

$$P_{l,m}(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) = \frac{(-1)^m}{2^l l!} (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2-1)^l. \quad (\text{C.97})$$

These are no longer polynomials for odd m and reduce to the Legendre polynomials Eq. for $m = 0$. (C.46). It applies

$$\begin{aligned} \frac{d}{dx} P_{l,m}(x) &= -mx(-1)^m (1-x^2)^{\frac{m-2}{2}} \frac{d^m}{dx^m} P_l(x) + (-1)^m (1-x^2)^{m/2} \frac{d^{m+1}}{dx^{m+1}} P_l(x) \\ &= -\frac{mx}{1-x^2} P_{l,m}(x) - \frac{1}{\sqrt{1-x^2}} P_{l,m+1}(x). \end{aligned} \quad (\text{C.98})$$

From Eq. (C.118) follows

$$\begin{aligned} \frac{d^n}{dx^n} (xf(x)) &= xf^{(n)} + nf^{(n-1)} \\ \Leftrightarrow xf^{(n)} &= \frac{d^n}{dx^n} (xf(x)) - nf^{(n-1)}. \end{aligned} \quad (\text{C.99})$$

Furthermore, with Eq. (C.77)

$$P_l = \frac{2l+3}{l+1} x P_{l+1} - \frac{l+2}{l+1} P_{l+2}. \quad (\text{C.100})$$

Thus you get

$$\begin{aligned}
 P_{l,m}(x) &= (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) = \frac{(-1)^m}{l+1} (1-x^2)^{m/2} \frac{d^m}{dx^m} [(2l+3)xP_{l+1}(x) - (l+2)P_{l+2}(x)], \\
 &= x \frac{(-1)^m (2l+3)}{l+1} (1-x^2)^{m/2} \frac{d^m}{dx^m} P_{l+1}(x) + m \frac{(-1)^m (2l+3)}{l+1} (1-x^2)^{m/2} \frac{d^{m-1}}{dx^{m-1}} P_{l+1}(x) \\
 &\quad - \frac{(-1)^m (l+2)}{l+1} (1-x^2)^{m/2} \frac{d^m}{dx^m} P_{l+2}(x) \\
 &= \frac{2l+3}{l+1} x P_{l+1,m} - m \frac{2l+3}{l+1} \sqrt{1-x^2} P_{l+1,m-1} - \frac{l+2}{l+1} P_{l+2,m} \\
 \Rightarrow x P_{l+1,m} &= \frac{l+1}{2l+3} P_{l,m} + m \sqrt{1-x^2} P_{l+1,m-1} + \frac{l+2}{2l+3} P_{l+2,m} \\
 \Rightarrow x P_{l,m} &= \frac{l}{2l+1} P_{l-1,m} + m \sqrt{1-x^2} P_{l,m-1} + \frac{l+1}{2l+1} P_{l+1,m}.
 \end{aligned} \tag{C.101}$$

It applies

$$P_{l,m-1}(x) = (-1)^{m-1} \frac{1}{2^l l!} (1-x^2)^{\frac{m-1}{2}} \frac{d^{l+m-1}}{dx^{l+m-1}} (x^2-1)^l. \tag{C.102}$$

Furthermore is

$$\begin{aligned}
 \frac{d^{l+m+1}}{dx^{l+m+1}} (x^2-1)^{l+1} &= \frac{d^{l+m}}{dx^{l+m}} 2(l+1)x(x^2-1)^l \\
 &= \frac{d^{l+m-1}}{dx^{l+m-1}} \left[2(l+1)(x^2-1)^l + 4x^2 l(l+1)(x^2-1)^{l-1} \right] \\
 &= \frac{d^{l+m-1}}{dx^{l+m-1}} \left[2(l+1)(x^2-1)^l + 4l(l+1)(x^2-1)^l + 4l(l+1)(x^2-1)^{l-1} \right] \\
 &= 2(1+2l)(l+1) \frac{d^{l+m-1}}{dx^{l+m-1}} \left[(x^2-1)^l + 4l(l+1)(x^2-1)^{l-1} \right].
 \end{aligned} \tag{C.103}$$

So it applies

$$\frac{d^{l+m-1}}{dx^{l+m-1}} (x^2-1)^l = \frac{1}{2(1+2l)(l+1)} \frac{d^{l+m+1}}{dx^{l+m+1}} (x^2-1)^{l+1} - \frac{2l}{(2l+1)} \frac{d^{l+m-1}}{dx^{l+m-1}} (x^2-1)^{l-1}. \tag{C.104}$$

This follows

$$\begin{aligned}
 (-1)^{m-1} \frac{1}{2^l l!} (1-x^2)^{\frac{m-1}{2}} \frac{d^{l+m-1}}{dx^{l+m-1}} (x^2-1)^l &= (-1)^{m-1} \frac{1}{2^{l+1}(l+1)!} (1-x^2)^{\frac{m-1}{2}} \frac{1}{(1+2l)} \frac{d^{l+m+1}}{dx^{l+m+1}} (x^2-1)^{l+1} \\
 - \frac{1}{2l+1} (-1)^{m-1} \frac{1}{2^{l-1}(l-1)!} (1-x^2)^{\frac{m-1}{2}} \frac{d^{l+m-1}}{dx^{l+m-1}} (x^2-1)^{l-1}.
 \end{aligned} \tag{C.105}$$

Thus you get

$$\sqrt{1-x^2} P_{l,m-1} = -\frac{1}{2l+1} P_{l+1,m} + \frac{1}{2l+1} P_{l-1,m}. \tag{C.106}$$

It follows

$$x P_{l,m} = \frac{l+m}{2l+1} P_{l-1,m} + \frac{l+1-m}{2l+1} P_{l+1,m}. \tag{C.107}$$

Herewith and with Eq. (C.101) follows

$$\begin{aligned}
\frac{l+m}{2l+1}P_{l-1,m} + \frac{l+1-m}{2l+1}P_{l+1,m} &= \frac{l}{2l+1}P_{l-1,m} + m\sqrt{1-x^2}P_{l,m-1} + \frac{l+1}{2l+1}P_{l+1,m} \\
&\Rightarrow \sqrt{1-x^2}P_{l,m-1} = \frac{1}{2l+1}P_{l-1,m} - \frac{1}{2l+1}P_{l+1,m} \\
&\Rightarrow \sqrt{1-x^2}P_{l,m} = \frac{1}{2l+1}P_{l-1,m+1} - \frac{1}{2l+1}P_{l+1,m+1}.
\end{aligned} \tag{C.108}$$

The normalization of the Legendre functions results in:

$$\begin{aligned}
\int_{-1}^1 P_{l,m}(x)^2 dx &= \frac{1}{2^l l!^2} \int_{-1}^{(1)} (1-x^2)^m \frac{d^{l+m}}{dx^{l+m}} (1-x^2)^l \frac{d^{l+m}}{dx^{l+m}} (1-x^2)^l dx \\
&\stackrel{m+l-\text{fache p.I.}}{=} \frac{1}{2^l l!^2} (-1)^{m+l} (-1)^{m+l} (m+l)! \frac{(2l)!}{(l-m)!} \int_{-1}^1 (1-x^2)^l dx \\
&= \frac{1}{2^l l!^2} \frac{(m+l)!}{(l-m)!} (2l)! \int_{-1}^1 (1+x)^l (1-x)^l dx \\
&\stackrel{l-\text{fache p.I.}}{=} \frac{1}{2^l l!^2} \frac{(m+l)!}{(l-m)!} (2l)! \frac{l!}{(2l)!} l! \int_{-1}^1 (1+x)^{2l} dx \\
&= \frac{1}{2^l} \frac{(m+l)!}{(l-m)!} \frac{2^{2l+1}}{2l+1} = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!}.
\end{aligned} \tag{C.109}$$

Furthermore, for $l \neq l'$ (otherwise one can assume $l < l'$):

$$\int_{-1}^1 P_{l,m}(x) P_{l',m}(x) dx \propto \int_{-1}^1 (1-x^2)^m \frac{d^{l+m}}{dx^{l+m}} (1-x^2)^l \frac{d^{l'+m}}{dx^{l'+m}} (1-x^2)^{l'} dx. \tag{C.110}$$

This is obtained by $m+l$ -fold partial integration, in which $(1-x^2)^m \frac{d^{l+m}}{dx^{l+m}}$ is derived and $\frac{d^{l'+m}}{dx^{l'+m}} (1-x^2)^{l'}$ is integrated

$$\int_{-1}^1 P_{l,m}(x) P_{l',m}(x) dx \propto \int_{-1}^1 \frac{d^{l'-l}}{dx^{l'-l}} (1-x^2)^{l'} dx = 0. \tag{C.111}$$

The term without an integral is omitted for each integration step, since it is evaluated at the edges ± 1 and terms $\propto (1-x^2)$ always appear there as factors. So it applies

$$\int_{-1}^1 P_{l,m}(x) P_{l',m}(x) dx = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{l,l'}. \tag{C.112}$$

C.3 Hermite polynomials

The *Hermite polynomials* are defined by their Rodrigues formula

$$H_n(x) := (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{C.113}$$

If you put in Eq. (4.69) $\tilde{E} - 1 = 2n$, you get the *Hermite's differential equation*

$$P_n'' - 2xP_n' + 2nP_n = 0. \tag{C.114}$$

Now we want to show that the Hermite polynomials according to Eq. (C.113) solve this DGL and thus also the recursion formula Eq. (4.77). Yes, they apply

$$\frac{dH_n}{dx}(x) = (-)^n e^{x^2} \left[2x \frac{d^n}{dx^n} e^{-x^2} + \frac{d^{n+1}}{dx^{n+1}} e^{-x^2} \right], \quad (\text{C.115})$$

$$\frac{d^2 H_n}{dx^2}(x) = (-)^n e^{x^2} \left[4x^2 \frac{d^n}{dx^n} e^{-x^2} + 4x \frac{d^{n+1}}{dx^{n+1}} e^{-x^2} + \frac{d^{n+2}}{dx^{n+2}} e^{-x^2} + 2 \frac{d^n}{dx^n} e^{-x^2} \right]. \quad (\text{C.116})$$

Plugging all of this into the left side of Hermite's DGL, you get

$$\begin{aligned} \left(\frac{d^n}{dx^n} e^{-x^2} \right) [2 + 2n] + \left(\frac{d^{n+1}}{dx^{n+1}} e^{-x^2} \right) [-2x + 4x] + \left(\frac{d^{n+2}}{dx^{n+2}} e^{-x^2} \right) &= 0 \\ \Leftrightarrow \left[2(1 + n) \frac{d^n}{dx^n} + 2x \frac{d^{n+1}}{dx^{n+1}} + \frac{d^{n+2}}{dx^{n+2}} \right] \exp(-x^2) &= 0. \end{aligned} \quad (\text{C.117})$$

This is true for $n = 0$. By differentiating the equation in terms of x one obtains the same statement for $n + 1$. The Hermite polynomials thus solve the Hermite differential equation, you can set $P_n(x) = H_n(x)$. Furthermore, it is clear that this applies

$$\begin{aligned} \frac{d^n}{dx^n} (f(x)g(x)) &= \frac{d^{n-1}}{dx^{n-1}} [f'g + fg'] = \frac{d^{n-2}}{dx^{n-2}} [f''g + 2f'g' + fg''] \\ &= \sum_{k=0}^n \binom{n}{k} f^{(k)} g^{(n-k)} \end{aligned} \quad (\text{C.118})$$

for $n \in \mathbb{N}$ and $f, g : \mathbb{R} \rightarrow \mathbb{R}$, n -fold differentiable. This can be shown formally via complete induction. For $n = 0$ the statement is correct. The statement applies to an $n \in \mathbb{N}$. Then applies

$$\begin{aligned} \frac{d^{n+1}}{dx^{n+1}} (fg) &= \frac{d}{dx} \left(\frac{d^n}{dx^n} (fg) \right) = \frac{d}{dx} \sum_{k=0}^n \binom{n}{k} f^{(k)} g^{(n-k)} \\ &= \sum_{k=0}^n \binom{n}{k} \left[f^{(k+1)} g^{(n-k)} + f^{(k)} g^{(n+1-k)} \right], \end{aligned} \quad (\text{C.119})$$

the rest follows analogous to the proof of the binomial theorem Eq. (A.17). This can be used to

$$\begin{aligned} H'_n(x) &= 2x (-)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} + (-)^n e^{x^2} \frac{d^{n+1}}{dx^{n+1}} e^{-x^2} \\ &= 2x (-)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} + (-)^n e^{x^2} \frac{d^n}{dx^n} (-2xe^{-x^2}) \end{aligned} \quad (\text{C.120})$$

to simplify. In the second summand, put in terms of Eq. (C.118) $f = -2x$ and $g = e^{-x^2}$, then only the terms with $k = 0$ and $k = 1$ play a role in the sum, so

$$\frac{d^n}{dx^n} (-2xe^{-x^2}) = -2x \frac{d^n}{dx^n} e^{-x^2} - 2n \frac{d^{n-1}}{dx^{n-1}} e^{-x^2}. \quad (\text{C.121})$$

It therefore applies

$$H'_n(x) = 2nH_{n-1}(x). \quad (\text{C.122})$$

It is immediately clear that this applies

$$H'_n = 2xH_n - H_{n+1} \Leftrightarrow nH_{n-1} + \frac{H_{n+1}}{2} = xH_n. \quad (\text{C.123})$$

The coefficient C_n before the highest power is $C_n = 2^n$, as can be easily seen. The following applies to the normalization of Hermite polynomials

$$\int_{-\infty}^{\infty} H_n^2(x) e^{-x^2} dx = \sqrt{\pi} 2^n n!. \quad (\text{C.124})$$

To show this, first make it clear that:

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 0, \quad (\text{C.125})$$

for $n \neq m$, since in this case $H_n(x) \exp(-\frac{x^2}{2})$ and $H_m(x) \exp(-\frac{x^2}{2})$ are two eigenfunctions of a Hermitian operator with different eigenvalues, and therefore orthogonal.

Now one can show the statement about complete induction. For $n = 0$, $H_n = 1$, so

$$\int_{-\infty}^{\infty} H_0^2(x) e^{-x^2} dx = \sqrt{\pi}. \quad (\text{C.126})$$

For $n = 1$, $H_1(x) = -2x$, so holds

$$\int_{-\infty}^{\infty} H_1^2 e^{-x^2} dx = 4 \int_{-\infty}^{\infty} x^2 e^{-x^2} dx = 2 \int_{-\infty}^{\infty} e^{-x^2} dx = 2\sqrt{\pi}. \quad (\text{C.127})$$

So for $n = 0$ and $n = 1$ the statement is true. Now the statement already applies to an n and also to $n - 1$. Then the equations (C.122) and (C.123) also follow

$$\begin{aligned} \int_{-\infty}^{\infty} H_{n+1}^2 e^{-x^2} dx &= 4 \int_{-\infty}^{\infty} [x^2 H_n^2 + n^2 H_{n-1}^2 - 2xn H_{n-1} H_n] e^{-x^2} dx \\ &= 4n^2 \sqrt{\pi} 2^{n-1} (n-1)! + 4 \int_{-\infty}^{\infty} x^2 H_n^2 e^{-x^2} dx - 4n \int_{-\infty}^{\infty} [H'_{n-1} H_n + H_{n-1} H'_n] e^{-x^2} dx \\ &= 2n \sqrt{\pi} 2^n n! + 2 \int_{-\infty}^{\infty} [2x H'_n H_n + H_n^2] e^{-x^2} dx - 8n^2 \sqrt{\pi} 2^{n-1} (n-1)! \\ &= (2n - 4n) \sqrt{\pi} 2^n n! + 2 \int_{-\infty}^{\infty} H_n^2 e^{-x^2} dx + 2\sqrt{\pi} 2^n n! \\ &= \sqrt{\pi} 2^n n! (2n) + 2\sqrt{\pi} 2^n n! = \sqrt{\pi} 2^{n+1} (n+1)!. \end{aligned} \quad (\text{C.128})$$

So the statement also applies to $n + 1$ and therefore to all $n \in \mathbb{N}$.

C.4 Laguerre polynomials

Laguerre's differential equation is:

$$xP'' + (k + 1 - x)P' + nP = 0 \quad (\text{C.129})$$

for $k \in \mathbb{N}$. A power series approach is made for $P(x)$,

$$P(x) = \sum_{i=0}^{\infty} a_i x^i. \quad (\text{C.130})$$

Follow with that

$$P'(x) = \sum_{i=0}^{\infty} i a_i x^{i-1} = \sum_{i=0}^{\infty} (i+1) a_{i+1} x^i, \quad (\text{C.131})$$

$$P''(x) = \sum_{i=0}^{\infty} i(i+1) a_{i+1} x^{i-1}. \quad (\text{C.132})$$

If you put this in, you get

$$i(i+1)a_{i+1} + (k+1)(i+1)a_{i+1} - ia_i + na_i = 0 \Leftrightarrow a_{i+1} = a_i \frac{i-n}{(i+1)(i+k+1)}. \quad (\text{C.133})$$

The factor $\frac{i-n}{(i+1)(i+k+1)}$ approaches zero for high i like $1/i$, the recursion must therefore terminate. So $n \in \mathbb{N}$ must be. n is the degree of the polynomial P . The polynomials

$$L_{n,k}(x) := \sum_{i=0}^n \binom{n+k}{n-i} \frac{(-)^{(i)}}{i!} x^{(i)}. \quad (\text{C.134})$$

solve Eq. (C.129) also, to show this, check their recurrence relation. First, they are polynomials of degree n . The coefficient before the highest power of x is $\frac{(-)^n}{n!}$, this implies normalization. It applies

$$\begin{aligned} a_i &= \frac{(n+k)!}{(n-i)!(k+i)!i!} (-)^{(i)} \\ \Leftrightarrow \frac{a_{i+1}}{a_i} &= -\frac{(n-i)!(k+i)!i!}{(n-i-1)!(k+i+1)!(i+1)!} = \frac{i-n}{(k+1+i)(i+1)}. \end{aligned} \quad (\text{C.135})$$

Therefore, one can use Eq. View (C.134) as the definition of the Laguerre polynomials. You can do all of this

$$n \rightarrow n_r, \quad k \rightarrow 2l+1 \quad (\text{C.136})$$

rewrite to

$$L_{n_r, 2l+1}(x) := \sum_{i=0}^{n_r} \binom{n_r+2l+1}{n_r-i} \frac{(-)^{(i)}}{i!} x^{(i)} \quad (\text{C.137})$$

and

$$xL''_{n_r, 2l+1} + (2l+2-x)L'_{n_r, 2l+1} + n_r L_{n_r, 2l+1} = 0. \quad (\text{C.138})$$

This is the formulation used in Section 4.8. The Rodrigues formula of Laguerre polynomials is

$$P_{n,k}(x) = \frac{e^x}{n!x^k} \frac{d^n}{dx^n} [e^{-x}x^{n+k}]. \quad (\text{C.139})$$

You can immediately see that these are polynomials of degree n . The coefficient in front of x^n is $\frac{(-)^n}{n!}$. For $l \in \mathbb{N}$ with $l \leq n$ holds

$$\frac{d^l}{dx^l} x^{n+k} = \frac{(n+k)!}{(n+k-l)!} x^{n+k-l} \quad (\text{C.140})$$

It follows

$$\frac{d^n}{dx^n} [e^{-x}x^{n+k}] = \sum_{i=0}^n (-)^i e^{-x} \binom{n}{i} \frac{(n+k)!}{(k+i)!} x^{k+i} = \sum_{i=0}^n (-)^i e^{-x} \frac{n!}{i!(n-i)!} \frac{(n+k)!}{(k+i)!} x^{k+i}. \quad (\text{C.141})$$

This gives you

$$P_{n,k}(x) = \sum_{i=0}^n (-)^i \frac{1}{i!(n-i)!} \frac{(n+k)!}{(k+i)!} x^i = \sum_{i=0}^n \binom{n+k}{n-i} \frac{(-)^{(i)}}{i!} x^{(i)}. \quad (\text{C.142})$$

The Rodrigues formula therefore corresponds to the explicit representation Eq. (C.134). The Laguerre polynomials satisfy the integral property

$$\int_0^\infty x^{k+1} e^{-x} L_{n,k}(x)^2 dx = \frac{(n+k)!}{n!} (2n+k+1). \quad (\text{C.143})$$

This is what you count on

$$\begin{aligned} \int_0^\infty x^{k+1} e^{-x} L_{n,k}(x)^2 dx &= \int_0^\infty x^{k+1} e^{-x} L_{n,k}(x) \frac{e^x}{n! x^k} \frac{d^n}{dx^n} [e^{-x} x^{n+k}] dx \\ &= \frac{1}{n!} \int_0^\infty x L_{n,k}(x) \frac{d^n}{dx^n} [e^{-x} x^{n+k}] dx = \frac{1}{n!} (-1)^n \int_0^\infty e^{-x} x^{n+k} \frac{d^n}{dx^n} x L_{n,k}(x) dx. \end{aligned} \quad (\text{C.144})$$

According to the explicit representation Eq. (C.134) applies

$$\begin{aligned} \frac{d^n}{dx^n} x L_{n,k}(x) &= (-1)^n (n+1) x + n! \frac{(-1)^{n-1}}{(n-1)!} \frac{(n+k)!}{(n+k-1)!} \\ &= (-1)^n (n+1) x + n (-1)^{n-1} (n+k). \end{aligned} \quad (\text{C.145})$$

With Eq. (A.96) follows

$$\begin{aligned} \int_0^\infty \dots dx &= \frac{(-1)^n}{n!} [(-1)^n (n+1) (n+k+1)! - n (-1)^n (n+k) (n+k)!] \\ &= \frac{(n+k)!}{n!} [(n+1) (n+k+1) - n (n+k)] = \frac{(n+k)!}{n!} (2n+k+1). \end{aligned} \quad (\text{C.146})$$

Furthermore, $k \geq 2$ applies

$$\int_0^\infty x^{k-2} [L_{n,k}(x)]^2 \exp(-x) dx = \frac{(n+k)!}{n!} \frac{2n+k+1}{(k-1)k(k+1)}. \quad (\text{C.147})$$

This is taken into account

$$\begin{aligned} \int_0^\infty x^{k-2} e^{-x} L_{n,k}(x)^2 dx &= \int_0^\infty x^{k-2} e^{-x} L_{n,k}(x) \frac{e^x}{n! x^k} \frac{d^n}{dx^n} [e^{-x} x^{n+k}] dx \\ &= \frac{1}{n!} \int_0^\infty \frac{1}{x^2} L_{n,k}(x) \frac{d^n}{dx^n} [e^{-x} x^{n+k}] dx = \frac{1}{n!} (-1)^n \int_0^\infty e^{-x} x^{n+k} \frac{d^n}{dx^n} \left[\frac{1}{x^2} L_{n,k}(x) \right] dx. \end{aligned} \quad (\text{C.148})$$

$L_{n,k}$ ist ein Polynom vom Grad n , also ist $L_{n,k}/x^2$ vom Grad $n-2$. Schreibe

$$L_{n,k} = a + bx + \mathcal{O}(x^2), \quad (\text{C.149})$$

applies accordingly

$$\frac{d}{dx^n} \frac{L_{n,k}}{x^2} = \frac{d}{dx^n} \left(\frac{a}{x^2} + \frac{b}{x} \right) = (-1)^n (a(n+1)! x^{-2-n} + n! b x^{-n-1}). \quad (\text{C.150})$$

According to the explicit representation Eq. (C.134) apply

$$a = \frac{(n+k)!}{n!k!}, \quad b = -\frac{(n+k)!}{(n-1)!(k+1)!}. \quad (\text{C.151})$$

Thus follows

$$\begin{aligned} \frac{d}{dx^n} \frac{L_{n,k}}{x^2} &= (-1)^n \left(\frac{(n+k)!}{n!k!} (n+1)! x^{-2-n} - \frac{(n+k)!}{(n-1)!(k+1)!} n! x^{-n-1} \right) \\ &= (-1)^n (n+k)! \left[\frac{(n+1)}{k!} x^{-2-n} - \frac{n}{(k+1)!} x^{-n-1} \right]. \end{aligned} \quad (\text{C.152})$$

This gives you

$$e^{-x} x^{n+k} \frac{d}{dx^n} \frac{L_{n,k}}{x^2} = e^{-x} (-)^n (n+k)! \left[\frac{(n+1)}{k!} x^{k-2} - \frac{n}{(k+1)!} x^{k-1} \right]. \quad (\text{C.153})$$

With Eq. (A.96) follows

$$\begin{aligned} \int_0^\infty \dots dx &= \frac{(n+k)!}{n!} \left[\frac{(n+1)}{k(k-1)} - \frac{n}{k(k+1)} \right] \\ &= \frac{(n+k)!}{n!} \left[\frac{(n+1)(k+1)}{k(k-1)(k+1)} - \frac{n(k-1)}{k(k+1)(k-1)} \right] \\ &= \frac{(n+k)!}{n!} \frac{2n+k+1}{k(k+1)(k-1)}. \end{aligned} \quad (\text{C.154})$$

C.5 Spherical surface functions

The dependencies of the solution Eq. (D.42) of $\cos(\theta)$ and φ are combined to $P_{l,m}(\cos(\theta)) \exp(im\varphi)$. The *spherical harmonics* are defined by

$$Y_{l,m}(\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l,m}(\cos(\theta)) \exp(im\varphi). \quad (\text{C.155})$$

with the associated Legendre functions $P_{l,m}(x)$, Eq. (C.97). The preliminary factors result from the normalization

$$\int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} |Y_{l,m}(\theta, \varphi)|^2 \sin(\theta) d\varphi d\theta \stackrel{!}{=} 1, \quad (\text{C.156})$$

which is now verified:

$$\begin{aligned} &\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} (P_{l,m}(\cos(\theta)))^2 \sin(\theta) d\varphi d\theta \\ &= \frac{2l+1}{2} \frac{(l-m)!}{(l+m)!} \int_{-1}^1 P_{l,m}(z)^2 dz = 1 \end{aligned} \quad (\text{C.157})$$

Furthermore, the spherical surface functions are orthogonal. For $m \neq m'$ holds:

$$\begin{aligned} &\int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} Y_{l,m}(\theta, \varphi)^* Y_{l',m'}(\theta, \varphi) \sin(\theta) d\varphi d\theta \\ &\propto \int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} \exp(i(m-m')\varphi) d\varphi P_{l,m}^*(\cos(\theta)) P_{l',m'}(\cos(\theta)) \sin(\theta) d\theta = 0. \end{aligned} \quad (\text{C.158})$$

For $l \neq l'$ one obtains

$$\int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} Y_{l,m}(\theta, \varphi)^* Y_{l',m}(\theta, \varphi) \sin(\theta) d\varphi d\theta = 2\pi \int_{-1}^1 P_{l,m}(z) P_{l',m}(z) dz \stackrel{\text{Glg. (C.111)}}{=} 0. \quad (\text{C.159})$$

In summary you get

$$\int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} Y_{l,m}(\theta, \varphi)^* Y_{l',m'}(\theta, \varphi) \sin(\theta) d\varphi d\theta = \delta_{l,l'} \delta_{m,m'}. \quad (\text{C.160})$$

Still applies

$$\Delta_{\theta,\varphi} Y_{l,m}(\theta, \varphi) = -l(l+1) Y_{l,m}(\theta, \varphi) \quad (\text{C.161})$$

with

$$\Delta_{\theta,\varphi} = \Delta_{\mu,\varphi} = \frac{\partial}{\partial \mu} (\mathbf{1} - \mu^2) \frac{\partial}{\partial \mu} + \frac{\mathbf{1}}{\mathbf{1} - \mu^2} \frac{\partial^2}{\partial \varphi^2}, \quad (\text{C.162})$$

as the angle component of the Laplace operator and $\mu = \cos(\theta)$. It applies

$$\frac{\partial^2}{\partial \varphi^2} Y_{l,m} = -m^2 Y_{l,m}(\theta, \varphi), \quad (\text{C.163})$$

thus is here

$$\Delta_{\mu,\varphi} = \frac{\partial}{\partial \mu} (\mathbf{1} - \mu^2) \frac{\partial}{\partial \mu} - \frac{m^2}{\mathbf{1} - \mu^2}. \quad (\text{C.164})$$

For the associated Legendre polynomials $P_{l,m}(\mu)$ the DGL (C.78) applies

$$\frac{d}{d\mu} (\mathbf{1} - \mu^2) P'_{l,m}(\mu) - \frac{m^2}{\mathbf{1} - \mu^2} P_{l,m}(\mu) = -l(l + \mathbf{1}) P_{l,m}(\mu). \quad (\text{C.165})$$

Thus follows

$$\Delta_{\theta,\varphi} Y_{l,m}(\theta, \varphi) = -l(l + \mathbf{1}) Y_{l,m}(\theta, \varphi). \quad (\text{C.166})$$

From Eq. (C.98) follows

$$\frac{\partial}{\partial \theta} Y_{l,m}(\theta, \varphi) = m \cot(\theta) Y_{l,m}(\theta, \varphi) + \sqrt{l^2 - m^2 + l - m} Y_{l,m+1}(\theta, \varphi) \exp(-i\varphi). \quad (\text{C.167})$$

Still applies

$$\frac{\partial}{\partial \varphi} Y_{l,m}(\theta, \varphi) = im Y_{l,m}(\theta, \varphi). \quad (\text{C.168})$$

This follows

$$\begin{aligned} \exp(\pm i\varphi) \left(i \cot(\theta) \frac{\partial}{\partial \varphi} \pm \frac{\partial}{\partial \theta} \right) Y_{l,m}(\theta, \varphi) &= -m \cot(\theta) \exp(\pm i\varphi) Y_{l,m}(\theta, \varphi) \\ &\pm \exp(\pm i\varphi) m \cot(\theta) Y_{l,m}(\cos(\theta)) \pm \sqrt{l^2 - m^2 + l - m} \exp(\pm i\varphi) Y_{l,m+1}(\theta, \varphi) \exp(-i\varphi) \end{aligned}$$

So it applies

$$\hat{L}_+ Y_{l,m}(\theta, \varphi) = \sqrt{l^2 - m^2 + l - m} Y_{l,m+1}(\theta, \varphi). \quad (\text{C.169})$$

This means that for the eigenstates $|n, l, m\rangle$ in the hydrogen atom

$$\hat{L}_+ |n, l, m\rangle = \sqrt{l^2 - m^2 + l - m} |n, l, m+1\rangle. \quad (\text{C.170})$$

From Eq. (C.107) follows

$$\begin{aligned}
\cos(\theta) Y_{l,m} &= \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \cos(\theta) P_{l,m}(\cos(\theta)) \exp(im\varphi) \\
&= \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \left[\frac{l+m}{2l+1} P_{l-1,m} + \frac{l-m+1}{2l+1} P_{l+1,m} \right] \exp(im\varphi) \\
&= \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \frac{l+m}{2l+1} P_{l-1,m} \exp(im\varphi) + \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \frac{l-m+1}{2l+1} P_{l+1,m} \exp(im\varphi) \\
&= \frac{l+m}{2l+1} \sqrt{\frac{2l+1}{2l-1} \frac{l-m}{l+m}} \sqrt{\frac{2l-1}{4\pi} \frac{(l-1-m)!}{(l-1+m)!}} P_{l-1,m} \exp(im\varphi) \\
&\quad + \frac{l-m+1}{2l+1} \sqrt{\frac{2l+1}{2l+3} \frac{l+1+m}{l+1-m}} \sqrt{\frac{2l+3}{4\pi} \frac{(l+1-m)!}{(l+1+m)!}} P_{l+1,m} \exp(im\varphi) \\
&= \frac{l+m}{2l+1} \sqrt{\frac{2l+1}{2l-1} \frac{l-m}{l+m}} Y_{l-1,m} + \frac{l-m+1}{2l+1} \sqrt{\frac{2l+1}{2l+3} \frac{l+1+m}{l+1-m}} Y_{l+1,m}.
\end{aligned}$$

Therefore applies

$$\cos(\theta) Y_{l,m} = \sqrt{\frac{l^2 - m^2}{4l^2 - 1}} Y_{l-1,m} + \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} Y_{l+1,m}. \quad (\text{C.171})$$

From Eq. (C.108) follows

$$\begin{aligned}
\sin(\theta) Y_{l,m} &= \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \sin(\theta) P_{l,m}(\cos(\theta)) \exp(im\varphi) \\
&= \frac{1}{2l+1} \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} [P_{l-1,m+1}(\cos(\theta)) - P_{l+1,m+1}(\cos(\theta))] \exp(im\varphi) \\
&= \frac{1}{2l+1} \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l-1,m+1}(\cos(\theta)) \exp(im\varphi) \\
&\quad - \frac{1}{2l+1} \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_{l+1,m+1}(\cos(\theta)) \exp(im\varphi) \\
&= \frac{1}{2l+1} \sqrt{\frac{2l+1}{2l-1} (l-m-1)(l-m)} \sqrt{\frac{2l-1}{4\pi} \frac{(l-m-2)!}{(l+m)!}} P_{l-1,m+1}(\cos(\theta)) \exp(im\varphi) \\
&\quad - \frac{1}{2l+1} \sqrt{\frac{2l+1}{2l+3} (l+m+1)(l+m+2)} \sqrt{\frac{2l+3}{4\pi} \frac{(l-m)!}{(l+m+2)!}} P_{l+1,m+1}(\cos(\theta)) \exp(im\varphi).
\end{aligned}$$

Therefore applies

$$\begin{aligned}
\sin(\theta) Y_{l,m} &= \sqrt{\frac{1}{4l^2 - 1} (l-m-1)(l-m)} e^{-i\varphi} Y_{l-1,m+1} \\
&\quad - \sqrt{\frac{1}{4l^2 + 8l + 3} (l+m+1)(l+m+2)} e^{-i\varphi} Y_{l+1,m+1}.
\end{aligned} \quad (\text{C.172})$$

C.5.1 Products

C.5.2 Transformation to geographical coordinates

Now the derived equations should be transformed to geographical coordinates (φ, λ) . Previously, $\theta = \pi/2 - \varphi$ was used instead of latitude φ . So they apply

$$\cos(\theta) = \cos\left(\frac{\pi}{2} - \varphi\right) = \sin(\varphi), \quad (\text{C.173})$$

$$\sin(\theta) = \sin\left(\frac{\pi}{2} - \varphi\right) = \cos(\varphi), \quad (\text{C.174})$$

$$\cot(\theta) = \tan(\varphi), \quad (\text{C.175})$$

$$\frac{\partial}{\partial \varphi} = \frac{\partial \theta}{\partial \varphi} \frac{\partial}{\partial \theta} = -\frac{\partial}{\partial \theta}, \quad (\text{C.176})$$

$$\mathcal{P}_{\text{sph. coord.}} = \lambda. \quad (\text{C.177})$$

From Eq. (C.167) follows

$$\frac{\partial}{\partial \varphi} Y_{l,m}(\theta, \varphi) = -m \tan(\varphi) Y_{l,m} - \sqrt{l^2 - m^2 + l - m} Y_{l,m+1} \exp(-i\lambda). \quad (\text{C.178})$$

From Eq. (C.168) follows

$$\frac{\partial}{\partial \lambda} Y_{l,m} = im Y_{l,m}. \quad (\text{C.179})$$

From Eq. (C.171) will

$$\sin(\varphi) Y_{l,m} = \sqrt{\frac{l^2 - m^2}{4l^2 - 1}} Y_{l-1,m} + \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} Y_{l+1,m}. \quad (\text{C.180})$$

From Eq. (C.172) will

$$\begin{aligned} \cos(\varphi) Y_{l,m} &= \sqrt{\frac{1}{4l^2 - 1}} (l - m - 1)(l - m) e^{-i\lambda} Y_{l-1,m+1} \\ &\quad - \sqrt{\frac{1}{4l^2 + 8l + 3}} (l + m + 1)(l + m + 2) e^{-i\lambda} Y_{l+1,m+1}. \end{aligned} \quad (\text{C.181})$$

D.1 Convention on coordinate systems

D.1.1 Resting coordinates

Here you choose a base $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, which is at the center of the earth and does not rotate with the earth. $\mathbf{e}_1$ and $\mathbf{e}_2$ lie in the equatorial plane, $\mathbf{e}_3$ points towards the North Pole. The wind field $\mathbf{v}$ is given as

$$\mathbf{v} = u_1 \mathbf{e}_1 + u_2 \mathbf{e}_2 + u_3 \mathbf{e}_3 \quad (\text{D.1})$$

written. The wind field is not the same as the particle movement measured in this system, as the rotation of the Earth is also superimposed.

Particle movement in stationary coordinates = wind field + earth rotation

D.1.2 Global coordinates

Here you choose a base $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$, which is at the center of the earth just like the base of the resting coordinates, but also rotates. $\mathbf{e}_x$ points in the direction of the intersection between the prime meridian and the equator, $\mathbf{e}_y$ points in the direction of the intersection between ninetyeth longitude and the equator and $\mathbf{e}_z$ points in the direction of the North Pole. The wind field is written as

$$\mathbf{v} = u_x \mathbf{e}_x + u_y \mathbf{e}_y + u_z \mathbf{e}_z. \quad (\text{D.2})$$

D.1.3 Geographic coordinates

Alternatively, you can also use *geographical coordinates* (r, φ, λ) , where $r \geq 0$ is the distance from the center of the Earth, $-\pi/2 \leq \varphi \leq \pi/2$ is the angle that a point makes with the equatorial plane (the geographical latitude assuming a spherical Earth) and $0 \leq \lambda < 2\pi$ is the angle a point with the xz plane includes (the geographical longitude). This can be transformed into ordinary spherical coordinates (r, θ, φ) , with $\theta + \varphi = \pi/2$

$$\sin(\varphi) = \sin(\pi/2 - \theta) = \cos(\theta), \quad (\text{D.3})$$

$$\cos(\varphi) = \cos(\pi/2 - \theta) = \sin(\theta), \quad (\text{D.4})$$

$$\tan(\theta) = \frac{\sin(\theta)}{\cos(\theta)} = \frac{\cos(\varphi)}{\sin(\varphi)} = \frac{1}{\tan(\varphi)}, \quad (\text{D.5})$$

$$v_\theta = -v_\varphi, \quad (\text{D.6})$$

$$\frac{\partial}{\partial \theta} = -\frac{\partial}{\partial \varphi}. \quad (\text{D.7})$$

Locally, the use of the spherical coordinate system is very confusing if you want to note vectors. Therefore, a Cartesian, right-handed coordinate system is used locally, which stands on the sphere and whose x-axis points to the east, y-axis to north and z-axis to the top. The respective basis vectors are called $\mathbf{i}, \mathbf{j}, \mathbf{k}$. The wind field $\mathbf{v}$ is written as

$$\mathbf{v} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}. \quad (\text{D.8})$$

D.2 Spherical geometry

D.2.1 Geodesics

Here we want to determine the shortest connecting line between two points (φ_i, λ_i) on a sphere with $i = 1, 2$ along the surface of the sphere. The length L of any connecting line is calculated as:

$$L = \int ds = \int_0^1 \left| \frac{d\mathbf{r}}{d\tau} \right| d\tau, \quad (\text{D.9})$$

where $\tau \in [0, 1]$ is a parameter that allows one to move along the connecting line and $\mathbf{r}(\tau)$ sets the trajectory. In particular, $\mathbf{r}(0) = \mathbf{r}(\varphi_1, \lambda_1)$ and $\mathbf{r}(1) = \mathbf{r}(\varphi_2, \lambda_2)$.

First start from the sphere, here to determine the functions $\varphi(\tau)$, $\mathcal{J}(\tau)$ you can first start from the unit sphere and ignore the radius. Then apply

$$\mathbf{r}(\mathbf{o}) = \begin{pmatrix} \cos(\varphi_1) \cos(\mathcal{J}_1) \\ \cos(\varphi_1) \sin(\mathcal{J}_1) \\ \sin(\varphi_1) \end{pmatrix}, \quad (\text{D.10})$$

$$\mathbf{r}(\mathbf{i}) = \begin{pmatrix} \cos(\varphi_2) \cos(\mathcal{J}_2) \\ \cos(\varphi_2) \sin(\mathcal{J}_2) \\ \sin(\varphi_2) \end{pmatrix}. \quad (\text{D.11})$$

Define a function

$$\mathbf{r}'(\tau') := \tau' \mathbf{r}(\mathbf{i}) + (\mathbf{i} - \tau') \mathbf{r}(\mathbf{o}). \quad (\text{D.12})$$

Then applies

$$\varphi(\tau') = \arcsin(\tau' \sin(\varphi_2) + (\mathbf{i} - \tau') \sin(\varphi_1)). \quad (\text{D.13})$$

Furthermore applies

$$\begin{aligned} \mathcal{J}(\tau') &= \arctan_2[\tau' \cos(\varphi_2) \sin(\mathcal{J}_2) + (\mathbf{i} - \tau') \cos(\varphi_1) \sin(\mathcal{J}_1), \\ &\quad \tau' \cos(\varphi_2) \cos(\mathcal{J}_2) + (\mathbf{i} - \tau') \cos(\varphi_1) \cos(\mathcal{J}_1)] (+2\pi \text{ im Fall } \arctan_2 < \mathbf{o}). \end{aligned} \quad (\text{D.14})$$

For the distance d between two points $(r_a, \varphi_a, \mathcal{J}_a)$ and $(r_b, \varphi_b, \mathcal{J}_b)$ applies

$$\begin{aligned} d &= \sqrt{(x_b - x_a)^2 + (y_b - y_a)^2 + (z_b - z_a)^2} \\ &= \sqrt{(r_b \cos(\varphi_b) \cos(\mathcal{J}_b) - r_a \cos(\varphi_a) \cos(\mathcal{J}_a))^2 + (r_b \cos(\varphi_b) \sin(\mathcal{J}_b) - r_a \cos(\varphi_a) \sin(\mathcal{J}_a))^2} \\ &\quad + (r_b \sin(\varphi_b) - r_a \sin(\varphi_a))^2 \\ &= \sqrt{r_b^2 \cos^2(\varphi_b) + r_a^2 \cos^2(\varphi_a) + r_b^2 \sin^2(\varphi_b) + r_a^2 \sin^2(\varphi_a) - 2r_a r_b \cos(\varphi_b) \cos(\mathcal{J}_b) \cos(\varphi_a) \cos(\mathcal{J}_a)} \\ &\quad - 2r_a r_b \cos(\varphi_b) \sin(\mathcal{J}_b) \cos(\varphi_a) \sin(\mathcal{J}_a) - 2r_b r_a \sin(\varphi_b) \sin(\varphi_a)} \\ &= \sqrt{r_a^2 + r_b^2 - 2r_a r_b \cos(\varphi_b) \cos(\varphi_a) (\cos(\mathcal{J}_b) \cos(\mathcal{J}_a) + \sin(\mathcal{J}_b) \sin(\mathcal{J}_a)) - 2r_b r_a \sin(\varphi_b) \sin(\varphi_a)} \\ &= \sqrt{r_a^2 + r_b^2 - 2r_a r_b (\cos(\varphi_a) \cos(\varphi_b) \cos(\mathcal{J}_a - \mathcal{J}_b) + \sin(\varphi_a) \sin(\varphi_b))} \end{aligned} \quad (\text{D.15})$$

In the case $r_a = r_b = r$ applies

$$d = r \sqrt{2 - 2(\cos(\varphi_a) \cos(\varphi_b) \cos(\mathcal{J}_a - \mathcal{J}_b) + \sin(\varphi_a) \sin(\varphi_b))}. \quad (\text{D.16})$$

The distance between two points on a sphere can be easily calculated from this. Let a sphere with radius r be given. Then the distance Δ between two points on the surface, measured along the surface, is given by

$$\Delta = r\theta, \quad (\text{D.17})$$

where θ is the angle between the two points, for this angle applies

$$\sin\left(\frac{\theta}{2}\right) = \frac{d}{2r}. \quad (\text{D.18})$$

So the equation applies because of $\frac{\theta}{2} \in [\mathbf{o}, \frac{\pi}{2}]$ for the distance Δ

$$\Delta = 2 \arcsin \left(\sqrt{\frac{1}{2} - \frac{1}{2} (\cos(\varphi_a) \cos(\varphi_b) \cos(\lambda_a - \lambda_b) + \sin(\varphi_a) \sin(\varphi_b))} \right). \quad (\text{D.19})$$

Now τ has to be converted into τ' . It applies

$$\begin{aligned} \tau &= \frac{1}{2} + \frac{1}{\theta} \arctan \left(\frac{\tau' - \frac{1}{2}}{\sqrt{r^2 - \frac{d^2}{4}}} d \right) = \frac{1}{2} + \frac{1}{\theta} \arctan \left(\frac{\tau' - \frac{1}{2}}{\sqrt{\frac{r^2}{d^2} - \frac{1}{4}}} \right) \\ \Leftrightarrow \tau - \frac{1}{2} &= \frac{1}{\theta} \arctan \left(\frac{\tau' - \frac{1}{2}}{\sqrt{\frac{r^2}{d^2} - \frac{1}{4}}} \right) \\ \Leftrightarrow \theta \left(\tau - \frac{1}{2} \right) &= \arctan \left(\frac{\tau' - \frac{1}{2}}{\sqrt{\frac{r^2}{d^2} - \frac{1}{4}}} \right) \\ \Leftrightarrow \tan \left[\theta \left(\tau - \frac{1}{2} \right) \right] &= \frac{\tau' - \frac{1}{2}}{\sqrt{\frac{r^2}{d^2} - \frac{1}{4}}} \\ \Leftrightarrow \sqrt{\frac{r^2}{d^2} - \frac{1}{4}} \tan \left[\theta \left(\tau - \frac{1}{2} \right) \right] &= \tau' - \frac{1}{2}. \end{aligned}$$

From this it follows

$$\tau' = \frac{1}{2} + \sqrt{\frac{r^2}{d^2} - \frac{1}{4}} \tan \left[\theta \left(\tau - \frac{1}{2} \right) \right]. \quad (\text{D.20})$$

$$(\text{D.21})$$

D.2.2 Vertical surfaces

For vertical surfaces A_v with the base length L and the same designation for the radii applies

$$A_v = \int_{r_o}^{r_1} L \frac{r}{r_o} dr = \frac{L}{2r_o} (r_1^2 - r_o^2). \quad (\text{D.22})$$

D.2.3 Volumes

Volumes V with the base area A , the inner radius r_o and the outer radius r_1 are calculated via

$$V = \int_{r_o}^{r_1} A \frac{r^2}{r_o^2} dr = \frac{A}{r_o^2} \frac{1}{3} (r_1^3 - r_o^3). \quad (\text{D.23})$$

D.2.4 Spherical triangles

D.2.5 Spherical Voronoi lattices

D.3 Earth's gravity field

D.3.1 Properties of ellipses and ellipsoids

An *ellipse* in the xz plane is described by

$$\frac{x^2}{a^2} + \frac{z^2}{c^2} = 1. \quad (\text{D.24})$$

Here, $a > 0$ is the *semi-major axis* (maximum extent of the ellipse in the x-direction) and $0 < c < a$ is the *semi-minor axis* (maximum extent of the ellipse in the z-direction). The *eccentricity* becomes

$$\varepsilon := \frac{a - c}{a} \quad (\text{D.25})$$

defined. This gives you

$$c = a(1 - \varepsilon). \quad (\text{D.26})$$

Follow in polar coordinates with

$$x = r \cos(\varphi), \quad z = r \sin(\varphi) \quad (\text{D.27})$$

the equations

$$\begin{aligned} \frac{r^2}{a^2} \cos^2(\varphi) + \frac{r^2}{c^2} \sin^2(\varphi) &= 1 \\ \Rightarrow r(\varphi) &= \left[\frac{\cos^2(\varphi)}{a^2} + \frac{\sin^2(\varphi)}{c^2} \right]^{-1/2} = a \left[\cos^2(\varphi) + \frac{a^2}{c^2} \sin^2(\varphi) \right]^{-1/2} \\ \Rightarrow r(\varphi) &= a \left[1 + \left(\frac{a^2}{c^2} - 1 \right) \sin^2(\varphi) \right]^{-1/2}. \end{aligned} \quad (\text{D.28})$$

With

$$\frac{a^2}{c^2} - 1 = \frac{1}{(1 - \varepsilon)^2} - 1 = \frac{1 - (1 - \varepsilon)^2}{(1 - \varepsilon)^2} = \frac{2\varepsilon - \varepsilon^2}{(1 - \varepsilon)^2} \quad (\text{D.29})$$

you can do this

$$r(\varphi) = a \left[1 + \frac{2\varepsilon - \varepsilon^2}{(1 - \varepsilon)^2} \sin^2(\varphi) \right]^{-1/2}. \quad (\text{D.30})$$

rewrite. It follows from equation (D.29)

$$a^2 - c^2 = c^2 \frac{2\varepsilon - \varepsilon^2}{(1 - \varepsilon)^2} = a^2 \varepsilon (2 - \varepsilon). \quad (\text{D.31})$$

A *ellipsoid of rotation* or simply *ellipsoid* is created by letting the ellipse just examined rotate around the z-axis. Its volume V is calculated as

$$\begin{aligned} V &= \int_{-c}^c \int_0^{a\sqrt{1-\frac{z^2}{c^2}}} 2\pi x dx dz = 2\pi \int_{-c}^c \left[\frac{1}{2} x^2 \right]_0^{a\sqrt{1-\frac{z^2}{c^2}}} dz \\ &= 2\pi \int_{-c}^c \frac{1}{2} a^2 \left(1 - \frac{z^2}{c^2} \right) dz = \pi \int_{-c}^c a^2 - \frac{a^2}{c^2} z^2 dz = \pi 2a^2 c - \pi \frac{a^2}{c^2} \frac{2}{3} c^3 \\ &= \pi 2a^2 c - \frac{2}{3} \pi a^2 c \end{aligned}$$

$$\Leftrightarrow V = \frac{4}{3} \pi a^2 c \quad (\text{D.32})$$

D.3.2 Gravity field of an ellipsoid

The ellipsoidal coordinates will be based on the Earth's geopotential φ_g , for which applies

$$\varphi_g = \varphi_z + \varphi_o, \quad (\text{D.33})$$

Here φ_z is the centrifugal potential and φ_o is the gravitational potential of the earth. The following applies to the fleeing potential

$$\varphi_z = -\frac{\mathbf{I}}{2} (\omega^2 (x^2 + y^2)), \quad (\text{D.34})$$

because gradient formation results in

$$-\nabla \varphi_z = \omega^2 \begin{pmatrix} x \\ y \\ 0 \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ \omega \end{pmatrix} \times \begin{pmatrix} -\omega y \\ \omega x \\ 0 \end{pmatrix} = -\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}). \quad (\text{D.35})$$

The context applies

$$\mathbf{a} = -\nabla \varphi_g \quad (\text{D.36})$$

between the gravitational potential φ_g and the gravitational acceleration $\mathbf{a}$. Newton's law of gravity can then be written as

$$\nabla \cdot \mathbf{a} = -4\pi G \varrho \quad (\text{D.37})$$

with ϱ as the mass distribution, because in the case of a point mass this results in M at the origin using Gauss's theorem

$$-4\pi G M = a 4\pi r^2 \Leftrightarrow a = -G \frac{M}{r^2}. \quad (\text{D.38})$$

In terms of the gravitational potential this becomes

$$\Delta \varphi_g = 4\pi G \varrho \quad (\text{D.39})$$

or

$$\Delta \varphi_g = 0 \quad (\text{D.40})$$

outside the earth. This is called a Laplace differential equation. This has to be solved in order to determine the gravitational potential of the earth. In general you can use an integral

$$\varphi_o(\mathbf{r}) = -G \int_E \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \quad (\text{D.41})$$

set up for this, here E is the earth, but this cannot be solved analytically in the case of an ellipsoidal set E . Therefore, φ_g is developed according to certain functions. The approach used is $\mu := \cos(\theta)$, a separation approach

$$\varphi_g(r, \mu, \varphi) = \frac{U(r)}{r} P(\mu) Q(\varphi). \quad (\text{D.42})$$

made. If you substitute this into $\Delta \varphi_g = 0$, you get with Eq. (B.91) and the statement

$$\frac{1}{r} \frac{\partial^2}{\partial r^2} (r f) = \frac{1}{r} \frac{\partial}{\partial r} (f + r f') = \frac{2}{r} f' + f'' = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right), \quad (\text{D.43})$$

here $f = f(r)$ and $f' := \frac{\partial f}{\partial r}$

$$\begin{aligned}
PQ \frac{U''}{r} + UQ \frac{1}{r^3} \frac{\partial}{\partial \mu} (1 - \mu^2) P' + \frac{UP}{r^3 (1 - \mu^2)} Q'' &= 0 \\
\Leftrightarrow r^2 (1 - \mu^2) \frac{1}{v} U'' + \frac{1}{P} (1 - \mu^2) \frac{\partial}{\partial \mu} (1 - \mu^2) P' &= -\frac{Q''}{Q}.
\end{aligned} \tag{D.44}$$

The left side of Eq. (D.44) does not depend on φ , while the right-hand side does not depend on μ and r , therefore both are equal to a separation constant m^2 . This therefore applies to Q

$$Q'' = -m^2 Q, \tag{D.45}$$

what is solved by

$$Q(\varphi) = \exp(im\varphi). \tag{D.46}$$

Since $Q(\varphi) = Q(\varphi + 2\pi)$, $m \in \mathbb{Z}$. Now divide Eq. (D.44) by $1 - \mu^2$ and sets the right side equal to m^2 , you then get

$$r^2 \frac{U''}{v} = -\frac{1}{P} \frac{\partial}{\partial \mu} (1 - \mu^2) P'(\mu) + \frac{m^2}{1 - \mu^2}. \tag{D.47}$$

Both sides are equal to a new separation constant λ . You get two differential equations, one for P and one for U , which reads for P

$$\frac{d}{d\mu} (1 - \mu^2) P'(\mu) = P \left(-\lambda + \frac{m^2}{1 - \mu^2} \right) \tag{D.48}$$

and that for U is

$$r^2 U'' - \lambda U = 0. \tag{D.49}$$

Cylindrical symmetry is sufficient for the geopotential, i.e. $m = 0$. Then you get

$$\frac{d}{d\mu} (1 - \mu^2) P'(\mu) = -\lambda P. \tag{D.50}$$

If you put in Eq. (D.49) $\lambda = n(n + 1)$, you get

$$r^2 U'' - n(n + 1) U = 0. \tag{D.51}$$

U depends on n , write U_n . It is found that

$$U_n(r) = r^{n+1} \tag{D.52}$$

and

$$U_n(r) = r^{-n} \tag{D.53}$$

solutions are and thus the general solution of the ordinary second-order DGL Eq. (D.52) is given by

$$U_n(r) = a_n r^{n+1} + \frac{b_n}{r^n}. \tag{D.54}$$

Now solutions are of the form

$$\mathcal{P}_g^{(n)}(r, \mu) = \frac{U_n(r)}{r} P_n(\mu) \tag{D.55}$$

found, since the Laplace equation (D.40) is linear in φ_g , any linear combinations of these are again solutions and one obtains as a general solution

$$\varphi_g(r, \mu) = \sum_{n=0}^{\infty} \left(a_n r^n + \frac{b_n}{r^{n+1}} \right) P_n(\mu). \quad (\text{D.56})$$

The specific solution for the rotating ellipsoid case is determined by the boundary conditions. This is:

$$\varphi_g(x, z) = 0 \quad (\text{D.57})$$

for

$$\frac{x^2}{a^2} + \frac{z^2}{c^2} = 1, \quad (\text{D.58})$$

Here a is the semi-major and c the semi-minor axis of the Earth. At this point the sum in Eq. (D.56) is terminated at $n = 2$ and only the gravitational component is considered:

$$\varphi_o = \left(a_o + \frac{b_o}{r} \right) P_o(\sin(\chi)) + \left(a_1 r + \frac{b_1}{r^2} \right) P_1(\sin(\chi)) + \left(a_2 r^2 + \frac{b_2}{r^3} \right) P_2(\sin(\chi)) \quad (\text{D.59})$$

χ is the geocentric latitude (as opposed to the geodetic latitude). We have $\chi + \theta = \pi/2$. The first three Legendre polynomials are

$$P_o(\sin(\chi)) = 1, \quad (\text{D.60})$$

$$P_1(\sin(\chi)) = \frac{1}{2} \sin(\chi) = \sin(\chi), \quad (\text{D.61})$$

$$P_2(\sin(\chi)) = \frac{1}{8} (12 \sin^2(\chi) - 4) = \frac{3}{2} \sin^2(\chi) - \frac{1}{2}. \quad (\text{D.62})$$

So the expression for φ_g is

$$\varphi_o = a_o + \frac{b_o}{r} + \left(a_1 r + \frac{b_1}{r^2} \right) \sin(\chi) + \left(\frac{a_2}{2} r^2 + \frac{b_2}{2r^3} \right) (3 \sin^2(\chi) - 1). \quad (\text{D.63})$$

The goal is now to calculate the coefficients $a_o, a_1, a_2, b_o, b_1, b_2$. However, because of the usual boundary condition $\lim_{r \rightarrow \infty} \varphi_o(r) = 0$ applies

$$a_o = a_1 = a_2 = 0, \quad (\text{D.64})$$

furthermore, the solution should become $-GM/r$ at an infinite distance, since the ellipsoidal mass distribution looks like a point mass from a distance, so it is expected

$$b_o = -GM. \quad (\text{D.65})$$

The coefficients b_1 and b_2 are still free:

$$\varphi_o = -\frac{GM}{r} + \frac{b_1}{r^2} \sin(\chi) + \frac{b_2}{2r^3} (3 \sin^2(\chi) - 1). \quad (\text{D.66})$$

To determine this, one calculates the gravitational potential on the z-axis ($z = r > c$). There we have $\chi = \pi/2$

$$\varphi_o(r) = -\frac{GM}{r} + \frac{b_1(\varepsilon)}{r^2} + \frac{b_2(\varepsilon)}{r^3}. \quad (\text{D.67})$$

It was assumed that the b_i depend on the eccentricity ε . So one assumes a homogeneous earth of density ρ and integrates

$$\begin{aligned}
\mathcal{P}_o(r) &= -G_\rho \int_{z=-c}^c \int_0^{a\sqrt{1-\frac{z^2}{c^2}}} \frac{1}{\sqrt{(r-z)^2 + x^2}} 2\pi x dx dz = -2\pi G_\rho \int_{z=-c}^c \left[\sqrt{(r-z)^2 + x^2} \right]_0^{a\sqrt{1-\frac{z^2}{c^2}}} dz \\
&= -2\pi G_\rho \int_{-c}^c \sqrt{(z-r)^2 + a^2 \left(1 - \frac{z^2}{c^2}\right)} - r + z dz = -2\pi G_\rho \int_{-c}^c \sqrt{r^2 + z^2 \left(1 - \frac{a^2}{c^2}\right) - 2zr + a^2 - r + z} dz \\
&= 2\pi G_\rho r 2c - 2\pi G_\rho \int_{-c}^c \sqrt{\left(1 - \frac{a^2}{c^2}\right) z^2 - 2zr + a^2 + r^2} dz \\
&= 4\pi G_\rho cr - 2\pi G_\rho \int_{-c}^c \sqrt{Az^2 + Bz + C} dz = 2\pi G_\rho \left(2cr - \int_{-c}^c \sqrt{Az^2 + Bz + C} dz \right) \tag{D.68}
\end{aligned}$$

with

$$A = 1 - \frac{a^2}{c^2}, \tag{D.69}$$

$$B = -2r, \tag{D.70}$$

$$C = a^2 + r^2. \tag{D.71}$$

This formula can first be checked for a simple limiting case, namely the case of a ball $a = c$. In this case you get

$$\begin{aligned}
\mathcal{P}_o(r) &= 2\pi G_\rho \left(2ar - \int_{-c}^c \sqrt{r^2 - 2zr + a^2} dz \right) = 2\pi G_\rho \left(2ar - \left[-\frac{1}{3r} (r^2 - 2zr + a^2)^{3/2} \right]_{-c}^c \right) \\
&= 2\pi G_\rho \left(2ar + \left[\frac{1}{3r} (r^2 - 2ar + a^2)^{3/2} - \frac{1}{3r} (r^2 + 2ar + a^2) \right] \right) \\
&= 2\pi G_\rho \left(2ar + \frac{1}{3r} [(r-a)^3 - (r+a)^3] \right) \\
&= 2\pi G_\rho \left(2ar + \frac{1}{3r} [(r^2 - a^2 - 2ar)(r-a) - (r^2 + a^2 + 2ar)(r+a)] \right) \\
&= 2\pi G_\rho \left(2ar + \frac{1}{3r} [r^3 + r^2a + a^2r - a^3 - 2ar^2 + 2a^2r - r^3 - r^2a - a^2r - a^3 - 2ar^2 - 2a^2r] \right) \\
&= 2\pi G_\rho \left(2ar + \frac{1}{3r} [-6r^2a - 2a^3] \right) = 2\pi G_\rho \left(2ar - 2ra - \frac{2}{3} \frac{a^3}{r} \right) = -\frac{4\pi G_\rho a^3}{3r} \\
&= -GM \frac{1}{r}. \tag{D.72}
\end{aligned}$$

The gravitational potential of a homogeneous solid sphere outside the sphere is equal to that of a point mass at the location of the sphere's center of gravity. According to [1] Eq. (3.3.37)

$$\int \sqrt{Ax^2 + Bx + C} dx = \frac{2Ax + B}{4A} \sqrt{Ax^2 + Bx + C} + \frac{4AC - B^2}{8A} \int \frac{dx}{\sqrt{Ax^2 + Bx + C}}. \tag{D.73}$$

Here is

$$\int \frac{dx}{\sqrt{Ax^2 + Bx + C}} = -\frac{1}{\sqrt{-A}} \arcsin \frac{2Ax + B}{\sqrt{B^2 - 4AC}}. \tag{D.74}$$

The requirements for this are

$$A < 0, \quad (D.75)$$

$$B^2 > 4AC \Leftrightarrow 4r^2 > \left(1 - \frac{a^2}{c^2}\right)(a^2 + r^2) \\ \Leftrightarrow r^2 > a^2 + r^2 - \frac{a^4}{c^2} - a^2 \frac{r^2}{c^2},$$

$$|2Ax + B| < \sqrt{B^2 - 4AC} \Leftrightarrow \left| 2 \left(1 - \frac{a^2}{c^2}\right)x - 2r \right| < \sqrt{4r^2 + 4(a^2 + r^2) \left(\frac{a^2}{c^2} - 1\right)} \\ \Leftrightarrow \left| x \left(1 - \frac{a^2}{c^2}\right) - r \right| < \sqrt{r^2 - a^2 - r^2 + \frac{a^4}{c^2} + r^2 \frac{a^2}{c^2}} \\ \Leftrightarrow c \left(\frac{a^2}{c^2} - 1\right) + r < a \sqrt{\frac{a^2}{c^2} - 1 + \frac{r^2}{c^2}}. \quad (D.76)$$

For $r = c$ the last two expressions become equal. The derivative of the left expression with respect to r is

$$\frac{d}{dr} \left(c \left(\frac{a^2}{c^2} - 1 \right) + r \right) = 1, \quad (D.77)$$

is the derivative of the right-hand expression with respect to r

$$\frac{d}{dr} a \sqrt{\frac{a^2}{c^2} - 1 + \frac{r^2}{c^2}} = a \frac{2r}{c^2} \frac{1}{\sqrt{\frac{a^2}{c^2} - 1 + \frac{r^2}{c^2}}} = \frac{ra}{c \sqrt{a^2 - c^2 + r^2}}. \quad (D.78)$$

This expression is equal to one for $r = c$ and $a/c > 1$ for $r \rightarrow \infty$, the derivative

$$\frac{d}{dr} \frac{ra}{c \sqrt{a^2 - c^2 + r^2}} \propto \frac{ac \sqrt{a^2 - c^2 + r^2} - racr \frac{1}{\sqrt{a^2 - c^2 + r^2}}}{ac(a^2 - c^2 + r^2) - r^2 ac} > 0 \quad (D.79)$$

is positive everywhere and therefore is

$$\frac{d}{dr} a \sqrt{\frac{a^2}{c^2} - 1 + \frac{r^2}{c^2}} > 1 \quad (D.80)$$

for $r > c$. Thus the inequality (16.242) for $r > c$ is satisfied and the integral formula

$$\int \sqrt{Ax^2 + Bx + C} dx = \frac{2Ax + B}{4A} \sqrt{Ax^2 + Bx + C} - \frac{4AC - B^2}{8A} \frac{1}{\sqrt{-A}} \arcsin \frac{2Ax + B}{\sqrt{B^2 - 4AC}} \quad (D.81)$$

can be applied. So it applies

$$\int_{-c}^c \sqrt{Ax^2 + Bx + C} dx \\ = \frac{2Ac + B}{4A} \cdot \sqrt{Ac^2 + Bc + C} - \frac{4AC - B^2}{8A} \frac{1}{\sqrt{-A}} \arcsin \left(\frac{2Ac + B}{\sqrt{B^2 - 4AC}} \right) - \frac{B - 2Ac}{4A} \cdot \sqrt{Ac^2 - Bc + C} \\ + \frac{4AC - B^2}{8A} \frac{1}{\sqrt{-A}} \arcsin \left(\frac{-2Ac + B}{\sqrt{B^2 - 4AC}} \right) = \frac{2Ac + B}{4A} \sqrt{Ac^2 + Bc + C} + \frac{4AC - B^2}{8A \sqrt{-A}} \\ \cdot \left[\arcsin \left(\frac{B - 2Ac}{\sqrt{B^2 - 4AC}} \right) - \arcsin \left(\frac{2Ac + B}{\sqrt{B^2 - 4AC}} \right) \right] - \frac{B - 2Ac}{4A} \sqrt{Ac^2 - Bc + C}. \quad (D.82)$$

Here you now insert A, B and C and get

$$\sqrt{Ac^2 + Bc + C} = \sqrt{c^2 - a^2 - 2rc + a^2 + r^2} = \sqrt{c^2 + r^2 - 2rc} = r - c, \quad (\text{D.83})$$

$$\sqrt{Ac^2 - Bc + C} = \sqrt{c^2 - a^2 + 2rc + a^2 + r^2} = r + c, \quad (\text{D.84})$$

$$B - 2Ac = -2r - 2c + 2\frac{a^2}{c} = 2\left(\frac{a^2}{c} - r - c\right), \quad (\text{D.85})$$

$$B + 2Ac = -2r + 2c - 2\frac{a^2}{c} = 2\left(c - r - \frac{a^2}{c}\right), \quad (\text{D.86})$$

$$B^2 - 4AC = 4r^2 - 4\left(1 - \frac{a^2}{c^2}\right)(a^2 + r^2) = -4a^2 + 4\frac{a^4}{c^2} + 4\frac{a^2r^2}{c^2} = 4\frac{a^2}{c^2}(a^2 + r^2 - c^2), \quad (\text{D.87})$$

$$\begin{aligned} & \frac{2Ac + B}{4A}\sqrt{Ac^2 + Bc + C} - \frac{B - 2Ac}{4A}\sqrt{Ac^2 - Bc + C} \\ &= \frac{2\left(c - r - \frac{a^2}{c}\right)}{4 - 4\frac{a^2}{c^2}}(r - c) - \frac{2\left(\frac{a^2}{c} - r - c\right)}{4 - 4\frac{a^2}{c^2}}(r + c) \\ &= \frac{4cr - 2a^2r/c}{2 - 2a^2/c^2} = \frac{2c^3r - a^2rc}{c^2 - a^2} = rc\frac{a^2 - 2c^2}{a^2 - c^2}, \end{aligned} \quad (\text{D.88})$$

$$\begin{aligned} \frac{4AC - B^2}{8A\sqrt{-A}} &= -\frac{4\frac{a^2}{c^2}(a^2 + r^2 - c^2)}{8\left(1 - \frac{a^2}{c^2}\right)\sqrt{\frac{a^2}{c^2} - 1}} = -\frac{a^2(a^2 + r^2 - c^2)}{2(c^2 - a^2)\sqrt{\frac{a^2}{c^2} - 1}} \\ &= -\frac{a^2 + r^2 - c^2}{2\left(\frac{c^2}{a^2} - 1\right)\sqrt{\frac{a^2}{c^2} - 1}} = a^2c\frac{a^2 + r^2 - c^2}{2(a^2 - c^2)\sqrt{a^2 - c^2}}, \end{aligned} \quad (\text{D.89})$$

$$\frac{B - 2Ac}{\sqrt{B^2 - 4AC}} = \frac{2\left(\frac{a^2}{c} - r - c\right)}{2\frac{a}{c}\sqrt{a^2 + r^2 - c^2}} = \frac{a^2 - rc - c^2}{a\sqrt{a^2 + r^2 - c^2}}, \quad (\text{D.90})$$

$$\frac{2Ac + B}{\sqrt{B^2 - 4AC}} = \frac{2\left(c - r - \frac{a^2}{c}\right)}{2\frac{a}{c}\sqrt{a^2 + r^2 - c^2}} = \frac{c^2 - rc - a^2}{a\sqrt{a^2 + r^2 - c^2}} \quad (\text{D.91})$$

the equation

$$\begin{aligned} \int_{-c}^c \dots dx &= a^2c\frac{a^2 + r^2 - c^2}{2(a^2 - c^2)^{3/2}} \cdot \left[\arcsin\left(\frac{a^2 - rc - c^2}{a\sqrt{a^2 + r^2 - c^2}}\right) - \arcsin\left(\frac{c^2 - rc - a^2}{a\sqrt{a^2 + r^2 - c^2}}\right) \right] \\ &+ rc\frac{a^2 - 2c^2}{a^2 - c^2}. \end{aligned} \quad (\text{D.92})$$

So for the gravitational potential on the z-axis it follows

$$4cr - 2cr\frac{a^2 - 2c^2}{a^2 - c^2} = rc\frac{4a^2 - 4c^2 - 2a^2 + 4c^2}{a^2 - c^2} = 2rc\frac{a^2}{a^2 - c^2} \quad (\text{D.93})$$

the bill

$$\begin{aligned} \varphi_o(r) &= \pi G\rho \left(4cr - 2rc\frac{a^2 - 2c^2}{a^2 - c^2} - a^2c\frac{a^2 + r^2 - c^2}{(a^2 - c^2)^{3/2}} \cdot \left[\arcsin\left(\frac{a^2 - rc - c^2}{a\sqrt{a^2 + r^2 - c^2}}\right) - \arcsin\left(\frac{c^2 - rc - a^2}{a\sqrt{a^2 + r^2 - c^2}}\right) \right] \right) \\ &= \pi G\rho \left(rc\frac{2a^2}{a^2 - c^2} - a^2c\frac{a^2 + r^2 - c^2}{(a^2 - c^2)^{3/2}} \cdot \left[\arcsin\left(\frac{a^2 - rc - c^2}{a\sqrt{a^2 + r^2 - c^2}}\right) - \arcsin\left(\frac{c^2 - rc - a^2}{a\sqrt{a^2 + r^2 - c^2}}\right) \right] \right) \\ &= \pi G\rho \frac{a^2c}{a^2 - c^2} \left(2r - \frac{a^2 + r^2 - c^2}{\sqrt{a^2 - c^2}} \cdot \left[\arcsin\left(\frac{a^2 - rc - c^2}{a\sqrt{a^2 + r^2 - c^2}}\right) - \arcsin\left(\frac{c^2 - rc - a^2}{a\sqrt{a^2 + r^2 - c^2}}\right) \right] \right). \end{aligned} \quad (\text{D.94})$$

Here you can see the mass of the earth

$$M = \frac{4}{3} \pi \rho a^2 c \Rightarrow \pi \rho a^2 c = \frac{3M}{4} \quad (\text{D.95})$$

install:

$$\begin{aligned} \varphi_o(r) = G \frac{M}{a^2 - c^2} & \left(\frac{3}{2} r - \frac{3}{4} \frac{a^2 + r^2 - c^2}{\sqrt{a^2 - c^2}} \cdot \right. \\ & \cdot \left[\arcsin \left(\frac{a^2 - rc - c^2}{a\sqrt{a^2 + r^2 - c^2}} \right) - \arcsin \left(\frac{c^2 - rc - a^2}{a\sqrt{a^2 + r^2 - c^2}} \right) \right] \right) \end{aligned} \quad (\text{D.96})$$

With Eq. (D.31) follows for the gravitational potential

$$\begin{aligned} \varphi_o(r) = G \frac{M}{a^2 \varepsilon (2 - \varepsilon)} & \left(\frac{3}{2} r - \frac{3}{4} \frac{a^2 \varepsilon (2 - \varepsilon) + r^2}{a\sqrt{\varepsilon (2 - \varepsilon)}} \cdot \right. \\ & \cdot \left[\arcsin \left(\frac{a^2 \varepsilon (2 - \varepsilon) - ra(1 - \varepsilon)}{a\sqrt{a^2 \varepsilon (2 - \varepsilon) + r^2}} \right) - \arcsin \left(-\frac{a^2 \varepsilon (2 - \varepsilon) + ra(1 - \varepsilon)}{a\sqrt{a^2 \varepsilon (2 - \varepsilon) + r^2}} \right) \right] \right) \\ = G \frac{M}{a \varepsilon (2 - \varepsilon)} & \left(\frac{3}{2} \frac{r}{a} - \frac{3}{4} \frac{\varepsilon (2 - \varepsilon) + r^2/a^2}{\sqrt{\varepsilon (2 - \varepsilon)}} \cdot \right. \\ & \cdot \left[\arcsin \left(\frac{\varepsilon (2 - \varepsilon) - \frac{r}{a} (1 - \varepsilon)}{\sqrt{\varepsilon (2 - \varepsilon) + \frac{r^2}{a^2}}} \right) - \arcsin \left(-\frac{\varepsilon (2 - \varepsilon) + \frac{r}{a} (1 - \varepsilon)}{\sqrt{\varepsilon (2 - \varepsilon) + \frac{r^2}{a^2}}} \right) \right] \right) \\ = \frac{3GM}{2a \varepsilon (2 - \varepsilon)} & \left(\frac{r}{a} - \frac{\varepsilon (2 - \varepsilon) + r^2/a^2}{2\sqrt{\varepsilon (2 - \varepsilon)}} \cdot \left[\arcsin \left(\frac{\varepsilon (2 - \varepsilon) - \frac{r}{a} (1 - \varepsilon)}{\sqrt{\varepsilon (2 - \varepsilon) + \frac{r^2}{a^2}}} \right) \right. \right. \\ & \left. \left. + \arcsin \left(\frac{\varepsilon (2 - \varepsilon) + \frac{r}{a} (1 - \varepsilon)}{\sqrt{\varepsilon (2 - \varepsilon) + \frac{r^2}{a^2}}} \right) \right] \right). \end{aligned} \quad (\text{D.97})$$

Eq. (D.97) is the basis for the theoretical investigation of the gravity field of an ellipsoid of revolution. It is exact for eccentricities $\varepsilon \neq 0$, but is not applicable for $\varepsilon = 0$. Unfortunately, the expression does not yet have the form of Equation. (D.67). To achieve this, it is expanded in the small parameter $\varepsilon \ll 1$. To do this, you define the abbreviations

$$f_1(\varepsilon) := \frac{\varepsilon (2 - \varepsilon) - \frac{r}{a} (1 - \varepsilon)}{\sqrt{\varepsilon (2 - \varepsilon) + \frac{r^2}{a^2}}}, \quad (\text{D.98})$$

$$f_2(\varepsilon) := \frac{\varepsilon (2 - \varepsilon) + \frac{r}{a} (1 - \varepsilon)}{\sqrt{\varepsilon (2 - \varepsilon) + \frac{r^2}{a^2}}}. \quad (\text{D.99})$$

Preparations are already underway

$$\begin{aligned}
f'_1(\varepsilon) &= \frac{(2 - 2\varepsilon + \frac{r}{a}) \sqrt{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}} - [\varepsilon(2 - \varepsilon) - \frac{r}{a}(1 - \varepsilon)]^{\frac{1}{2}} (2 - 2\varepsilon) \frac{1}{\sqrt{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}}}}{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}} \\
&= \frac{(2 - 2\varepsilon + \frac{r}{a}) (\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}) - [\varepsilon(2 - \varepsilon) - \frac{r}{a}(1 - \varepsilon)] (1 - \varepsilon)}{[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}]^{3/2}} \\
&= \frac{2(1 - \varepsilon)\varepsilon(2 - \varepsilon) + 2(1 - \varepsilon)\frac{r^2}{a^2} + \frac{r}{a}\varepsilon(2 - \varepsilon) + \frac{r^3}{a^3} - \varepsilon(2 - \varepsilon)(1 - \varepsilon) + \frac{r}{a}(1 - \varepsilon)^2}{[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}]^{3/2}} \\
&= \frac{\varepsilon(1 - \varepsilon)(2 - \varepsilon) + \frac{r^3}{a^3} + \frac{r^2}{a^2}2(1 - \varepsilon) + \frac{r}{a}}{[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}]^{3/2}} \tag{D.100}
\end{aligned}$$

and

$$\begin{aligned}
f'_2(\varepsilon) &= \frac{(2 - 2\varepsilon - \frac{r}{a}) \sqrt{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}} - [\varepsilon(2 - \varepsilon) + \frac{r}{a}(1 - \varepsilon)]^{\frac{1}{2}} (2 - 2\varepsilon) \frac{1}{\sqrt{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}}}}{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}} \\
&= \frac{(2 - 2\varepsilon - \frac{r}{a}) (\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}) - [\varepsilon(2 - \varepsilon) + \frac{r}{a}(1 - \varepsilon)] (1 - \varepsilon)}{[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}]^{3/2}} \\
&= \frac{2(1 - \varepsilon)\varepsilon(2 - \varepsilon) + 2(1 - \varepsilon)\frac{r^2}{a^2} - \frac{r}{a}\varepsilon(2 - \varepsilon) - \frac{r^3}{a^3} - \varepsilon(2 - \varepsilon)(1 - \varepsilon) - \frac{r}{a}(1 - \varepsilon)^2}{[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}]^{3/2}} \\
&= \frac{\varepsilon(1 - \varepsilon)(2 - \varepsilon) - \frac{r^3}{a^3} + \frac{r^2}{a^2}2(1 - \varepsilon) - \frac{r}{a}}{[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}]^{3/2}}. \tag{D.101}
\end{aligned}$$

The gravitational potential is written as:

$$\varphi_o(r) = \frac{3GM}{2a} \frac{2\frac{r}{a}(\varepsilon(2 - \varepsilon))^{1/2} - (\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}) [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]}{2(\varepsilon(2 - \varepsilon))^{3/2}}. \tag{D.102}$$

This will be with

$$g(\varepsilon) := 2\frac{r}{a}(\varepsilon(2 - \varepsilon))^{1/2} - \left(\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}\right) [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))], \tag{D.103}$$

$$h(\varepsilon) := 2(\varepsilon(2 - \varepsilon))^{3/2}, \tag{D.104}$$

$$F(\varepsilon) := \frac{g(\varepsilon)}{h(\varepsilon)} \tag{D.105}$$

to

$$\varphi_o(r) = \frac{3GM}{2a} \frac{g(\varepsilon)}{h(\varepsilon)} = \frac{3}{2} \frac{GM}{a} F(\varepsilon). \tag{D.106}$$

The goal now is to expand $F(\varepsilon)$ to the first order in ε :

$$\varphi_o(r) = \frac{3}{2} \frac{GM}{a} (F(o) + F'(o)\varepsilon + \mathcal{O}(\varepsilon^2)) \tag{D.107}$$

Because $h(o) = o$ this is not possible directly, but you have to do the replacements

$$F(o) \rightarrow \lim_{x \downarrow o} F(x), F'(o) \rightarrow \lim_{x \downarrow o} F'(x) \tag{D.108}$$

make. It's because

$$f_1(\mathbf{o}) = -\mathbf{1} = -f_2(\mathbf{o}) \quad (\text{D.109})$$

also

$$g(\mathbf{o}) = \mathbf{o}, \quad (\text{D.110})$$

So one can apply L'Hospital's rule to find $\lim_{\varepsilon \rightarrow 0} \frac{g(\varepsilon)}{h(\varepsilon)}$. It applies

$$\begin{aligned} g'(\varepsilon) &= \mathbf{2} \frac{r}{a} \frac{\mathbf{1}}{\mathbf{2}} (\mathbf{2} - \mathbf{2}\varepsilon) \frac{\mathbf{1}}{\sqrt{\varepsilon(\mathbf{2} - \varepsilon)}} - (\mathbf{2} - \mathbf{2}\varepsilon) [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))], \\ &\quad - \left(\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2} \right) \left[f'_1(\varepsilon) \frac{\mathbf{1}}{\sqrt{\mathbf{1} - f_1^2(\varepsilon)}} + f'_2(\varepsilon) \frac{\mathbf{1}}{\sqrt{\mathbf{1} - f_2^2(\varepsilon)}} \right] \\ &= \frac{2r(\mathbf{1} - \varepsilon)}{a\sqrt{\varepsilon(\mathbf{2} - \varepsilon)}} - \mathbf{2}(\mathbf{1} - \varepsilon) [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))] \\ &\quad - \left(\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2} \right) \left[f'_1(\varepsilon) \frac{\mathbf{1}}{\sqrt{\mathbf{1} - f_1^2(\varepsilon)}} + f'_2(\varepsilon) \frac{\mathbf{1}}{\sqrt{\mathbf{1} - f_2^2(\varepsilon)}} \right]. \end{aligned} \quad (\text{D.111})$$

They apply

$$f_1^2(\varepsilon) = \frac{\varepsilon^2(\mathbf{2} - \varepsilon)^2 + \frac{r^2}{a^2}(\mathbf{1} - \varepsilon)^2 - \mathbf{2}\varepsilon(\mathbf{2} - \varepsilon)\frac{r}{a}(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} \quad (\text{D.112})$$

and

$$f_2^2(\varepsilon) = \frac{\varepsilon^2(\mathbf{2} - \varepsilon)^2 + \frac{r^2}{a^2}(\mathbf{1} - \varepsilon)^2 + \mathbf{2}\varepsilon(\mathbf{2} - \varepsilon)\frac{r}{a}(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}}. \quad (\text{D.113})$$

Follow from this

$$\begin{aligned} \mathbf{1} - f_1^2(\varepsilon) &= \frac{\varepsilon(\mathbf{2} - \varepsilon)(\mathbf{1} - \varepsilon(\mathbf{2} - \varepsilon)) + \frac{r^2}{a^2}(\mathbf{1} - (\mathbf{1} - \varepsilon)^2) + \mathbf{2}\varepsilon(\mathbf{2} - \varepsilon)\frac{r}{a}(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} \\ &= \frac{\varepsilon(\mathbf{2} - \varepsilon)(\mathbf{1} - \mathbf{2}\varepsilon + \varepsilon^2) + \frac{r^2}{a^2}(\mathbf{1} - \mathbf{1} - \varepsilon^2 + \mathbf{2}\varepsilon) + \mathbf{2}\varepsilon(\mathbf{2} - \varepsilon)\frac{r}{a}(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} \\ &= \frac{\varepsilon(\mathbf{2} - \varepsilon)(\mathbf{1} - \varepsilon)^2 + \frac{r^2}{a^2}\varepsilon(\mathbf{2} - \varepsilon) + \mathbf{2}\varepsilon\frac{r}{a}(\mathbf{2} - \varepsilon)(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} = (\mathbf{2} - \varepsilon)\varepsilon \frac{(\mathbf{1} - \varepsilon)^2 + \frac{r^2}{a^2} + \mathbf{2}\frac{r}{a}(\mathbf{1} - \varepsilon)}{(\mathbf{2} - \varepsilon)\varepsilon + \frac{r^2}{a^2}} \\ &= (\mathbf{2} - \varepsilon)\varepsilon \frac{\left[(\mathbf{1} - \varepsilon) + \frac{r}{a} \right]^2}{(\mathbf{2} - \varepsilon)\varepsilon + \frac{r^2}{a^2}} \end{aligned} \quad (\text{D.114})$$

and

$$\begin{aligned} \mathbf{1} - f_2^2(\varepsilon) &= \frac{\varepsilon(\mathbf{2} - \varepsilon)(\mathbf{1} - \varepsilon(\mathbf{2} - \varepsilon)) + \frac{r^2}{a^2}(\mathbf{1} - (\mathbf{1} - \varepsilon)^2) - \mathbf{2}\varepsilon(\mathbf{2} - \varepsilon)\frac{r}{a}(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} \\ &= \frac{\varepsilon(\mathbf{2} - \varepsilon)(\mathbf{1} - \mathbf{2}\varepsilon + \varepsilon^2) + \frac{r^2}{a^2}(\mathbf{1} - \mathbf{1} - \varepsilon^2 + \mathbf{2}\varepsilon) - \mathbf{2}\varepsilon(\mathbf{2} - \varepsilon)\frac{r}{a}(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} \\ &= \frac{\varepsilon(\mathbf{2} - \varepsilon)(\mathbf{1} - \varepsilon)^2 + \frac{r^2}{a^2}\varepsilon(\mathbf{2} - \varepsilon) - \mathbf{2}\varepsilon\frac{r}{a}(\mathbf{2} - \varepsilon)(\mathbf{1} - \varepsilon)}{\varepsilon(\mathbf{2} - \varepsilon) + \frac{r^2}{a^2}} = (\mathbf{2} - \varepsilon)\varepsilon \frac{(\mathbf{1} - \varepsilon)^2 + \frac{r^2}{a^2} - \mathbf{2}\frac{r}{a}(\mathbf{1} - \varepsilon)}{(\mathbf{2} - \varepsilon)\varepsilon + \frac{r^2}{a^2}} \\ &= (\mathbf{2} - \varepsilon)\varepsilon \frac{\left[(\mathbf{1} - \varepsilon) - \frac{r}{a} \right]^2}{(\mathbf{2} - \varepsilon)\varepsilon + \frac{r^2}{a^2}}. \end{aligned} \quad (\text{D.115})$$

Follow from this

$$\frac{\mathbf{I}}{\sqrt{\mathbf{I} - f_1^2(\varepsilon)}} = \frac{\mathbf{I}}{\mathbf{I} - \varepsilon + \frac{r}{a}} \sqrt{\frac{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}}{\varepsilon(2 - \varepsilon)}} \quad (\text{D.116})$$

and

$$\frac{\mathbf{I}}{\sqrt{\mathbf{I} - f_2^2(\varepsilon)}} = \frac{\mathbf{I}}{\varepsilon + \frac{r}{a} - \mathbf{I}} \sqrt{\frac{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}}{\varepsilon(2 - \varepsilon)}}. \quad (\text{D.117})$$

It follows

$$\begin{aligned} & \left(\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2} \right) \left(f_1'(\varepsilon) \frac{\mathbf{I}}{\sqrt{\mathbf{I} - f_1^2(\varepsilon)}} + f_2'(\varepsilon) \frac{\mathbf{I}}{\sqrt{\mathbf{I} - f_2^2(\varepsilon)}} \right) \\ &= \frac{\left[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2} \right]^{3/2}}{\sqrt{\varepsilon(2 - \varepsilon)}} \cdot \frac{\mathbf{I}}{\left[\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2} \right]^{3/2}} \cdot \left[\frac{\varepsilon(\mathbf{I} - \varepsilon)(2 - \varepsilon) + \frac{r^3}{a^3} + \frac{r^2}{a^2} 2(\mathbf{I} - \varepsilon) + \frac{r}{a}}{\mathbf{I} - \varepsilon + \frac{r}{a}} \right. \\ &+ \left. \frac{\varepsilon(\mathbf{I} - \varepsilon)(2 - \varepsilon) - \frac{r^3}{a^3} + \frac{r^2}{a^2} 2(\mathbf{I} - \varepsilon) - \frac{r}{a}}{\varepsilon + \frac{r}{a} - \mathbf{I}} \right] \\ &= \frac{\mathbf{I}}{\sqrt{\varepsilon(2 - \varepsilon)}} \left[\frac{\varepsilon(\mathbf{I} - \varepsilon)(2 - \varepsilon) + \frac{r^3}{a^3} + \frac{r^2}{a^2} 2(\mathbf{I} - \varepsilon) + \frac{r}{a}}{\mathbf{I} - \varepsilon + \frac{r}{a}} + \frac{\varepsilon(\mathbf{I} - \varepsilon)(2 - \varepsilon) - \frac{r^3}{a^3} + \frac{r^2}{a^2} 2(\mathbf{I} - \varepsilon) - \frac{r}{a}}{\varepsilon + \frac{r}{a} - \mathbf{I}} \right] \\ &= \frac{\mathbf{I}}{\sqrt{\varepsilon(2 - \varepsilon)}} \frac{2\frac{r}{a}\varepsilon(\mathbf{I} - \varepsilon)(2 - \varepsilon) + 4(\mathbf{I} - \varepsilon)\frac{r^3}{a^3} - 2(\mathbf{I} - \varepsilon)\frac{r^3}{a^3} - 2\frac{r}{a}(\mathbf{I} - \varepsilon)}{\frac{r^2}{a^2} - \mathbf{I} - \varepsilon^2 + 2\varepsilon} \\ &= \frac{2\frac{r}{a}(\mathbf{I} - \varepsilon)}{\sqrt{\varepsilon(2 - \varepsilon)}} \frac{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2} - \mathbf{I}}{\frac{r^2}{a^2} - \mathbf{I} - \varepsilon^2 + 2\varepsilon} = \frac{2\frac{r}{a}(\mathbf{I} - \varepsilon)}{\sqrt{\varepsilon(2 - \varepsilon)}}. \end{aligned} \quad (\text{D.118})$$

So you have

$$g'(\varepsilon) = \frac{2r(\mathbf{I} - \varepsilon)}{a\sqrt{\varepsilon(2 - \varepsilon)}} - 2(\mathbf{I} - \varepsilon) [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))], \quad (\text{D.119})$$

$$- \frac{2\frac{r}{a}(\mathbf{I} - \varepsilon)}{\sqrt{\varepsilon(2 - \varepsilon)}} = -2(\mathbf{I} - \varepsilon) [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]. \quad (\text{D.120})$$

Still applies

$$h'(\varepsilon) = 2\frac{3}{2}\sqrt{\varepsilon(2 - \varepsilon)}(2 - 2\varepsilon) = 6\sqrt{\varepsilon(2 - \varepsilon)}(\mathbf{I} - \varepsilon). \quad (\text{D.121})$$

So it applies

$$\frac{g'(\varepsilon)}{h'(\varepsilon)} = -\frac{\mathbf{I}}{3\sqrt{\varepsilon(2 - \varepsilon)}} [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]. \quad (\text{D.122})$$

Here you have to apply L'Hospital's rule again, it applies

$$\frac{d}{d\varepsilon} [\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))] = \frac{\mathbf{I}}{\varepsilon(2 - \varepsilon) + \frac{r^2}{a^2}} \frac{2\frac{r}{a}(\mathbf{I} - \varepsilon)}{\sqrt{\varepsilon(2 - \varepsilon)}} \quad (\text{D.123})$$

as well as

$$\frac{d}{d\varepsilon} \sqrt{\varepsilon(2 - \varepsilon)} = \frac{\mathbf{I} - \varepsilon}{\sqrt{\varepsilon(2 - \varepsilon)}}. \quad (\text{D.124})$$

This follows

$$\lim_{\varepsilon \rightarrow 0} \frac{g'(\varepsilon)}{h'(\varepsilon)} = -\frac{1}{3} \frac{2 \frac{r}{a}}{\frac{r^2}{a^2}} = -\frac{2a}{3r}. \quad (\text{D.125})$$

and thus

$$\lim_{\varepsilon \rightarrow 0} F(\varepsilon) = -\frac{2a}{3r}. \quad (\text{D.126})$$

In the case of a sphere, the correct limiting case results. For the derivation of F applies

$$\begin{aligned} F'(\varepsilon) &= \frac{g'(\varepsilon)h(\varepsilon) - g(\varepsilon)h'(\varepsilon)}{h(\varepsilon)^2} = \frac{-2(1-\varepsilon)[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]2(\varepsilon(2-\varepsilon))^{3/2}}{4(\varepsilon(2-\varepsilon))^3} \\ &\quad - \frac{\left(2\frac{r}{a}(\varepsilon(2-\varepsilon))^{1/2} - (\varepsilon(2-\varepsilon) + \frac{r^2}{a^2})[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]\right)6(1-\varepsilon)\sqrt{\varepsilon(2-\varepsilon)}}{4(\varepsilon(2-\varepsilon))^3} \\ &= \frac{(1-\varepsilon)[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]}{2(\varepsilon(2-\varepsilon))^{3/2}} + \frac{3r^2(1-\varepsilon)[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]}{2a^2(\varepsilon(2-\varepsilon))^{5/2}} \\ &\quad - 3\frac{r}{a}\frac{1-\varepsilon}{(\varepsilon(2-\varepsilon))^2}. \end{aligned} \quad (\text{D.127})$$

Due to the calculation rules for function limits, $\lim_{\varepsilon \rightarrow 0} F'(\varepsilon) = \frac{1}{4\sqrt{2}} \lim_{\varepsilon \rightarrow 0} G(\varepsilon)$ with

$$\begin{aligned} G(\varepsilon) &:= \frac{(2-\varepsilon)[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]}{2\varepsilon^{3/2}} + \frac{3r^2 \arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))}{2a^2 \varepsilon^{5/2}} - 3\frac{r\sqrt{2-\varepsilon}}{a\varepsilon^2} \\ &= \frac{(a^2\varepsilon(2-\varepsilon) + 3r^2)[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))] - 6ra\sqrt{\varepsilon(2-\varepsilon)}}{2a^2\varepsilon^{5/2}}. \end{aligned} \quad (\text{D.128})$$

It applies with L'Hospital's rule

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} G(\varepsilon) &= \lim_{\varepsilon \rightarrow 0} \frac{2a^2(1-\varepsilon)[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]}{5a^2\varepsilon^{3/2}} \\ &\quad + \frac{(a^2\varepsilon(2-\varepsilon) + 3r^2)\frac{1}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}}\frac{2\frac{r}{a}(1-\varepsilon)}{\sqrt{\varepsilon(2-\varepsilon)}}}{5a^2\varepsilon^{3/2}} - \frac{6ra\frac{1-\varepsilon}{\sqrt{\varepsilon(2-\varepsilon)}}}{5a^2\varepsilon^{3/2}} \\ &= \frac{2}{5a^2} \lim_{\varepsilon \rightarrow 0} \frac{a^2[\arcsin(f_1(\varepsilon)) + \arcsin(f_2(\varepsilon))]}{\varepsilon^{3/2}} + \frac{(a^2\varepsilon(2-\varepsilon) + 3r^2)\frac{1}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}}\frac{\frac{r}{a}}{\sqrt{\varepsilon(2-\varepsilon)}}}{\varepsilon^{3/2}} - 3\frac{ra}{\sqrt{\varepsilon(2-\varepsilon)}} \\ &= \frac{4}{15a^2} \lim_{\varepsilon \rightarrow 0} \frac{2a^2}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}}\frac{2\frac{r}{a}(1-\varepsilon)}{\varepsilon\sqrt{2-\varepsilon}} + 3\frac{ra(1-\varepsilon)}{\varepsilon^2(2-\varepsilon)^{3/2}} \\ &\quad - (a^2\varepsilon(2-\varepsilon) + 3r^2)\frac{2(1-\varepsilon)}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2}\frac{\frac{r}{a}}{\varepsilon\sqrt{2-\varepsilon}} - \frac{a^2\varepsilon(2-\varepsilon) + 3r^2}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}}\frac{\frac{r}{a}(1-\varepsilon)}{\varepsilon^2(2-\varepsilon)^{3/2}}. \end{aligned} \quad (\text{D.129})$$

With

$$\begin{aligned}
& \frac{2a^2}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}} \frac{2\frac{r}{a}(1-\varepsilon)}{\varepsilon\sqrt{2-\varepsilon}} - (a^2\varepsilon(2-\varepsilon) + 3r^2) \frac{2(1-\varepsilon)}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \frac{\frac{r}{a}}{\varepsilon\sqrt{2-\varepsilon}} \\
&= \frac{2\frac{r}{a}(1-\varepsilon)a^2}{\varepsilon\sqrt{(2-\varepsilon)}} \frac{1}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \left[2\varepsilon(2-\varepsilon) + 2\frac{r^2}{a^2} - \varepsilon(2-\varepsilon) - \frac{3r^2}{a^2} \right] \\
&= \frac{2\frac{r}{a}(1-\varepsilon)a^2}{\varepsilon\sqrt{2-\varepsilon}} \frac{1}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \left[-\frac{r^2}{a^2} + \varepsilon(2-\varepsilon) \right] \\
&= -\frac{2r^3(1-\varepsilon)}{a\varepsilon\sqrt{2-\varepsilon}} \frac{1}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} + \frac{2\frac{r}{a}(1-\varepsilon)a^2\sqrt{2-\varepsilon}}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2}
\end{aligned} \tag{D.130}$$

and

$$\begin{aligned}
& 3 \frac{ra(1-\varepsilon)}{\varepsilon^2(2-\varepsilon)^{3/2}} - \frac{a^2\varepsilon(2-\varepsilon) + 3r^2}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}} \frac{\frac{r}{a}(1-\varepsilon)}{\varepsilon^2(2-\varepsilon)^{3/2}} \\
&= ra \frac{1-\varepsilon}{\varepsilon^2(2-\varepsilon)^{3/2}} \left[3 - \frac{\varepsilon(2-\varepsilon) + 3\frac{r^2}{a^2}}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}} \right] = \frac{ra}{\varepsilon^2(2-\varepsilon)^{3/2}} \frac{2\varepsilon(2-\varepsilon)}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}}
\end{aligned} \tag{D.131}$$

follows

$$\begin{aligned}
\lim_{\varepsilon \rightarrow 0} G(\varepsilon) &= \frac{4}{15a^2\sqrt{2}} \lim_{\varepsilon \rightarrow 0} -\frac{1r^3}{a\varepsilon[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} + \frac{ra}{\varepsilon^2(2-\varepsilon)} \frac{2\varepsilon(2-\varepsilon)}{\varepsilon(2-\varepsilon) + r^2} + \frac{2\frac{r}{a}(1-\varepsilon)a^2(2-\varepsilon)}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \\
&= \frac{4r}{15a^2\sqrt{2}} \lim_{\varepsilon \rightarrow 0} -\frac{2r^2}{a\varepsilon[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} + \frac{a}{\varepsilon} \frac{2}{\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}} + \frac{2\frac{1}{a}(1-\varepsilon)a^2(2-\varepsilon)}{[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \\
&= \frac{4}{15r\sqrt{2}} \lim_{\varepsilon \rightarrow 0} -\frac{2r^2}{a\varepsilon[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]} + \frac{2a}{\varepsilon} + \frac{2r^2(1-\varepsilon)(2-\varepsilon)}{a[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \\
&= \frac{4}{15r\sqrt{2}} \lim_{\varepsilon \rightarrow 0} \frac{-2\frac{r^2}{a} + 2a\varepsilon(2-\varepsilon) + 2\frac{r^2}{a}}{\varepsilon(\varepsilon(2-\varepsilon) + \frac{r^2}{a^2})} + \frac{2r^2(1-\varepsilon)(2-\varepsilon)}{a[\varepsilon(2-\varepsilon) + \frac{r^2}{a^2}]^2} \\
&= \frac{4}{15r\sqrt{2}} \left[\frac{4a}{\frac{r^2}{a^2}} + \frac{4r^2}{a\frac{r^4}{a^4}} \right] = \frac{4}{15r\sqrt{2}} \frac{8a^3}{r^2} = \frac{32}{15\sqrt{2}} \frac{a^3}{r^3}.
\end{aligned} \tag{D.132}$$

Thus follows

$$\lim_{\varepsilon \rightarrow 0} F'(\varepsilon) = \frac{4}{15} \frac{a^3}{r^3}. \tag{D.133}$$

Analogously, the higher order coefficients can be determined in ε . So you have

$$\varphi_o(r) = \frac{3GM}{2a} \left[-\frac{2a}{3r} + \varepsilon \frac{4a^3}{15r^3} \right] = -\frac{GM}{r} + \varepsilon \frac{2GM}{5r^3} a^2, \tag{D.134}$$

the terms $\mathcal{O}(\varepsilon^2)$ were neglected. It therefore applies in terms of Eq. (D.67)

$$b_1 = 0, \tag{D.135}$$

$$b_2(\varepsilon) = \varepsilon \frac{2GMa^2}{5}. \tag{D.136}$$

This therefore applies to the gravitational component of the Earth's gravity potential

$$\varphi_o(r, \chi) = -\frac{GM}{r} + \frac{b_2}{2r^3} (3\sin^2(\chi) - 1) = -\frac{GM}{r} + \varepsilon \frac{GMa^2}{5r^3} (3\sin^2(\chi) - 1). \tag{D.137}$$

Now the centrifugal force is taken into account. Define

$$m := \frac{\omega^2 a^3}{GM}. \quad (\text{D.138})$$

Then the centrifugal component φ_z is written using Eq. (D.34) as

$$\varphi_z = -\frac{\mathbf{1}}{\mathbf{2}}\omega^2 r^2 \cos^2(\chi) = -\frac{\mathbf{1}}{\mathbf{2}}\frac{GMm}{a^3}r^2 \cos^2(\chi) = \frac{GMm}{\mathbf{2}a^3}r^2 (\sin^2(\chi) - \mathbf{1}). \quad (\text{D.139})$$

For the gravity potential one obtains

$$\begin{aligned} \varphi_g(r, \chi) &= \varphi_o(r, \chi) + \varphi_z(r, \chi) = -\frac{GM}{r} + \varepsilon \frac{GMa^2}{5r^3} (3\sin^2(\chi) - \mathbf{1}) + \frac{GMm}{\mathbf{2}a^3}r^2 (\sin^2(\chi) - \mathbf{1}) \\ &= \frac{GM}{r} \left[\left\{ \frac{3a^2\varepsilon}{5r^2} + \frac{mr^3}{\mathbf{2}a^3} \right\} \sin^2(\chi) - \mathbf{1} \right] - \frac{GM}{a} \left\{ \frac{a^3}{5r^3}\varepsilon + \frac{mr^2}{\mathbf{2}a^2} \right\}. \end{aligned} \quad (\text{D.140})$$

An additional condition is now required that the surface of the ellipsoid of revolution is an equipotential surface, i.e

$$\varphi_g(r, \chi) = \text{const.} \quad (\text{D.141})$$

for

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{c^2} = \mathbf{1}. \quad (\text{D.142})$$

A necessary condition for this is that the geopotential at the equator corresponds to that at the pole, i.e

$$\begin{aligned} -\frac{GM}{a} - \frac{GM}{a} \left[\frac{\varepsilon}{5} + \frac{m}{\mathbf{2}} \right] &= \frac{GM}{c} \left[\frac{3a^2\varepsilon}{5c^2} + \frac{mc^3}{\mathbf{2}a^3} - \mathbf{1} \right] - \frac{GM}{a} \left[\frac{\varepsilon a^3}{5c^3} + \frac{mc^2}{\mathbf{2}a^2} \right] \\ \Leftrightarrow \mathbf{1} + \frac{\varepsilon}{5} + \frac{m}{\mathbf{2}} &= -\frac{3a^3}{5c^3}\varepsilon - \frac{mc^2}{\mathbf{2}a^2} + \frac{a}{c} + \frac{\varepsilon a^3}{5c^3} + \frac{mc^2}{\mathbf{2}a^2} \\ \Leftrightarrow \mathbf{1} + \frac{\varepsilon}{5} + \frac{m}{\mathbf{2}} &= -\frac{\mathbf{2}a^3}{5c^3}\varepsilon + \frac{\mathbf{1}}{\mathbf{1}-\varepsilon} \\ \Leftrightarrow -\varepsilon + (\mathbf{1}-\varepsilon) \left(\frac{\varepsilon}{5} + \frac{m}{\mathbf{2}} \right) &= -(\mathbf{1}-\varepsilon) \frac{\mathbf{2}a^3}{5c^3}\varepsilon = -\varepsilon(\mathbf{1}-\varepsilon) \frac{\mathbf{2}}{5} (\mathbf{1}-\varepsilon)^3. \end{aligned} \quad (\text{D.143})$$

If you neglect all the terms $\mathcal{O}(\varepsilon^2)$ and also $\mathcal{O}(\varepsilon m)$, you get

$$-\varepsilon + \frac{\varepsilon}{5} + \frac{m}{\mathbf{2}} = -\varepsilon \frac{\mathbf{2}}{5} \Leftrightarrow \frac{m}{\mathbf{2}} = \varepsilon \frac{\mathbf{2}}{5}. \quad (\text{D.144})$$

So it applies in the equilibrium case

$$\varepsilon = \varepsilon(m) = \frac{5m}{4}. \quad (\text{D.145})$$

Given a semi-major axis, the semi-minor axis c is fixed:

$$c = a(\mathbf{1} - \varepsilon(m)) = a \left(\mathbf{1} - \frac{5m}{4} \right). \quad (\text{D.146})$$

You use it

$$\frac{3\varepsilon}{5} = \varepsilon - \frac{\mathbf{2}}{5}\varepsilon = \varepsilon - \frac{m}{\mathbf{2}} = \frac{\mathbf{2}\varepsilon - m}{\mathbf{2}} \quad (\text{D.147})$$

to simplify the expression for the gravity potential:

$$\mathcal{P}_g(r, \chi) = \frac{GM}{r} \left[\left\{ \left(\frac{2\varepsilon - m}{2} \right) \frac{a^2}{r^2} + \frac{m}{2} \frac{r^3}{a^3} \right\} \sin^2(\chi) - 1 \right] - \frac{GM}{a} \left\{ \left(\frac{2\varepsilon - m}{6} \right) \frac{a^3}{r^3} + \frac{m}{2} \frac{r^2}{a^2} \right\} \quad (\text{D.148})$$

This is the formula that will be used from now on. Since it is first order in ε and m , all subsequent approximations are also only made in first order in ε and m .

D.3.3 Requirements for non-spherical coordinates

For the development of a meteorological coordinate system, it is practical if the surfaces with the same vertical coordinate are equipotential surfaces in the gravity field (see section 13.2). It is also expected to be advantageous for these surfaces to be ellipsoidal. For the development of a non-spherical coordinate system, it is also important to be able to specify the trajectories perpendicular to all potential surfaces in terms of the basic functions. In addition, the geopotential approximation used must be as consistent as possible with real physics and at the same time can be treated analytically. This means that the correct Clairaut ratio results again, and that $c = a(1 - \varepsilon)$.

The requirements for an approximation of the gravity field are:

1. Possibility of analytically specifying the vertical trajectories
2. ellipsoidal contour surfaces
3. correct Clairaut ratio
4. correct semi-axis ratio

D.3.4 Ellipsoidal approximation of the gravity field

The first question that arises is whether all contour surfaces of Eq. (D.148) are ellipsoids. For the surface of the Earth (without orography) this has already been ensured to the first order in ε and m by $\varepsilon = \frac{5}{4}m$. With $r = \sqrt{x^2 + y^2 + z^2}$ one can derive an expression for the distance r from the center of an ellipsoid of revolution with a semi-major axis A and a semi-minor axis C as a function of the geocentric angle χ at a given eccentricity:

$$\begin{aligned} 1 &= \frac{r^2 \cos^2(\chi)}{A^2} + \frac{r^2 \sin^2(\chi)}{C^2} = \frac{r^2}{A^2} \left(\cos^2(\chi) + A^2 \frac{\sin^2(\chi)}{C^2} \right) \\ \Leftrightarrow r(\chi) &= A \left[\cos^2(\chi) + A^2 \frac{\sin^2(\chi)}{C^2} \right]^{-1/2} \end{aligned} \quad (\text{D.149})$$

With $A = a$, $C = c = a(1 - \varepsilon)$ it follows

$$r(\chi) = a(1 - \varepsilon) \left[(1 - \varepsilon)^2 + (1 - (1 - \varepsilon)^2) \sin^2(\chi) \right]^{-1/2} \quad (\text{D.150})$$

Eq. (D.148) is not of this form: If you keep the left side of the equation constant and multiply by r^3 , you get a fifth degree polynomial in r , which can generally only be solved numerically.

So one has to use an ellipsoidal approximation of Eq. (D.148). The following discussion is based on [34]. First of all, make it clear how you can designate a specific geopotential surface. The equatorial radius R of the surface is suitable for this. For him applies

$$\mathcal{P}_R = -\frac{GM}{R} \left[1 + \left(\frac{2\varepsilon - m}{6} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right]. \quad (\text{D.151})$$

If you now want to specify this area more precisely, i.e. specify its distance $r = r(\chi)$ from the center of the earth at a geocentric latitude φ , you simply write

$$\begin{aligned} \frac{1}{R} \left[1 + \left(\frac{2\varepsilon - m}{6} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right] &= \frac{1}{r} \left[1 - \left\{ \left(\frac{2\varepsilon - m}{2} \right) \frac{a^2}{r^2} + \frac{m}{2} \frac{r^3}{a^3} \right\} \sin^2(\chi) \right] \\ &+ \frac{1}{a} \left\{ \left(\frac{2\varepsilon - m}{6} \right) \frac{a^3}{r^3} + \frac{m}{2} \frac{r^2}{a^2} \right\}. \end{aligned} \quad (\text{D.152})$$

Now one makes the assumption that this applies

$$\frac{r}{R} = \mathbf{1} + \frac{r-R}{R} = \mathbf{1} + \mathcal{O}(\varepsilon), \quad (\text{D.153})$$

It is valid

$$\frac{r-R}{R} \lesssim \frac{c-a}{a} = -\varepsilon, \quad (\text{D.154})$$

at least within the weather-relevant atmosphere. You can now write first

$$\begin{aligned} \mathcal{P}_g(r, \chi) &= -\frac{GM}{r} + \frac{GM}{R} \frac{\mathbf{1}}{r/R} \left[\left(\frac{2\varepsilon - m}{2} \right) \frac{a^2}{R^2} \frac{R^2}{r^2} + \frac{m}{2} \frac{R^3}{a^3} \frac{r^3}{R^3} \right] \sin^2(\chi) \\ &\quad - \frac{GM}{a} \left[\left(\frac{2\varepsilon - m}{6} \right) \frac{a^3}{R^3} \frac{R^3}{r^3} + \frac{m}{2} \frac{R^2}{a^2} \frac{r^2}{R^2} \right] \\ &= -\frac{GM}{r} + \frac{GM}{R} \left(\mathbf{1} + \frac{r-R}{R} \right)^{-1} \left[\left(\frac{2\varepsilon - m}{2} \right) \frac{a^2}{R^2} \left(\mathbf{1} + \frac{r-R}{R} \right)^{-2} \right. \\ &\quad \left. + \frac{m}{2} \frac{R^3}{a^3} \left(\mathbf{1} + \frac{r-R}{R} \right)^3 \right] \sin^2(\chi) - \frac{GM}{a} \left[\left(\frac{2\varepsilon - m}{6} \right) \frac{a^3}{R^3} \left(\mathbf{1} + \frac{r-R}{R} \right)^{-3} \right. \\ &\quad \left. + \frac{m}{2} \frac{R^2}{a^2} \left(\mathbf{1} + \frac{r-R}{R} \right)^2 \right]. \end{aligned} \quad (\text{D.155})$$

By neglecting terms $\mathcal{O}(\varepsilon^2, m^2, \varepsilon m)$ this becomes initially the case

$$\begin{aligned} \mathcal{P}_g(\chi, R) &= -\frac{GM}{r(\chi, R)} + \frac{GM}{R} \left[\mathbf{1} + \left\{ \left(\frac{2\varepsilon - m}{2} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right\} \sin^2(\chi) \right] \\ &\quad - \frac{GM}{R} \left[\mathbf{1} + \left(\frac{2\varepsilon - m}{6} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right] + \mathcal{O}(\varepsilon^2, m^2, \varepsilon m) \end{aligned} \quad (\text{D.156})$$

and then continue to

$$\begin{aligned} \mathcal{P}_g(\chi, R) &\approx -\frac{GM}{r(\chi, R)} + \frac{GM}{R} \left[\mathbf{1} + \left\{ (2\varepsilon - m) \frac{a^2}{R^2} + m \frac{R^3}{a^3} \right\} \sin^2(\chi) \right]^{1/2} \\ &\quad - \frac{GM}{R} \left[\mathbf{1} + \left(\frac{2\varepsilon - m}{6} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right]. \end{aligned} \quad (\text{D.157})$$

The contour surfaces of this are already ellipsoids. To show this, determine the geocentric distance r as a function of latitude given the equatorial radius R :

$$\begin{aligned} &-\frac{GM}{R} + \frac{GM}{R} - \frac{GM}{R} - \frac{GM}{R} \left[\left(\frac{2\varepsilon - m}{6} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right] \\ &= -\frac{GM}{r} + \frac{GM}{R} \left[\mathbf{1} + \left\{ (2\varepsilon - m) \frac{a^2}{R^2} + m \frac{R^3}{a^3} \right\} \sin^2(\chi) \right]^{1/2} - \frac{GM}{R} - \frac{GM}{R} \left[\left(\frac{2\varepsilon - m}{6} \right) \frac{a^2}{R^2} + \frac{m}{2} \frac{R^3}{a^3} \right] \\ \Leftrightarrow \mathbf{1} &= \frac{R}{r} - \left[\mathbf{1} + \sin^2(\chi) \left\{ (2\varepsilon - m) \frac{a^2}{R^2} + m \frac{R^3}{a^3} \right\} \right]^{1/2} + \mathbf{1} \\ \Leftrightarrow r &= R \frac{\mathbf{1}}{\left[\mathbf{1} + \sin^2(\chi) \left\{ (2\varepsilon - m) \frac{a^2}{R^2} + m \frac{R^3}{a^3} \right\} \right]^{1/2}} \\ \Leftrightarrow r(R, \chi) &= R \left[\cos^2(\chi) + \sin^2(\chi) \left\{ (2\varepsilon - m) \frac{a^2}{R^2} + m \frac{R^3}{a^3} + \mathbf{1} \right\} \right]^{-1/2} \end{aligned} \quad (\text{D.158})$$

If one sets $R = A$ and $C = A \left\{ (2\varepsilon - m) \frac{a^2}{R^2} + m \frac{R^3}{a^3} + \mathbf{1} \right\}^{-1/2}$ in Eq. (D.149) you get exactly this result. Unfortunately, the trajectories orthogonal to the contour sets of this potential cannot be determined analytically, so Eq.

(D.155) needs to be further approximated. To do this, the terms $\frac{a^2}{R^2}$ and $\frac{R^3}{a^3}$ are expanded by $R^2 = a^2$: This is justified because of $\frac{R-a}{a} \lesssim \mathbf{1} \mathbf{o}^{-2}$.

$$\frac{a^2}{R^2} \approx \mathbf{1} - \frac{\mathbf{1}}{a^2} (R^2 - a^2) = \mathbf{2} - \frac{R^2}{a^2}, \quad (\text{D.159})$$

$$\frac{R^3}{a^3} = \frac{(R^2)^{3/2}}{a^3} \approx \mathbf{1} + \frac{\mathbf{3}}{\mathbf{2}} \frac{R^2 - a^2}{a^2} = -\frac{\mathbf{1}}{\mathbf{2}} + \frac{\mathbf{3}}{\mathbf{2}} \frac{R^2}{a^2} \quad (\text{D.160})$$

Putting this into Eq. (D.155), you get

$$\begin{aligned} \varphi_g(\chi, R) \approx & -\frac{GM}{r(\chi, R)} + \frac{GM}{R} \left[\mathbf{1} + \left\{ \left(\frac{8\varepsilon - 5m}{\mathbf{2}} \right) + \left(\frac{5m - 4\varepsilon}{\mathbf{2}} \right) \frac{R^2}{a^2} \right\} \sin^2(\chi) \right]^{1/2} \\ & - \frac{GM}{R} \left[\mathbf{1} + \left(\frac{8\varepsilon - 7m}{\mathbf{12}} \right) + \left(\frac{\mathbf{11}m - 4\varepsilon}{\mathbf{12}} \right) \frac{R^2}{a^2} \right]. \end{aligned} \quad (\text{D.161})$$

This leads to

$$r(\chi, R) = R \left[\cos^2(\chi) + \sin^2(\chi) \left\{ \left(\frac{8\varepsilon - 5m}{\mathbf{2}} \right) + \left(\frac{5m - 4\varepsilon}{\mathbf{2}} \right) \frac{R^2}{a^2} + \mathbf{1} \right\} \right]^{-1/2}, \quad (\text{D.162})$$

with Eq. (D.149) will do this

$$C = R \left\{ \mathbf{1} + \left(\frac{8\varepsilon - 5m}{\mathbf{2}} \right) + \left(\frac{5m - 4\varepsilon}{\mathbf{2}} \right) \frac{R^2}{a^2} \right\}^{-1/2}. \quad (\text{D.163})$$

However, a self-consistency problem arises here. If you set $R = a$ in Eq. (D.162), you get

$$r(\chi, a) = a \left[\mathbf{1} + \mathbf{2}\varepsilon \sin^2(\chi) \right]^{-1/2}. \quad (\text{D.164})$$

This expression describes the earth's surface without orography. You receive

$$r(\mathbf{o}, a) = a, \quad r(\pi/\mathbf{2}, a) = a \frac{\mathbf{1}}{\sqrt{\mathbf{1} + \mathbf{2}\varepsilon}}. \quad (\text{D.165})$$

With

$$\frac{d}{d\varepsilon} \frac{\mathbf{1}}{\sqrt{\mathbf{1} + \mathbf{2}\varepsilon}} = -\frac{\mathbf{1}}{(\mathbf{1} + \mathbf{2}\varepsilon)^{3/2}} \quad (\text{D.166})$$

follows

$$r(\pi/\mathbf{2}) = a - a\varepsilon + \mathcal{O}(\varepsilon^2) \approx a(\mathbf{1} - \varepsilon), \quad (\text{D.167})$$

So not the desired exact result $r(\pi/\mathbf{2}) = a(\mathbf{1} - \varepsilon)$. To solve this problem, define

$$\widetilde{\varepsilon} := \frac{a^2 - c^2}{\mathbf{2}c^2} = \frac{\mathbf{1} - (\mathbf{1} - \varepsilon)^2}{\mathbf{2}(\mathbf{1} - \varepsilon)^2}. \quad (\text{D.168})$$

Define the auxiliary function $f(\varepsilon)$ by

$$f(\varepsilon) := \frac{\mathbf{1} - (\mathbf{1} - \varepsilon)^2}{\mathbf{2}(\mathbf{1} - \varepsilon)^2}, \quad (\text{D.169})$$

then applies

$$f'(\varepsilon) = \frac{4(1-\varepsilon)^3 - [1 - (1-\varepsilon)^2] 2(1-\varepsilon)^2}{4(1-\varepsilon)^4} \Rightarrow f'(0) = 1. \quad (\text{D.170})$$

So is

$$\tilde{\varepsilon} = \varepsilon + \mathcal{O}(\varepsilon^2). \quad (\text{D.171})$$

So in first order you can replace ε with $\tilde{\varepsilon}$ everywhere. You receive

$$\begin{aligned} \varphi_g(\chi, R) \approx & -\frac{GM}{r(\chi, R)} + \frac{GM}{R} \left[1 + \left\{ \left(\frac{8\tilde{\varepsilon} - 5m}{2} \right) + \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) \frac{R^2}{a^2} \right\} \sin^2(\chi) \right]^{1/2} \\ & - \frac{GM}{R} \left[1 + \left(\frac{8\tilde{\varepsilon} - 7m}{12} \right) + \left(\frac{11m - 4\tilde{\varepsilon}}{12} \right) \frac{R^2}{a^2} \right]. \end{aligned} \quad (\text{D.172})$$

With this formula you also get ellipsoidal contour surfaces,

$$r(\chi, R) = R \left[1 + \sin^2(\chi) \left\{ \left(\frac{8\tilde{\varepsilon} - 5m}{2} \right) + \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) \frac{R^2}{a^2} \right\} \right]^{-1/2}, \quad (\text{D.173})$$

and also

$$r(\chi, a) = a \left[1 + 2\tilde{\varepsilon} \sin^2(\chi) \right]^{-1/2} = a(1-\varepsilon) \left[(1-\varepsilon)^2 + (1 - (1-\varepsilon)^2) \sin^2(\chi) \right]^{-1/2}. \quad (\text{D.174})$$

This is the desired result, see Eq. (D.150).

The *Clairaut's theorem* is a statement about the connection between eccentricity ε , angular velocity ω and the ratio of gravity g_a, g_p at the equator and pole. At the pole, the geopotential is $\varphi_g = \varphi_g^{(p)}$ with Eq. (D.148)

$$\varphi_g^{(p)} = -\frac{GM}{r} + \frac{GM}{r^3} a^2 \left(\frac{2\varepsilon - m}{3} \right), \quad (\text{D.175})$$

applies at the equator

$$\varphi_g^{(a)} = -\frac{GM}{r} - \frac{GM}{a} \left\{ \left(\frac{2\varepsilon - m}{6} \right) \frac{a^3}{r^3} + \frac{m}{2} \frac{r^2}{a^2} \right\}. \quad (\text{D.176})$$

Therefore apply

$$\frac{d\varphi_g^{(a)}}{dr} = \frac{GM}{r^2} - \frac{GM}{a} \left\{ -3 \left(\frac{2\varepsilon - m}{6} \right) \frac{a^3}{r^4} + m \frac{r}{a^2} \right\}, \quad (\text{D.177})$$

$$\frac{d\varphi_g^{(p)}}{dr} = \frac{GM}{r^2} - 3 \frac{GM}{r^4} a^2 \left(\frac{2\varepsilon - m}{3} \right). \quad (\text{D.178})$$

This results in $r = a$ or $r = c = a(1-\varepsilon)$

$$g_a = \frac{GM}{a^2} \left[1 + \varepsilon - 3 \frac{m}{2} \right], \quad (\text{D.179})$$

$$g_p = \frac{GM}{a^2(1-\varepsilon)^2} \left[1 - \frac{2\varepsilon}{(1-\varepsilon)^2} + \frac{m}{(1-\varepsilon)^2} \right]. \quad (\text{D.180})$$

It follows

$$\begin{aligned}\frac{g_p - g_a}{g_a} &= \frac{\frac{1}{(1-\varepsilon)^2} \left[1 - \frac{2}{(1-\varepsilon)^2} \varepsilon + \frac{m}{(1-\varepsilon)^2} \right] - 1 - \varepsilon + 3\frac{m}{2}}{1 + \varepsilon - 3\frac{m}{2}} \\ &\approx \frac{1 - \frac{2}{(1-\varepsilon)^2} \varepsilon + \frac{m}{(1-\varepsilon)^2} - 1 - \varepsilon + 3\frac{m}{2} + 2\varepsilon}{1 - \varepsilon - 3\frac{m}{2}},\end{aligned}\quad (\text{D.181})$$

where again terms $\mathcal{O}(\varepsilon^2, \varepsilon m, m^2)$ were neglected. With

$$\frac{d}{d\varepsilon} \frac{1}{(1-\varepsilon)^2} = \frac{2(1-\varepsilon)}{(1-\varepsilon)^4} = \frac{2}{(1-\varepsilon)^3} \quad (\text{D.182})$$

follows

$$\frac{1}{(1-\varepsilon)^2} \approx 1 + 2\varepsilon \quad (\text{D.183})$$

and thus

$$\frac{g_p - g_a}{g_a} \approx \frac{1 - 2\varepsilon + m - 1 - \varepsilon + 3\frac{m}{2} + 2\varepsilon}{1 - \varepsilon - \frac{3m}{2}} = \frac{\frac{5m}{2} - \varepsilon}{1 - \varepsilon - \frac{3m}{2}}. \quad (\text{D.184})$$

If you insert $\varepsilon \approx \frac{5m}{4}$ here, you get

$$\frac{g_p - g_a}{g_a} \approx m \frac{\frac{5}{4}}{1 - m \left(\frac{5}{4} - \frac{3}{2} \right)} = \frac{m}{4} \frac{5}{1 + \frac{m}{4}} = \frac{5m}{4 + m}. \quad (\text{D.185})$$

Define $f(m) := \frac{5m}{4+m}$, then holds

$$\frac{df}{dm} = 5 \frac{4 + m - m}{(4 + m)^2}, \quad (\text{D.186})$$

so

$$\frac{df}{dm}(m=0) = \frac{5}{4}. \quad (\text{D.187})$$

This follows

$$\frac{g_p - g_a}{g_a} \approx 5 \frac{m}{4}. \quad (\text{D.188})$$

So that applies

$$\frac{a-c}{c} + \frac{g_p - g_a}{g_a} \approx \frac{5}{2} m = \frac{5\omega^2 a^3}{2GM}. \quad (\text{D.189})$$

This is Clairaut's theorem. This should now be done for Eq. (D.172) can be recalculated. All that needs to be shown is that Eq. (D.188) still applies. At the equator applies

$$\varphi_g^{(a)} = -\frac{GM}{r} - \frac{GM r}{a^2} \left[\left(\frac{8\tilde{\varepsilon} - 7m}{12} \right) + \left(\frac{11m - 4\tilde{\varepsilon}}{12} \right) \right]. \quad (\text{D.190})$$

It follows

$$g_a = \frac{GM}{a^2} \left[\mathbf{1} + \left(\frac{8\tilde{\varepsilon} - 7m}{\mathbf{12}} \right) + \left(\frac{\mathbf{11}m - 4\tilde{\varepsilon}}{\mathbf{12}} \right) \right]. \quad (\text{D.191})$$

At the pole applies

$$\begin{aligned} \varphi_g(\pi/2, R) &\approx -\frac{GM}{r(\pi/2, R)} + \frac{GM}{R} \left[\mathbf{1} + \left\{ \left(\frac{8\tilde{\varepsilon} - 5m}{2} \right) + \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) \frac{R^2}{a^2} \right\} \right]^{1/2} \\ &\quad - \frac{GM}{R} \left[\mathbf{1} + \left(\frac{8\tilde{\varepsilon} - 7m}{\mathbf{12}} \right) + \left(\frac{\mathbf{11}m - 4\tilde{\varepsilon}}{\mathbf{12}} \right) \frac{R^2}{a^2} \right]. \end{aligned} \quad (\text{D.192})$$

It follows

$$g_p = \frac{d\varphi_g}{dr} = \frac{\partial R}{\partial r} \frac{d\varphi_g}{dR} = \frac{\mathbf{1}}{\partial r / \partial R} \frac{d\varphi_g}{dR} = \frac{\mathbf{1}}{\partial r / \partial R} g_a. \quad (\text{D.193})$$

For dr/dR it follows from Eq. (D.173)

$$\begin{aligned} \frac{\partial r}{\partial R} &= \left[\mathbf{1} + \left\{ \left(\frac{8\tilde{\varepsilon} - 5m}{2} \right) + \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) \frac{R^2}{a^2} \right\} \sin^2(\chi) \right]^{-1/2} \\ &\quad - \frac{R^2}{a^2} \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) \left[\mathbf{1} + \left\{ \left(\frac{8\tilde{\varepsilon} - 5m}{2} \right) + \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) \frac{R^2}{a^2} \right\} \sin^2(\chi) \right]^{-3/2}. \end{aligned} \quad (\text{D.194})$$

At the point $\chi = \pi/2$, $R = a$ this becomes

$$\begin{aligned} \frac{\partial r}{\partial R}(R = a, \chi = \pi/2) &= [\mathbf{1} + 2\tilde{\varepsilon}]^{-1/2} - \left(\frac{5m - 4\tilde{\varepsilon}}{2} \right) [\mathbf{1} + 2\tilde{\varepsilon}]^{-3/2} \\ &= (\mathbf{1} + 2\tilde{\varepsilon})^{-3/2} \left[\mathbf{1} + 4\tilde{\varepsilon} - 5\frac{m}{2} \right]. \end{aligned} \quad (\text{D.195})$$

So you get

$$g_p = \frac{GM}{a^2} \left[\mathbf{1} + \left(\frac{8\tilde{\varepsilon} - 7m}{\mathbf{12}} \right) + \left(\frac{\mathbf{11}m - 4\tilde{\varepsilon}}{\mathbf{12}} \right) \right] (\mathbf{1} + 2\tilde{\varepsilon})^{3/2} \frac{\mathbf{1}}{\mathbf{1} + 4\tilde{\varepsilon} - 5\frac{m}{2}}. \quad (\text{D.196})$$

This leads to

$$\frac{g_p - g_a}{g_a} = \frac{\partial R}{\partial r} - \mathbf{1} = \frac{(\mathbf{1} + 2\tilde{\varepsilon})^{3/2}}{\mathbf{1} + 4\tilde{\varepsilon} - 5\frac{m}{2}} - \mathbf{1}. \quad (\text{D.197})$$

Define

$$f(x, y) := \frac{(\mathbf{1} + 2x)^{3/2}}{\mathbf{1} + 4x - 5\frac{y}{2}}, \quad (\text{D.198})$$

then $f(\mathbf{o}) = \mathbf{1}$ and

$$\frac{\partial f}{\partial x} = \frac{3\sqrt{\mathbf{1} + 2x} (\mathbf{1} + 4x - 5\frac{y}{2}) - (\mathbf{1} + 2x)^{3/2} 4}{(\mathbf{1} + 4x - 5\frac{y}{2})^2}, \quad (\text{D.199})$$

so

$$\frac{\partial f}{\partial x}(\mathbf{o}) = -\mathbf{1}, \quad (\text{D.200})$$

as well as

$$\frac{\partial f}{\partial y} = \frac{5}{2} (\mathbf{1} + 2x)^{3/2} \frac{\mathbf{1}}{(\mathbf{1} + 4x - 5\frac{y}{2})^2}, \quad (\text{D.201})$$

so

$$\frac{\partial f}{\partial y}(\mathbf{o}) = \frac{5}{2}. \quad (\text{D.202})$$

This follows

$$\frac{g_p - g_a}{g_a} \approx \frac{5m}{2} - \tilde{\varepsilon} \approx \frac{5m}{2} - \varepsilon, \quad (\text{D.203})$$

so with Eq. (D.172) also satisfies Clairaut's theorem. As a note, it should be said: Eq. (D.172) is first-order exact in ε and m and therefore no better or worse than Eq. (D.148).

D.3.5 Vertical trajectories

Since horizontal derivatives in a suitable geophysical coordinate system refer to equipotential surfaces in the gravity field, vertical derivatives (if the KS is orthogonal) are perpendicular to this and therefore aligned in the direction of the gravity field. So it's important to know this direction. For this purpose, the trajectories perpendicular to the equipotential surfaces are determined in this section.

Eq. (D.173) describes the equipotential surfaces in the gravity field, more precisely their distance r from the center of the Earth for a given equatorial radius R and geocentric latitude χ . This equation is:

$$r(\chi, R) = R \left[\mathbf{1} + \sin^2(\chi) \left\{ \mu + r \frac{R^2}{a^2} \right\} \right]^{-1/2} \quad (\text{D.204})$$

This was done

$$\mu := \frac{8\tilde{\varepsilon} - 5m}{2}, r := \frac{5m - 4\tilde{\varepsilon}}{2} \quad (\text{D.205})$$

defined. This can be transformed into:

$$r(\chi, R) = \frac{RC(R)}{\sqrt{R^2 \sin^2(\chi) + C^2(R) \cos^2(\chi)}} \quad (\text{D.206})$$

with

$$C(R) := R \frac{\mathbf{1}}{\sqrt{\mathbf{1} + \mu + r \frac{R^2}{a^2}}}. \quad (\text{D.207})$$

Fulfill ellipsoids

$$\frac{r^2 \cos^2(\chi)}{R^2} + \frac{r^2 \sin^2(\chi)}{c^2} = \mathbf{1} \quad (\text{D.208})$$

with semi-major axis R and semi-minor axis c . If you put Eq. (D.206), you get

$$\frac{\mathbf{1}}{R^2} \frac{R^2 C^2 \cos^2(\chi)}{R^2 \sin^2(\chi) + C^2 \cos^2(\chi)} + \frac{\mathbf{1}}{c^2} \frac{R^2 C^2 \sin^2(\chi)}{R^2 \sin^2(\chi) + C^2 \cos^2(\chi)} \stackrel{!}{=} \mathbf{1}. \quad (\text{D.209})$$

One sees that this is true for $c = C$. C is therefore the semi-minor axis of the equipotential surfaces.

Since an ellipsoid is rotationally symmetrical, it is sufficient to first determine the vertical trajectories in the meridian plane $\mathcal{A} = \mathfrak{o}$. Here you can simply look at ellipses and fulfill them

$$\frac{x^2}{R^2} + \frac{z^2}{C^2} = \mathbf{1}. \quad (\text{D.210})$$

If you insert the definition of C here, it follows

$$x^2 + \left(\mathbf{1} + \mu + r \frac{R^2}{a^2} \right) z^2 = R^2. \quad (\text{D.211})$$

If you convert this to R^2 , you get

$$R^2 = \frac{x^2 + (\mathbf{1} + \mu) z^2}{\mathbf{1} - r \frac{z^2}{a^2}}. \quad (\text{D.212})$$

Furthermore, it follows from this

$$\begin{aligned} \mathbf{1} + \mu + r \frac{x^2}{a^2} &= \mathbf{1} + \mu + \frac{x^2}{z^2} - \frac{x^2}{z^2} + r \frac{x^2}{a^2} = R^2 \frac{\mathbf{1}}{z^2} \left(\mathbf{1} - r \frac{z^2}{a^2} \right) - \frac{x^2}{z^2} \left(\mathbf{1} - r \frac{z^2}{a^2} \right) \\ &= \left(\mathbf{1} - r \frac{z^2}{a^2} \right) \frac{R^2 - x^2}{z^2} = \left(\mathbf{1} - r \frac{z^2}{a^2} \right) \left(\mathbf{1} + \mu + r \frac{R^2}{a^2} \right). \end{aligned} \quad (\text{D.213})$$

If R is fixed, the coordinate z of an ellipse in a half-space can be understood as a function of x . This function $z(x)$ satisfies Eq. (D.210). Differentiating this equation in terms of x gives us

$$\frac{dz}{dx} = - \frac{C^2}{R^2} \frac{x}{z}. \quad (\text{D.214})$$

This is a directional derivative along the potential surface. Geometrically it is clear that the local perpendicular to the potential surface applies

$$\frac{dz}{dx} = \frac{R^2}{C^2} \frac{z}{x}. \quad (\text{D.215})$$

With the definition of C follows

$$\frac{R^2}{C^2} = \mathbf{1} + \mu + r \frac{R^2}{a^2}, \quad (\text{D.216})$$

therefore applies

$$\frac{dz}{dx} = \left(\mathbf{1} + \mu + r \frac{R^2}{a^2} \right) \frac{z}{x} = \frac{\mathbf{1} + \mu + r \frac{x^2}{a^2}}{\mathbf{1} - r \frac{z^2}{a^2}} \frac{z}{x}. \quad (\text{D.217})$$

This can be solved using the method of separating the variables presented in Section A.7. $z(x)$ is bijective, so the requirements are met. First you do the math

$$\left(\mathbf{1} - r \frac{z^2}{a^2} \right) \frac{dz}{dx} = \frac{z}{x} \left(\mathbf{1} + \mu + r \frac{x^2}{a^2} \right) \Leftrightarrow \left(\frac{\mathbf{1}}{z} - r \frac{z}{a^2} \right) \frac{dz}{dx} = \frac{\mathbf{1} + \mu}{x} + r \frac{x}{a^2}. \quad (\text{D.218})$$

So follow

$$\begin{aligned}
& \int \frac{1}{z} - r \frac{z}{a^2} dz = \int \frac{1+\mu}{x} + r \frac{x}{a^2} dx \\
& \Leftrightarrow \frac{1}{a} \int \frac{a}{z} - r \frac{z}{a} d\left(\frac{z}{a}\right) = \frac{1}{a} \int (1+\mu) \frac{a}{x} + r \frac{x}{a} d\left(\frac{x}{a}\right) \\
& \Leftrightarrow \ln \frac{z}{a} - \frac{r}{2} \frac{z^2}{a^2} = D' + (1+\mu) \ln \left(\frac{x}{a}\right) + \frac{r}{2a^2} x^2 \\
& \Leftrightarrow \frac{z}{a} = \exp \left(D' + (1+\mu) \ln \left(\frac{x}{a}\right) + \frac{r}{2a^2} x^2 + \frac{r}{2} \frac{z^2}{a^2} \right) \\
& \Leftrightarrow z = aD \left(\frac{x}{a}\right)^{1+\mu} \exp \left[\frac{r}{2a^2} (x^2 + z^2) \right]
\end{aligned} \tag{D.219}$$

with an integration constant $D := \exp(D') > 0$ with $D' \in \mathbb{R}$. For a given x , by solving this equation one can find the z which lies on the desired orthogonal trajectory. Which trajectory this is is determined by the number D , so D is a function of a width φ , it is $D = D(\varphi)$. The exact form of this function $D = D(\varphi)$ is by convention. Here it is determined by the intersection of the trajectory with the WGS 84. Let $(x_S, z_S)^T$ be this intersection. Then applies

$$\begin{aligned}
|z_S| &= aD \left(\frac{x_S}{a}\right)^{1+\mu} \exp \left[\frac{r}{2a^2} (x_S^2 + z_S^2) \right] \\
\Rightarrow D &= \frac{|z_S|}{a} \left(\frac{a}{x_S}\right)^{1+\mu} \exp \left[-\frac{r}{2a^2} (x_S^2 + z_S^2) \right].
\end{aligned} \tag{D.220}$$

The following equation thus determines the vertical trajectories sought:

$$\frac{z}{z_S} = \left(\frac{x}{x_S}\right)^{1+\mu} \exp \left[\frac{r}{2a^2} (x^2 + z^2) - \frac{r}{2a^2} (x_S^2 + z_S^2) \right] \tag{D.221}$$

D.4 GREAT-Koordinaten

The GREAT coordinates are described in [34]. They are suitable for expressing differential operators in ellipsoidal geometries. They are also orthogonal.

First, all lengths are scaled to the semi-major axis of the Earth a :

$$\frac{x}{a} \rightarrow x, \quad \frac{y}{a} \rightarrow y, \quad \frac{z}{a} \rightarrow z, \quad \frac{R}{a} \rightarrow R \tag{D.222}$$

Eq. (D.221) is then

$$\frac{z}{z_S} = \left(\frac{x}{x_S}\right)^{1+\mu} \exp \left[\frac{r}{2} (x^2 + z^2) - \frac{r}{2} (x_S^2 + z_S^2) \right] \tag{D.223}$$

D.4.1 Vertical coordinate

In spherical coordinates, the radial coordinate r denotes a spherical surface. In GREAT coordinates, the radial coordinate R denotes a specific ellipsoid, R has already been introduced as the equatorial radius of the corresponding ellipsoid. This is the vertical coordinate in the GREAT system.

D.4.2 Zonal coordinate

The zonal coordinate λ of a location $\mathbf{r}$ is the angle by which one must rotate the xz plane about the z axis until $\mathbf{r}$ lies in this plane. This is analogous to the azimuth angle in ordinary spherical coordinates.

D.4.3 Meridional coordinate

To ensure consistency with measurement data, the geographical latitude φ is chosen as the meridional coordinate. The geographical latitude of a point $\mathbf{r}$ outside the Earth can be found as follows:

- Find the vertical trajectory on which $\mathbf{r}$ lies.
- Follow this vertical trajectory to its intersection $\mathbf{r}_s$ with the WGS 84.
- Find the perpendicular direction $\mathbf{s}$ to the WGS 84 at the point $\mathbf{r}_s$ and form the straight line $\mathbf{g} = \mathbf{r}_s + \gamma \mathbf{s}$ with $\gamma \in \mathbb{R}$.
- Trace the line $\mathbf{g}$ to its intersection $\mathbf{r}_o$ with the xy-plane of the global coordinates. The angle that $\mathbf{r}_o$ makes with the xy plane is the latitude φ .

D.4.4 Metric tensor

In order to be able to express the governing equations in GREAT coordinates, the differential operators must be expressed by partial derivatives with respect to φ, λ, R . To do this, some preparatory work must first be done. So let a point $\mathbf{r} = (x, y, z)^T$ be given in global coordinates, $\mathbf{r}$ has the GREAT coordinates (R, φ, λ) . The transformation of all differential operators is based on the metric factors $h_\lambda, h_\varphi, h_R > 0$, defined by

$$h_\lambda^2 = \left(\frac{\partial x}{\partial \lambda} \right)^2 + \left(\frac{\partial y}{\partial \lambda} \right)^2 + \left(\frac{\partial z}{\partial \lambda} \right)^2, \quad (\text{D.224})$$

$$h_\varphi^2 = \left(\frac{\partial x}{\partial \varphi} \right)^2 + \left(\frac{\partial y}{\partial \varphi} \right)^2 + \left(\frac{\partial z}{\partial \varphi} \right)^2, \quad (\text{D.225})$$

$$h_R^2 = \left(\frac{\partial x}{\partial R} \right)^2 + \left(\frac{\partial y}{\partial R} \right)^2 + \left(\frac{\partial z}{\partial R} \right)^2. \quad (\text{D.226})$$

To determine h_R and h_φ , an observation in the meridional plane $\lambda = 0$ is sufficient. If you apply the rescaling equations (D.222) - (D.222) to the equations (D.211) and (D.219), you get

$$x^2 + (\mathbf{1} + \mu + rR^2) z^2 = R^2, \quad (\text{D.227})$$

$$z = D(\varphi) x^{\mathbf{1}+\mu} \exp \left[\frac{r}{2} (x^2 + z^2) \right]. \quad (\text{D.228})$$

If you take this logarithm, you get

$$\ln(z^2) = \ln(R^2 - x^2) - \ln(\mathbf{1} + \mu + rR^2), \quad (\text{D.229})$$

$$\ln(z) = \ln[D(\varphi)] + (\mathbf{1} + \mu) \ln(x) + \frac{r}{2} (x^2 + z^2). \quad (\text{D.230})$$

$D(\varphi)$ results from Eq. (D.220), which reads rescaled

$$D(\varphi) = \frac{|z_S(\varphi)|}{x_S(\varphi)^{\mathbf{1}+\mu}} \exp \left[-\frac{r}{2} (x_S(\varphi)^2 + z_S(\varphi)^2) \right]. \quad (\text{D.231})$$

Now one differentiates Equation (D.231) partially according to R :

$$\begin{aligned} \frac{2}{z} \frac{\partial z}{\partial R} &= -\frac{\partial x}{\partial R} \frac{\mathbf{1}}{R^2 - x^2} + \frac{\mathbf{1}}{R^2 - x^2} - \frac{\mathbf{1}}{R^2 - x^2} \frac{\partial R}{\partial R} \\ \Leftrightarrow (\mathbf{1} + \mu + rR^2) z \frac{\partial z}{\partial R} &= -\frac{\partial x}{\partial R} (\mathbf{1} + \mu + rR^2) \frac{xz^2}{R^2 - x^2} + (\mathbf{1} + \mu + rR^2) \frac{Rz^2}{R^2 - x^2} - rRz^2. \end{aligned} \quad (\text{D.232})$$

If you put Eq. (D.227), you get

$$(\mathbf{1} + \mu + rR^2) z \frac{\partial z}{\partial R} + x \frac{\partial x}{\partial R} = R(\mathbf{1} - rz^2). \quad (\text{D.233})$$

If you differentiate Eq. (D.230) partial to R , we get:

$$\begin{aligned}
& \frac{1}{z} \frac{\partial z}{\partial R} = (1 + \mu) \frac{1}{x} \frac{\partial x}{\partial R} + r \left(x \frac{\partial x}{\partial R} + z \frac{\partial z}{\partial R} \right) \\
& \Leftrightarrow (1 + \mu) \frac{1}{x} \frac{\partial x}{\partial R} - \frac{1}{z} \frac{\partial z}{\partial R} = -r \left(x \frac{\partial x}{\partial R} + z \frac{\partial z}{\partial R} \right) \\
& \Leftrightarrow (1 + \mu + rR^2) \frac{1}{x} \frac{\partial x}{\partial R} - \frac{1}{z} \frac{\partial z}{\partial R} = -r \left(x \frac{\partial x}{\partial R} + z \frac{\partial z}{\partial R} \right) + rR^2 \frac{1}{x} \frac{\partial x}{\partial R} \\
& \Leftrightarrow (1 + \mu + rR^2) \frac{1}{x} \frac{\partial x}{\partial R} - \frac{1}{z} \frac{\partial z}{\partial R} = \frac{r}{x} \frac{\partial x}{\partial R} (R^2 - x^2) - rz \frac{\partial z}{\partial R}.
\end{aligned} \tag{D.234}$$

If you put Eq. (D.227), you get

$$\begin{aligned}
& \Leftrightarrow (1 + \mu + rR^2) \frac{1}{x} \frac{\partial x}{\partial R} - \frac{1}{z} \frac{\partial z}{\partial R} = \frac{r}{x} \frac{\partial x}{\partial R} (1 + \mu + rR^2) z^2 - rz \frac{\partial z}{\partial R} \\
& \Leftrightarrow (1 + \mu + rR^2) \frac{1}{x} \frac{\partial x}{\partial R} - \frac{1}{z} \frac{\partial z}{\partial R} = rz^2 \left[\frac{1}{x} \frac{\partial x}{\partial R} (1 + \mu + rR^2) z^2 - \frac{1}{z} \frac{\partial z}{\partial R} \right] \\
& \Leftrightarrow (1 + \mu + rR^2) \frac{1}{x} \frac{\partial x}{\partial R} - \frac{1}{z} \frac{\partial z}{\partial R} = 0.
\end{aligned} \tag{D.235}$$

If you convert this to $\frac{\partial z}{\partial R}$, you get

$$\frac{\partial z}{\partial R} = \frac{z}{x} (1 + \mu + rR^2) \frac{\partial x}{\partial R}. \tag{D.236}$$

Putting this into Eq. (D.233), you get

$$\begin{aligned}
& (1 + \mu + rR^2)^2 \frac{z^2}{x} \frac{\partial x}{\partial R} + x \frac{\partial x}{\partial R} = R(1 - rz^2) \\
& \Leftrightarrow x \frac{\partial x}{\partial R} \left[1 + \frac{z^2}{x^2} (1 + \mu + rR^2)^2 \right] = R(1 - rz^2) \\
& \Leftrightarrow \frac{\partial x}{\partial R} = \frac{R(1 - rz^2) x^2}{x [x^2 + z^2 (1 + \mu + rR^2)^2]} \\
& \Leftrightarrow \frac{\partial x}{\partial R} = \frac{R(1 - rz^2) (R^2 - (1 + \mu + rR^2) z^2)}{x [R^2 - (1 + \mu + rR^2) z^2 + z^2 (1 + \mu + rR^2)^2]} \\
& \Leftrightarrow \frac{\partial x}{\partial R} = \frac{R(1 - rz^2) (R^2 - (1 + \mu + rR^2) z^2)}{x [R^2 + z^2 (1 + \mu + rR^2) (\mu + rR^2)]}.
\end{aligned} \tag{D.237}$$

Equation was again used. (D.227) is used. If you put Eq. (D.237) in Eq. (D.236) and uses Eq. (D.229), follows

$$\frac{\partial z}{\partial R} = \frac{zR(1 - rz^2) (1 + \mu + rR^2)}{R^2 + z^2 (1 + \mu + rR^2) (\mu + rR^2)}. \tag{D.238}$$

So with Eq. (D.227)

$$h_R = \sqrt{\left(\frac{\partial x}{\partial R} \right)^2 + \left(\frac{\partial z}{\partial R} \right)^2} = \frac{R(1 - rz^2) \sqrt{z^2 (1 + \mu + rR^2)^2 + x^2}}{R^2 + z^2 (1 + \mu + rR^2) (\mu + rR^2)}$$

$$\boxed{\Leftrightarrow h_R = \frac{R(1 - rz^2)}{[R^2 + z^2 (1 + \mu + rR^2) (\mu + rR^2)]^{1/2}}.} \tag{D.239}$$

Now one differentiates Eq. (D.229) partial to φ :

$$\frac{z}{z} \frac{\partial z}{\partial \varphi} = -\frac{2x}{R^2 - x^2} \frac{\frac{\partial x}{\partial \varphi}}{\frac{\partial x}{\partial \varphi}} \Leftrightarrow \frac{R^2 - x^2}{z} \frac{\partial z}{\partial \varphi} = -x \frac{\partial x}{\partial \varphi}. \quad (\text{D.240})$$

If you put Eq. (D.227), you get

$$(\mathbf{1} + \mu + rR^2) z \frac{\partial z}{\partial \varphi} + x \frac{\partial x}{\partial \varphi} = \mathbf{0}. \quad (\text{D.241})$$

Proceed analogously with Eq. (D.230), you get

$$\begin{aligned} \frac{\mathbf{1}}{z} \frac{\partial z}{\partial \varphi} &= \frac{d \ln [D(\varphi)]}{d\varphi} + \frac{\mathbf{1} + \mu}{x} \frac{\partial x}{\partial \varphi} + rx \frac{\partial x}{\partial \varphi} + rz \frac{\partial z}{\partial \varphi} \\ &\Leftrightarrow [\mathbf{1} + \mu + rx^2] \frac{\mathbf{1}}{x} \frac{\partial x}{\partial \varphi} - [\mathbf{1} - rz^2] \frac{\mathbf{1}}{z} \frac{\partial z}{\partial \varphi} = -\frac{d \ln [D(\varphi)]}{d\varphi} \\ &\Leftrightarrow \frac{\mathbf{1} + \mu + rx^2}{\mathbf{1} - rz^2} \frac{\mathbf{1}}{x} \frac{\partial x}{\partial \varphi} - \frac{\mathbf{1}}{z} \frac{\partial z}{\partial \varphi} = -\frac{\mathbf{1}}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi} \\ &\Leftrightarrow (\mathbf{1} + \mu + rR^2) \frac{\mathbf{1}}{x} \frac{\partial x}{\partial \varphi} - \frac{\mathbf{1}}{z} \frac{\partial z}{\partial \varphi} = -\frac{\mathbf{1}}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi}. \end{aligned} \quad (\text{D.242})$$

In the last step, the version of Eq. rescaled using the equations (D.222) - (D.222) was used. (D.220) used. If you convert this to $\frac{\partial z}{\partial \varphi}$, you get

$$\frac{\partial z}{\partial \varphi} = z (\mathbf{1} + \mu + rR^2) \frac{\mathbf{1}}{x} \frac{\partial x}{\partial \varphi} + \frac{z}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi}. \quad (\text{D.243})$$

Putting this into Eq. (D.241), follows

$$\begin{aligned} (\mathbf{1} + \mu + rR^2)^2 z^2 \frac{\mathbf{1}}{x} \frac{\partial x}{\partial \varphi} + z^2 \frac{\mathbf{1} + \mu + rR^2}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi} + x \frac{\partial x}{\partial \varphi} &= \mathbf{0} \\ \Leftrightarrow \frac{\partial x}{\partial \varphi} \left(x + \frac{z^2}{x} (\mathbf{1} + \mu + rR^2)^2 \right) &= -\frac{z^2 (\mathbf{1} + \mu + rR^2)}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi} \\ \Leftrightarrow \frac{\partial x}{\partial \varphi} (x^2 + z^2 (\mathbf{1} + \mu + rR^2)^2) &= -\frac{xz^2 (\mathbf{1} + \mu + rR^2)}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi} \\ \Leftrightarrow \frac{\partial x}{\partial \varphi} (x^2 + z^2 (\mathbf{1} + \mu + rR^2) (\mu + rR^2) + z^2 (\mathbf{1} + \mu + rR^2)) & \\ = -\frac{xz^2 (\mathbf{1} + \mu + rR^2)}{\mathbf{1} - rz^2} \frac{d \ln [D(\varphi)]}{d\varphi}. \end{aligned} \quad (\text{D.244})$$

If you put Eq. (D.227), you get

$$\frac{\partial x}{\partial \varphi} = -\frac{xz^2 (\mathbf{1} + \mu + rR^2)}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \frac{d \ln [D(\varphi)]}{d\varphi}. \quad (\text{D.245})$$

Putting this into Eq. (D.243) and uses Eq. (D.227), so follows

$$\begin{aligned}
\frac{\partial z}{\partial \varphi} &= -\frac{z^3 (\mathbf{1} + \mu + rR^2)^2}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \frac{d\ln [D(\varphi)]}{d\varphi} + \frac{z}{\mathbf{1} - rz^2} \frac{d\ln [D(\varphi)]}{d\varphi} \\
&= \frac{zR^2 + z^3 (\mathbf{1} + \mu + rR^2) (\mu + rR^2) - z^3 (\mathbf{1} + \mu + rR^2)^2}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \frac{d\ln [D(\varphi)]}{d\varphi} \\
&\Leftrightarrow \frac{\partial z}{\partial \varphi} = \frac{zR^2 - z^3 (\mathbf{1} + \mu + rR^2)}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \frac{d\ln [D(\varphi)]}{d\varphi} \\
&\Leftrightarrow \frac{\partial z}{\partial \varphi} = \frac{zx^2}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \frac{d\ln [D(\varphi)]}{d\varphi}.
\end{aligned} \tag{D.246}$$

This means that again with Eq. (D.227)

$$\begin{aligned}
h_\varphi &= \sqrt{\left(\frac{\partial x}{\partial \varphi}\right)^2 + \left(\frac{\partial \varphi}{\partial z\varphi}\right)^2} = \frac{xz\sqrt{x^2 + z^2 (\mathbf{1} + \mu + rR^2)^2}}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \left| \frac{d\ln [D(\varphi)]}{d\varphi} \right| \\
&\Leftrightarrow h_\varphi = \frac{xz\sqrt{R^2 + z^2 (\mu + rR^2) (\mathbf{1} + \mu + rR^2)}}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)} \left| \frac{d\ln [D(\varphi)]}{d\varphi} \right|
\end{aligned}$$

$$h_\varphi = \frac{xz}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)^{1/2}} \left| \frac{d\ln [D(\varphi)]}{d\varphi} \right|. \tag{D.247}$$

If you logarithm both sides of Eq. (D.229), you get

$$\ln(D) = \ln(|z_S|) - (\mathbf{1} + \mu) \ln(x_S) - \frac{r}{2} (x_S^2 + z_S^2). \tag{D.248}$$

If you differentiate this, it follows

$$\begin{aligned}
\frac{d\ln(D)}{d\varphi} &= \frac{d\ln(|z_S|)}{d\varphi} - (\mathbf{1} + \mu) \frac{d\ln(x_S)}{d\varphi} - rx_S \frac{dx_S}{d\varphi} - rz_S \frac{dz_S}{d\varphi} \\
&= \frac{d\ln(|z_S|)}{d\varphi} (\mathbf{1} - rz_S^2) - \frac{d\ln(x_S)}{d\varphi} (\mathbf{1} + \mu + rx_S^2).
\end{aligned} \tag{D.249}$$

This equation can be used to express $\frac{d\ln(D)}{d\varphi}$ in terms of $\frac{dx_S}{d\varphi}$ and $\frac{dz_S}{d\varphi}$:

$$h_\varphi = \frac{xz}{(\mathbf{1} - rz^2) (R^2 + (\mu + rR^2) (\mathbf{1} + \mu + rR^2) z^2)^{1/2}} \left| \frac{d\ln(|z_S|)}{d\varphi} (\mathbf{1} - rz_S^2) - \frac{d\ln(x_S)}{d\varphi} (\mathbf{1} + \mu + rx_S^2) \right| \tag{D.250}$$

They apply

$$x = \sqrt{x^2 + y^2} \cos \lambda, \quad y = \sqrt{x^2 + y^2} \sin \lambda. \tag{D.251}$$

Thus follows

$$h_\lambda = \sqrt{\left(\frac{\partial x}{\partial \lambda}\right)^2 + \left(\frac{\partial y}{\partial \lambda}\right)^2} = \sqrt{x^2 + y^2} = r_\perp. \tag{D.252}$$

For the determinant g of the metric tensor of the GREAT coordinates holds

$$\begin{aligned}
\sqrt{g} &= h_R h_\lambda h_\varphi = h_R r_\perp h_\varphi = h_R r_\perp \frac{r_\perp z}{(\mathbf{1} - rz^2)(R^2 + (\mu + rR^2)(\mathbf{1} + \mu + rR^2)z^2)^{1/2}} \left| \frac{d \ln [D(\varphi)]}{d\varphi} \right| \\
&= h_R \frac{r_\perp^2 z}{(\mathbf{1} - rz^2)(R^2 + (\mu + rR^2)(\mathbf{1} + \mu + rR^2)z^2)^{1/2}} \left| \frac{d \ln [D(\varphi)]}{d\varphi} \right| \\
&= \frac{R(\mathbf{1} - rz^2)}{[R^2 + z^2(\mathbf{1} + \mu + rR^2)(\mu + rR^2)]^{1/2}} \frac{r_\perp^2 z}{(\mathbf{1} - rz^2)(R^2 + (\mu + rR^2)(\mathbf{1} + \mu + rR^2)z^2)^{1/2}} \left| \frac{d \ln [D(\varphi)]}{d\varphi} \right| \\
&= \frac{R}{[R^2 + z^2(\mathbf{1} + \mu + rR^2)(\mu + rR^2)]^{1/2}} \frac{r_\perp^2 z}{(R^2 + (\mu + rR^2)(\mathbf{1} + \mu + rR^2)z^2)^{1/2}} \left| \frac{d \ln [D(\varphi)]}{d\varphi} \right| \\
&= \frac{Rr_\perp^2 z}{R^2 + (\mu + rR^2)(\mathbf{1} + \mu + rR^2)z^2} \left| \frac{d \ln [D(\varphi)]}{d\varphi} \right|
\end{aligned}$$

$$\begin{aligned}
\Leftrightarrow \sqrt{g} &= \frac{Rr_\perp^2 z}{R^2 + (\mu + rR^2)(\mathbf{1} + \mu + rR^2)z^2} \cdot \\
&\cdot \left| \frac{\mathbf{1}}{\sin(\varphi) \cos(\varphi)} + \mu \tan(\varphi) \frac{c^2}{\cos^2(\varphi) + c^2 \sin^2(\varphi)} + r \frac{\sin(\varphi) \cos(\varphi) c^2 (\mathbf{1} - c^2)}{(\cos^2(\varphi) + c^2 \sin^2(\varphi))^2} \right|. \quad (\text{D.253})
\end{aligned}$$

D.4.5 Transformation von GREAT-Koordinaten in globale Koordinaten

Let a point $\mathbf{r}$ with the GREAT coordinates (R, φ, λ) be given. One wants to determine the global coordinates $(x, y, z)^T$ of this point. First assume $\lambda = \mathbf{o}$. If you square Eq. (D.228), you get

$$z^2 = D(\varphi)^2 (x^2)^{1+\mu} \exp[r(x^2 + z^2)]. \quad (\text{D.254})$$

If you put Eq. (D.230), follows

$$z^2 = D(\varphi)^2 [R^2 - z^2(\mathbf{1} + \mu + rR^2)]^{1+\mu} \exp[r(R^2 - z^2(\mu + rR^2))]. \quad (\text{D.255})$$

This equation is implicit and therefore has to be solved iteratively. $D(\varphi)$ and R are constants, z^2 is the only remaining quantity to be determined. About Eq. (D.230) can then be determined x^2 . The sign of z is the sign of φ . In the case $\lambda \neq \mathbf{o}$

$$x^2 \rightarrow r_\perp^2 \quad (\text{D.256})$$

to replace so that one

$$x = r_\perp \cos(\lambda), \quad (\text{D.257})$$

$$y = r_\perp \sin(\lambda) \quad (\text{D.258})$$

receives.

D.4.6 Transformation von globalen Koordinaten in GREAT-Koordinaten

Given a point $\mathbf{r}$ with global coordinates $(x, y, z)^T$, one wants to determine the GREAT coordinates (R, φ, λ) of $\mathbf{r}$. If you write down Eq. (D.212) with the replacement equations (D.222) - (D.222), one obtains

$$R^2 = \frac{x^2 + y^2 + (\mathbf{1} + \mu)z^2}{\mathbf{1} - rz^2}. \quad (\text{D.259})$$

$x^2 \rightarrow x^2 + y^2$ was replaced because the general case $\lambda \neq \mathbf{o}$ is assumed. λ is obtained via

$$\lambda = \text{sign}(y) \arccos \left(\frac{x}{\sqrt{x^2 + y^2}} \right). \quad (\text{D.260})$$

To determine φ , one first sets Eq. (D.228) to D and replaces $x^2 \rightarrow x^2 + y^2$ again:

$$D = \frac{z}{\sqrt{x^2 + y^2 + \mu}} \exp \left(-\frac{r}{2} (x^2 + y^2 + z^2) \right) \quad (\text{D.261})$$

Now you put in Eq. (D.255) $R = \mathbf{i}$, which corresponds to the surface of the WGS 84, and solves numerically for z_S^2 , the sign of z_S is identical to the sign of z . Now you can use Eq. Use (D.227) with $R = \mathbf{i}$, $z = z_S$ and $x^2 \rightarrow x_S^2 + y_S^2$ to determine $x_S^2 + y_S^2$. About the equation

$$\varphi = \arctan \left[\frac{a^2}{c^2} \frac{z_S}{\sqrt{x^2 + y^2}} \right] \quad (\text{D.262})$$

one can finally determine φ . Eq. (D.262) should now be derived. Please consider o. B. d. A. the plane $\lambda = \mathbf{o}$, therefore $y = \mathbf{o}$. The intersection of the WGS 84 with this plane is given by (note the scaling)

$$x^2 + \frac{z^2}{c^2} = \mathbf{i}. \quad (\text{D.263})$$

Define

$$f(x, z) := x^2 + \frac{z^2}{c^2}, \quad (\text{D.264})$$

then applies

$$\nabla f = \left(\frac{2x}{2z} \frac{z}{c^2} \right). \quad (\text{D.265})$$

The WGS 84 is given by the contour set $f = \mathbf{i}$. Define the line $\mathbf{g}$ in the xz plane of the global coordinates by

$$\mathbf{g} = \begin{pmatrix} x_S \\ z_S \end{pmatrix} + \gamma \begin{pmatrix} x_S \\ \frac{z_S}{c^2} \end{pmatrix} \quad (\text{D.266})$$

with $\gamma \in \mathbb{R}$. The intersection of $\mathbf{g}$ with the x-axis is given by in the case $z_S \neq \mathbf{o}$

$$\mathbf{o} = z_S + \gamma \frac{z_S}{c^2} \Rightarrow \gamma = -c^2. \quad (\text{D.267})$$

For the x coordinate of this point we get

$$x = x_S (\mathbf{i} - c^2). \quad (\text{D.268})$$

So it applies

$$\tan(\varphi) = \frac{z_S}{x_S c^2}. \quad (\text{D.269})$$

With Eq. (D.263) follows

$$z_S^2 = c^2 (\mathbf{i} - x_S^2) \quad (\text{D.270})$$

and therefore applies

$$\begin{aligned}\tan(\varphi) &= \frac{c\sqrt{1-x_S^2}}{x_S c^2} = \frac{\sqrt{1-x_S^2}}{x_S c} \Leftrightarrow \tan^2(\varphi) = \frac{1-x_S^2}{x_S^2 c^2} \Leftrightarrow x_S^2 (c^2 \tan^2(\varphi) + 1) = 1 \\ \Leftrightarrow x_S^2 &= \frac{\cos^2(\varphi)}{c^2 \sin^2(\varphi) + \cos^2(\varphi)}.\end{aligned}\quad (\text{D.271})$$

With $x_S > 0$ follows

$$x_S = \frac{\cos(\varphi)}{\sqrt{c^2 \sin^2(\varphi) + \cos^2(\varphi)}}. \quad (\text{D.272})$$

If you put Eq. (D.263) to x_S is obtained

$$x_S = \sqrt{1 - \frac{z_S^2}{c^2}}. \quad (\text{D.273})$$

Putting this into Eq. (D.269), you get

$$\begin{aligned}\tan(\varphi) &= \frac{z_S}{c^2 \sqrt{1 - \frac{z_S^2}{c^2}}} \Leftrightarrow c^4 \tan^2(\varphi) \left(1 - \frac{z_S^2}{c^2}\right) = z_S^2 \\ \Leftrightarrow z_S^2 (1 + c^2 \tan^2(\varphi)) &= c^4 \tan^2(\varphi) \Leftrightarrow z_S^2 = \frac{c^4 \sin^2(\varphi)}{\cos^2(\varphi) + c^2 \sin^2(\varphi)} \\ \Leftrightarrow z_S &= \text{sign}(\varphi) \frac{c^2 \sin(\varphi)}{\sqrt{\cos^2(\varphi) + c^2 \sin^2(\varphi)}}.\end{aligned}\quad (\text{D.274})$$

It therefore applies

$$\frac{z_S}{x_S} = \frac{c^2}{a^2} \tan(\varphi), \quad (\text{D.275})$$

with the generalization $x_S \rightarrow \sqrt{x_S^2 + y_S^2}$ follows Eq. (D.262).

Now we need to find an explicit expression for $D(\varphi)$. To do this, put the equations (D.272) and (D.274) with $y = 0$ in Eq. (D.261):

$$\begin{aligned}D(\varphi) &= \frac{|z_S|}{x_S^{1+\mu}} \exp\left(-\frac{r}{2}(x_S^2 + z_S^2)\right) \\ &= \frac{c^2 \sin(\varphi) (\cos^2(\varphi) + c^2 \sin^2(\varphi))^{\mu/2}}{(\cos(\varphi))^{1+\mu}} \exp\left[-\frac{r}{2} \left(\frac{\cos^2(\varphi) + c^4 \sin^2(\varphi)}{\cos^2(\varphi) + c^2 \sin^2(\varphi)}\right)\right].\end{aligned}\quad (\text{D.276})$$

If you take this logarithm, it follows

$$\begin{aligned}\ln[D(\varphi)] &= \ln(c) + \ln(\sin(\varphi)) + \frac{\mu}{2} \ln(\cos^2(\varphi) + c^2 \sin^2(\varphi)) - (1 + \mu) \ln(\cos(\varphi)) \\ &\quad - \frac{r}{2} \left(\frac{\cos^2(\varphi) + c^4 \sin^2(\varphi)}{\cos^2(\varphi) + c^2 \sin^2(\varphi)}\right).\end{aligned}\quad (\text{D.277})$$

Thus you get

$$\begin{aligned}
\frac{d \ln [D(\varphi)]}{d\varphi} &= \frac{\cos(\varphi)}{\sin(\varphi)} + \frac{\mu}{2} \frac{-2\sin(\varphi)\cos(\varphi) + c^2 2\cos(\varphi)\sin(\varphi)}{\cos^2(\varphi) + c^2\sin^2(\varphi)} + (\mathbf{1} + \mu) \frac{\sin(\varphi)}{\cos(\varphi)} \\
&- \frac{r}{2} \frac{(-2\cos(\varphi)\sin(\varphi) + 2c^4\cos(\varphi)\sin(\varphi))(\cos^2(\varphi) + c^2\sin^2(\varphi))}{(\cos^2(\varphi) + c^2\sin^2(\varphi))^2} \\
&+ \frac{r}{2} \frac{(\cos^2(\varphi) + c^4\sin^2(\varphi))(-2\sin(\varphi)\cos(\varphi) + c^2 2\cos(\varphi)\sin(\varphi))}{(\cos^2(\varphi) + c^2\sin^2(\varphi))^2} \\
&= \frac{\mathbf{1}}{\sin(\varphi)} \left(\cos(\varphi) + \frac{\sin^2(\varphi)}{\cos(\varphi)} \right) + \mu \sin(\varphi) \cos(\varphi) \frac{c^2 - \mathbf{1} + \mathbf{1} + c^2 \tan^2(\varphi)}{\cos^2(\varphi) + c^2\sin^2(\varphi)} \\
&+ r \frac{(\cos(\varphi)\sin(\varphi) - c^4\cos(\varphi)\sin(\varphi))(\cos^2(\varphi) + c^2\sin^2(\varphi))}{(\cos^2(\varphi) + c^2\sin^2(\varphi))^2} \\
&+ r \frac{(\cos^2(\varphi) + c^4\sin^2(\varphi))(-\sin(\varphi)\cos(\varphi) + c^2\cos(\varphi)\sin(\varphi))}{(\cos^2(\varphi) + c^2\sin^2(\varphi))^2} \\
&= \frac{\mathbf{1}}{\sin(\varphi)\cos(\varphi)} + \mu \tan(\varphi) \frac{c^2}{\cos^2(\varphi) + c^2\sin^2(\varphi)} \\
&+ r \frac{\sin(\varphi)\cos(\varphi)(c^2(\sin^2(\varphi) + \cos^2(\varphi)) + c^4(-\sin^2(\varphi) - \cos^2(\varphi)))}{(\cos^2(\varphi) + c^2\sin^2(\varphi))^2}
\end{aligned}$$

$$\Leftrightarrow \frac{d \ln [D(\varphi)]}{d\varphi} = \frac{\mathbf{1}}{\sin(\varphi)\cos(\varphi)} + \mu \tan(\varphi) \frac{c^2}{\cos^2(\varphi) + c^2\sin^2(\varphi)} + r \frac{\sin(\varphi)\cos(\varphi)c^2(\mathbf{1} - c^2)}{(\cos^2(\varphi) + c^2\sin^2(\varphi))^2} \quad (\text{D.278})$$

D.5 Ellipsoidal geometry

D.5.1 Ellipsoidal geodesics

D.5.2 Ellipsoidal triangles

An area A on an ellipsoid is usually calculated using an *area-conformal projection*. The basic procedure is to transform each vertex (φ_i, λ_i) into the projection plane, i.e. to determine its coordinates (x_i, y_i) , and then calculate the area A' in plane geometry. Area-conformal projections are exactly those for which $A = A'$ holds.

The *Lambert azimuthal projection* is used here as the surface-conformal projection.

D.5.3 Ellipsoidal Voronoi lattices

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