Wolfgang Nolting

Theoretical Physics 6

Quantum Mechanics - Basics

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General Preface

The nine volumes of the series *Basic Course: Theoretical Physics* are thought to be text book material for the study of university level physics. They are aimed to impart, in a compact form, the most important skills of theoretical physics which can be used as basis for handling more sophisticated topics and problems in the advanced study of physics as well as in the subsequent physics research. The conceptual design of the presentation is organized in such a way that

Classical Mechanics (volume 1)
Analytical Mechanics (volume 2)
Electrodynamics (volume 3)
Special Theory of Relativity (volume 4)
Thermodynamics (volume 5)

are considered as the theory part of an *integrated course* of experimental and theoretical physics as is being offered at many universities starting from the first semester. Therefore, the presentation is consciously chosen to be very elaborate and self-contained, sometimes surely at the cost of certain elegance, so that the course is suitable even for self-study, at first without any need of secondary literature. At any stage, no material is used which has not been dealt with earlier in the text. This holds in particular for the mathematical tools, which have been comprehensively developed starting from the school level, of course more or less in the form of recipes, such that right from the beginning of the study, one can solve problems in theoretical physics. The mathematical insertions are always then plugged in when they become indispensable to proceed further in the program of theoretical physics. It goes without saying that in such a context, not all the mathematical statements can be proved and derived with absolute rigor. Instead, sometimes a reference must be made to an appropriate course in mathematics or to an advanced textbook in mathematics. Nevertheless, I have tried for a reasonably balanced representation so that the mathematical tools are not only applicable but also appear at least "plausible".

The mathematical interludes are of course necessary only in the first volumes of this series, which incorporate more or less the material of a bachelor program. In the second part of the series which comprises the modern aspects of theoretical physics,

Quantum Mechanics: Basics (volume 6)
Quantum Mechanics: Methods and Applications (volume 7)
Statistical Physics (volume 8)
Many-Body Theory (volume 9),

mathematical insertions are no longer necessary. This is partly because, by the time one comes to this stage, the obligatory mathematics courses one has to take in order to study physics would have provided the required tools. The fact that training in theory has already started in the first semester itself permits inclusion of parts of quantum mechanics and statistical physics in the bachelor program itself. It is clear that the content of the last three volumes cannot be part of an *integrated course* but rather the subject matter of pure theory lectures. This holds in particular for *Many-Body Theory* which is offered, sometimes under different names, e.g., *Advanced Quantum Mechanics*, in the eighth or so semester of study. In this part, new methods and concepts beyond basic studies are introduced and discussed which are developed in particular for correlated many particle systems which in the meantime have become indispensable for a student pursuing a master's or a higher degree and for being able to read current research literature.

In all the volumes of the series *Theoretical Physics*, numerous exercises are included to deepen the understanding and to help correctly apply the abstractly acquired knowledge. It is obligatory for a student to attempt on his own to adapt and apply the abstract concepts of theoretical physics to solve realistic problems. Detailed solutions to the exercises are given at the end of each volume. The idea is to help a student to overcome any difficulty at a particular step of the solution or to check one's own effort. Importantly these solutions should not seduce the student to follow the *easy way out* as a substitute for his own effort. At the end of each bigger chapter, I have added self-examination questions which shall serve as a self-test and may be useful while preparing for examinations.

I should not forget to thank all the people who have contributed one way or another to the success of the book series. The single volumes arose mainly from lectures which I gave at the universities of Muenster, Wuerzburg, Osnabrueck, and Berlin (Germany), Valladolid (Spain), and Warangal (India). The interest and constructive criticism of the students provided me the decisive motivation for preparing the rather extensive manuscripts. After the publication of the German version, I received a lot of suggestions from numerous colleagues for improvement, and this helped to further develop and enhance the concept and the performance of the series. In particular, I appreciate very much the support by Prof. Dr. A. Ramakanth, a long-standing scientific partner and friend, who helped me in many respects, e.g., what concerns the checking of the translation of the German text into the present English version.

Special thanks are due to the Springer company, in particular to Dr. Th. Schneider and his team. I remember many useful motivations and stimulations. I have the feeling that my books are well taken care of.

Berlin, Germany Wolfgang Nolting
August 2016

Preface to Volume 6

The main goal of the present volume 6 (*Quantum Mechanics: Basics*) corresponds exactly to that of the total basic course in *Theoretical Physics*. It is thought to be accompanying textbook material for the study of university-level physics. It is aimed to impart, in a compact form, the most important skills of theoretical physics which can be used as basis for handling more sophisticated topics and problems in the advanced study of physics as well as in the subsequent physics research. It is presented in such a way that it enables self-study without the need for a demanding and laborious reference to secondary literature. For the understanding of the text it is only presumed that the reader has a good grasp of what has been elaborated in the preceding volumes. Mathematical interludes are always presented in a compact and functional form and practiced when they appear indispensable for the further development of the theory. For the whole text it holds that I had to focus on the essentials, presenting them in a detailed and elaborate form, sometimes consciously sacrificing certain elegance. It goes without saying, that after the basic course, secondary literature is needed to deepen the understanding of physics and mathematics.

For the treatment of *Quantum Mechanics* also, we have to introduce certain new mathematical concepts. However now, the special demands may be of rather *conceptual nature*. The *Quantum Mechanics* utilizes novel *'models of thinking'*, which are alien to Classical Physics, and whose understanding and applying may raise difficulties to the *'beginner'*. Therefore, in this case, it is especially mandatory to use the exercises, which play an indispensable role for an effective learning and therefore are offered after all important subsections, in order to become familiar with the at first unaccustomed principles and concepts of the *Quantum Mechanics*. The elaborate solutions to exercises at the end of the book should not keep the learner from attempting an independent treatment of the problems, but should only serve as a checkup of one's own efforts.

This volume on *Quantum Mechanics* arose from lectures I gave at the German universities in Würzburg, Münster, and Berlin. The animating interest of the students in my lecture notes has induced me to prepare the text with special care. The present

one as well as the other volumes is thought to be the textbook material for the study of basic physics, primarily intended for the students rather than for the teachers.

The wealth of subject matter has made it necessary to divide the presentation of *Quantum Mechanics* into two volumes, where the first part deals predominantly with the basics. In a rather extended first chapter, an inductive reasoning for *Quantum Mechanics* is presented, starting with a critical inspection of the *'pre-quantum-mechanical time'*, i.e., with an analysis of the problems encountered by the physicists at the beginning of the twentieth century. Surely, opinions on the value of such a historical introduction may differ. However, I think it leads to a profound understanding of *Quantum Mechanics*.

The presentation and interpretation of the *Schrödinger equation*, the fundamental equation of motion of *Quantum Mechanics*, which replaces the classical equations of motion (*Newton, Lagrange, Hamilton*), will be the central topic of the second chapter. The Schrödinger equation cannot be derived in a mathematically strict sense, but has rather to be introduced, more or less, by analogy considerations. For this purpose one can, for instance, use the *Hamilton-Jacobi theory* (section 3, Vol. 2), according to which the *Quantum Mechanics* should be considered as something like a super-ordinate theory, where the *Classical Mechanics* plays a similar role in the framework of *Quantum Mechanics* as the geometrical optics plays in the general theory of light waves. The *particle-wave dualism* of matter, one of the most decisive scientific findings of physics in the twentieth century, will already be indicated via such an *'extrapolation'* of *Classical Mechanics*.

The second chapter will reveal why the state of a system can be described by a *'wave function'*, the statistical character of which is closely related to typical quantum-mechanical phenomena as the *Heisenberg uncertainty principle*. This statistical character of *Quantum Mechanics*, in contrast to *Classical Physics*, allows for only probability statements. Typical determinants are therefore *probability distributions, average values, and fluctuations*.

The *Schrödinger wave mechanics* is only one of the several possibilities to represent *Quantum Mechanics*. The complete abstract basics will be worked out in the third chapter. While in the first chapter the *Quantum Mechanics* is reasoned inductively, which eventually leads to the Schrödinger version in the second chapter, now, opposite, namely, the *deductive* way will be followed. Fundamental terms such as *state* and *observable* are introduced axiomatically as *elements* and *operators* of an abstract *Hilbert space*. *'Measuring'* means *'operation'* on the *'state'* of the system, as a result of which, in general, the state is changed. This explains why the describing mathematics represents an *operator theory*, which at this stage of the course has to be introduced and exercised. The third chapter concludes with some considerations on the *correspondence principle* by which once more ties are established to *Classical Physics*.

In the fourth chapter, we will interrupt our general considerations in order to deepen the understanding of the abstract theory by some relevant applications to *simple potential problems*. As immediate results of the model calculations, we will encounter some novel, typical quantum-mechanical phenomena. Therewith the first part of the introduction to *Quantum Mechanics* will end. Further applications, in-

depth studies, and extensions of the subject matter will then be offered in the second part: *Theoretical Physics 7: Quantum Mechanics—Methods and Applications*.

I am thankful to the Springer company, especially to Dr. Th. Schneider, for accepting and supporting the concept of my proposal. The collaboration was always delightful and very professional. A decisive contribution to the book was provided by Prof. Dr. A. Ramakanth from the Kakatiya University of Warangal (India). Many thanks for it!

Berlin, Germany Wolfgang Nolting
November 2016

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Chapter 1
Inductive Reasons for the Wave Mechanics

In this chapter we present a critical survey of the *'pre-quantum-mechanics'* time. We are thereby not so much focused on historical exactness but rather on a physical analysis of the problems and challenges which the scientist encountered at the beginning of the twentieth century, and which, in the end, enforced the development of the Quantum Mechanics in its still today valid and successful form. The didactic value of such a *historical* introduction can of course be debatable. The reader, who wants to straight away deal with the quantum-mechanical principles and concepts, may skip this introductory chapter and start directly with Chap. 2. Although Chap. 1 is thought, in a certain sense, only as introduction or *'attunement'* into the complex of problems, we do not want, however, to deviate from the basic intention of our ground course in Theoretical Physics, representing even here the important connections and relationships in such a detailed manner that they become understandable without the use of secondary literature.

At the beginning of the twentieth century, the physics saw itself in dire straits. The *Classical Physics*, as we call it today, was essentially understood and had proven its worth. But at the same time, one got to know unequivocally reproducible experiments, whose results, in certain regions, were running blatantly contrary to Classical Physics. This concerned, e.g., the **heat radiation** (Sect. 1.2) which was not to be explained by classical concepts. Planck's revolutionary assumption of an **energy quantization** which is connected to the **quantum of action** $\hbar$, was, at that time, not strictly provable, but explained quantitatively correctly the experimental findings and has to be considered today as the hour of the birth of modern physics. The exploration of the atomic structure (Sect. 1.3) paved the way to a new and at first incomprehensible world. It was recognized that the atom is not at all indivisible but consists of (today of course well-known) sub-structures. In the (sub-)atomic region, one detected novel **quantum phenomena**, a particular example of which is the stationarity of the electron orbits.

Diffraction and interference *prove* the wave character of the light. Both phenomena are understandable in the framework of classical electrodynamics without any evidence for a quantum nature of electromagnetic radiation. The photoelectric

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effect and the Compton effect, on the other hand, are explainable only by means of Einstein's **light quantum hypothesis**. Light obviously behaves in certain situations like a wave, but however, exhibits in other contexts unambiguously particle character. The classically incomprehensible **particle-wave dualism** of the light was born (Sect. 1.4). The realization of this dualism even for matter (Sect. 2.1) certainly belongs to the greatest achievements in physics in the twentieth century.

Semi-classical theories (Sect. 1.5) tried to *satisfy* these novel experimental findings with the aid of *postulates* which are based on *bold plausibility*, sometimes even in strict contradiction to Classical Theoretical Physics, as e.g. the Bohr atom model. The conclusions drawn from such postulates provoked new experiments (Franck-Hertz experiment), which, on their part, impressively supported the postulates. The challenge was to construct a novel *'atom mechanics'* which was able to explain stable, stationary electron states with discrete energy values. This could be satisfactorily accomplished only by the actual Quantum Theory. It was clear that the *new* theory must contain the Classical Mechanics as the macroscopically correct limiting case. This fact was exploited in the form of a **correspondence principle** (Sect. 1.5.3) in order to *guess* the *new* theory from the known results and statements of Classical Physics. However, it is of course very clear that, in the final analysis, such semi-empirical ansatzes can not be fully convincing; the *older* Quantum Mechanics was therefore not a self-contained theory.

1.1 Limits of Classical Physics

One denotes as *Classical Mechanics* (see Vol. 1) the theory of the motions of physical bodies in space and time under the influence of forces, developed in the seventeenth century by Galilei, Huygens, Newton,.... In its original form it is valid, as one knows today, only when the relative velocities v are small compared to the **velocity of light:**

$$c = 2.9979 \cdot 10^{10} \frac{\text{cm}}{\text{s}} \tag{1.1}$$

Einstein (1905) succeeded in extending the mechanics to arbitrary velocities, where, however, c appears as the absolute limiting velocity. The *Theory of Relativity*, developed by him, is today considered as part of the *Classical Physics* (see Vol. 4).

A characteristic feature of the *classical theories* is their **determinism**, according to which the knowledge of all the quantities, which define the *state of the system* at a certain point in time, fixes already uniquely and with full certainty the *state* at **all later** times. This means, in particular, that all basic equations of the classical theories refer to physical quantities which are basically and without restriction, accessible, i.e. measurable. In this sense a system is described in **Classical Mechanics** by its Hamilton function $H(\mathbf{q}, \mathbf{p}, t)$. The *state* of a mechanical system corresponds to a

point $\boldsymbol{\pi} = \boldsymbol{\pi}(t)$,

$$\boldsymbol{\pi} = (q_1, q_2, \ldots, q_s, p_1, p_2, \ldots, p_s) \ , \tag{1.2}$$

in the state space (see Sect. 2.4.1, Vol. 2). The partial derivatives of the Hamilton function with respect to the *generalized coordinates* q_j and the *generalized momenta* $p_j (j = 1, \ldots, s)$ lead to a set of 2 s equations of motion, which can be integrated with a corresponding number of initial conditions (e.g. $\boldsymbol{\pi}_0 = \boldsymbol{\pi}(t_0)$) and therewith fixes for all times t the *mechanical state* $\boldsymbol{\pi}(t)$. In Electrodynamics we need for fixing the *state of the system* in particular the fields **E** and **B** and in Thermodynamics we have to know the thermodynamic potentials U, F, G, H, S.

The requirement of the in principle and unrestrictively possible measurability of such fundamental quantities, though, has not proven to be tenable. The Classical Mechanics, for instance, appears to be correct in the region of visible, macrophysical bodies, but fails drastically at *atomic dimensions*. Where are the limits of the region of validity? Why are there limits at all? In what follows we are going to think in-depth about these questions. An important keyword in this connection will be the *measuring process*. In order to get information about a system one has to perform a measurement. That means in the final analysis, we have to *disturb* the system. Consequently one might agree upon the following schedule line:

$$\textit{small system} \Longleftrightarrow \textit{disturbance} \text{ perceptible} \ ,$$

$$\textit{large} \text{ system} \Longleftrightarrow \textit{disturbance} \text{ unimportant} \ .$$

In classical physics, it underlies the prospect that each system can be treated in such a way that it can be considered as *large*. This prospect, however, turns out to fail for processes in *atomic dimensions* (typical: masses from 10^{-30} kg to 10^{-25} kg, linear dimensions from 10^{-15} m to 10^{-9} m). A complete theory is desirable as well as necessary which does not need any idealizations as those implied by the classical ansatzes. The

Quantum Mechanics

has proven in this sense to be a consistent framework for the description of all physical experiences known to date. It contains the Classical Physics as a special case. Its development started in the year 1900 with Planck's description of the heat (cavity) radiation, which is based on the assumption, which is not compatible with Classical Electrodynamics, that electromagnetic radiation of the frequency ω can be emitted only as integer multiples of $\hbar\omega$. The term **energy quantum** was born and simultaneously a new universal constant was discovered,

Definition 1.1.1

$$h = 6.624 \cdot 10^{-34} \, \mathrm{J\,s} \ , \tag{1.3}$$

$$\hbar = \frac{h}{2\pi} = 1.055 \cdot 10^{-34} \, \mathrm{J\,s} \ , \tag{1.4}$$

which today is called *Planck's quantum of action*. If one considers physical processes, whose dynamical extensions are so small, that the macroscopically tiny quantum of action h can no longer be treated as *relatively small*, then there appear certain

quantum phenomena ,

which are not explainable by means of Classical Physics. (The most important phenomena of this kind are commented on in the next sections!) In such situations, each measurement represents a massive disturbance, which, contrary to the *classical frame*, can not be neglected. In order to classify this issue, one conveniently utilizes the term, proposed by Heisenberg in 1927, namely

uncertainty, indeterminacy

Therewith the following is meant: In Classical Mechanics the canonical space and momentum coordinates $\mathbf{q}$ and $\mathbf{p}$ have, at any point of time t, well-defined real numerical values. The system runs in the phase space along a sharp **trajectory** $\boldsymbol{\pi}(t) = (\mathbf{q}(t),\ \mathbf{p}(t))$. The actual course may be unknown in detail, but is, however, even then considered as in principle determined. If the intrinsically strictly defined trajectory is only imprecisely known then one has to properly average over all remaining *thinkable* possibilities, i.e., one has to apply *Classical Statistical Mechanics*. In spite of this statistical character, Classical Mechanics remains in principle deterministic, since its fundamental equations of motion (Newton, Lagrange, Hamilton) can be uniquely integrated provided that sufficiently many initial conditions are known.

In contrast, a profound characteristic of Quantum Mechanics is the concept that the dynamical variables $\mathbf{q}$ and $\mathbf{p}$ in general do not have exactly defined values but are afflicted with **indeterminacies** $\Delta\mathbf{p}$ and $\Delta\mathbf{q}$. How large these are depends on the actual situation where, however, always the

Heisenberg Uncertainty Principle (Relation)

$$\Delta q_i \Delta p_i \geq \frac{\hbar}{2}\ ; \quad i = 1, 2, \ldots, s \tag{1.5}$$

is fulfilled. The space coordinate can thus assume under certain conditions—as a limiting case—sharp values, but then the canonically conjugated momentum coordinates are completely undetermined, and vice versa. An approximate determination of q_i allows for a correspondingly approximate determination of p_i, under regard of the uncertainty principle.

The relation (1.5), which we will be able to reason more precisely at a later stage, must not be interpreted in such a way that the items of physics possess in principle simultaneously sharp values for momentum and space coordinate, but we are not

(perhaps not yet) able to measure them exactly. Since the measurement is **fundamentally** impossible it makes no sense to speak of simultaneously sharp momentum and position. The uncertainty relation expresses a genuine indeterminacy, not an inability.

1.1.1 Exercises

Exercise 1.1.1 Determine by use of the uncertainty relation the lowest limiting value for the possible energies of the harmonic oscillator!

Exercise 1.1.2 The hydrogen atom consists of a proton and an electron. Because of its approximately two thousand times heavier mass the proton can be considered *at rest* at the origin. On the electron the attractive Coulomb potential of the proton acts (Fig. 1.1). Classically arbitrarily low energy states should therefore be realizable. Show by use of the uncertainty relation that in reality a finite energy minimum exists!

Exercise 1.1.3 Estimate by use of the uncertainty principle, how large the kinetic energy of a nucleon ($m = 1.7 \cdot 10^{-27}$ kg) in a nucleus (radius $R = 10^{-15}$ m) is at the least.

Exercise 1.1.4 Estimate by application of the uncertainty relation the ground state energy of the one-dimensional motion of a particle with the mass m which moves under the potential

$$V(x) = V_0 \left(\frac{x}{a}\right)^{2n} .$$

Let V_0 be positive and n a natural number. Discuss the special cases

$$n = 1 \quad \text{and} \quad n = \infty .$$

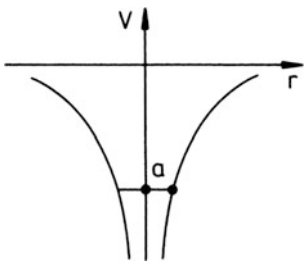

Fig. 1.1 Potential of the electron in the Coulomb field of the proton

1.2 Planck's Quantum of Action

At the turn of the century ($\approx$ 1900) physics was in a nasty dilemma. There existed a series of credible experimental observations which could only be interpreted by hypotheses which were in blatant contradiction to Classical Physics. This led to the compelling necessity to create a new self-consistent theory, which could turn these hypotheses into provable physical laws, but simultaneously should also contain the macroscopically correct Classical Physics as a valid limiting case. The result of an ingenious concurrence of theory and experiment was eventually the **Quantum Mechanics**. Let us try to retrace the dilemma of the Classical Physics mentioned above, in order to reveal the conceptually new aspects of the Quantum Theory that we are discussing. Of course her we are not so much focused on a detailed historical accuracy, but rather on the connections which have been important for the development of the understanding of physics.

The discovery of the universal quantum of action h, whose numerical value is already given in (1.3), is considered, not without good reason, as the hour of the birth of the Quantum Theory. Max Planck postulated its existence in his derivation of the spectral distribution of the intensity of the heat radiation. Because of the immense importance of his conclusions for the total subsequent physics, we want to dedicate a rather broad space to Planck's ideas.

1.2.1 Laws of Heat Radiation

The daily experience teaches us that a solid *'glows'* at high temperatures, i.e., emits visible light. At lower temperatures, however, it sends out energy in form of **heat radiation**, which can not be seen by the human eye, but is of course of the same physical origin. It is also nothing else but electromagnetic radiation. The term *heat radiation* only refers to the kind of its emergence. A first systematic theory of heat radiation was offered in 1859 by G. Kirchhoff. His considerations concerned the so-called **black body**. By this one understands a body which absorbs all the radiation incident it. This of course is, strictly speaking, an idealization, which, however, can be realized approximately by a hollow cavity with a small hole. Because of the multiple possibilities of absorption of radiation inside the hollow, it is rather unlikely that radiation which enters through the small hole will later be able to escape again. The area of the hole is therefore a quasi-ideal absorber. The radiation that nevertheless comes out of the hole is denoted as **black (or temperature) radiation**. It will be identical to the heat radiation which is inside the hollow and impinges on its walls. Let us thus imagine such a hollow with heat-impermeable walls which are kept at a constant temperature T. The walls emit and absorb electromagnetic radiation such that at thermodynamic equilibrium emission and absorption balance each other. Inside the hollow there will be established an electromagnetic field of

constant energy density ((4.46), Vol. 3):

$$w = \frac{1}{2}(\mathbf{E}\cdot\mathbf{D} + \mathbf{H}\cdot\mathbf{B}) \tag{1.6}$$

The heat radiation possesses a continuous spectrum which contains all frequencies from 0 to ∞. To describe the spectral distribution of the radiation one introduces the **spectral energy density** w_ν:

$$w_\nu = \frac{dw}{d\nu} \,. \tag{1.7}$$

The total spatial energy density follows from it by integration over all frequencies ν:

$$w = \int dw = \int_0^\infty w_\nu d\nu \,. \tag{1.8}$$

Using the second law of thermodynamics Kirchhoff proved that the radiation in the hollow is isotropic and homogeneous, i.e., being independent of the direction and equal at all points in the hollow. Furthermore, the spectral energy density w_ν can not depend, at constant temperature, T on the special constitution of the walls. Therefore, it is about a **universal function** of the frequency ν and the temperature T:

$$w_\nu \equiv f(\nu, T) \,. \tag{1.9}$$

We do not want to perform here the explicit proof of this assertion, not any more than the conclusion of W. Wien (1896), who by using a combination of thermodynamics and electromagnetic light theory, achieved a significant progress regarding the nature of the universal function f. He stated that the function f of **two** variables ν and T can be expressed in terms of a function g of only **one** variable ν/T,

$$f(\nu, T) = \nu^3 g\left(\frac{\nu}{T}\right) \,. \tag{1.10}$$

This is denoted as **Wien's law**. If one measures, for instance, the spectral energy density at different temperatures, one finds indeed for $f(\nu, T)/\nu^3$ as function of ν/T always the same shape of the curve. Via Wien's law (1.10), from the spectral distribution of the *black radiation*, measured at a given temperature, one can calculate the distribution for all other temperatures. Assume, for instance, that f is measured at the temperature T as function of ν, then it holds at the temperature T', if one understands ν' as $\nu' = \nu\frac{T'}{T}$:

$$f(\nu', T') = \nu'^3 g\left(\frac{\nu'}{T'}\right) = \nu'^3 g\left(\frac{\nu}{T}\right) = \left(\frac{T'}{T}\right)^3 \nu^3 g\left(\frac{\nu}{T}\right) = \left(\frac{T'}{T}\right)^3 f(\nu, T)$$

In spite of the indeterminacy of the function $g(\nu/T)$ some rather concrete statements can be derived from Wien's law. With the substitution of variables $x = \nu/T$ it follows from (1.8) and (1.10):

$$w = \int_0^\infty \nu^3 g\left(\frac{\nu}{T}\right) d\nu = T^4 \int_0^\infty x^3 g(x) dx \,. \tag{1.11}$$

The integral on the right-hand side yields only a numerical value α. Equation (1.11) is therewith the well-known

Stefan-Boltzmann Law

$$w(T) = \alpha T^4 \,. \tag{1.12}$$

If the spectral energy density w_ν possesses a maximum as function of ν at $\nu_{\max}$ then it must hold

$$\left.\frac{dw_\nu}{d\nu}\right|_{\nu_{\max}} = \left[3\nu^2 g\left(\frac{\nu}{T}\right) + \frac{\nu^3}{T} g'\left(\frac{\nu}{T}\right)\right]_{\nu_{\max}} \stackrel{!}{=} 0$$

or equivalently to that:

$$\frac{3}{x} g(x) + g'(x) \stackrel{!}{=} 0 \,.$$

The solution of this equation is a definite numerical value x_0:

$$\frac{\nu_{\max}}{T} \equiv x_0 = \text{const} \,. \tag{1.13}$$

This is **Wien's displacement law**. The frequency which corresponds to the maximal spectral energy density is directly proportional to the temperature.

The results of our considerations so far document that the Classical Physics can provide very detailed and far-reaching statements on the heat radiation. The laws (1.10), (1.12), and (1.13) are uniquely confirmed by the experiment, which must be valued as strong support of the concepts of Classical Physics. However, considerations going beyond this lead also to some blatant contradictions!

1.2.2 The Failure of Classical Physics

After the last section, the task that still remains consists in the determination of the universal Kirchhoff function $f(\nu, T) = \nu^3 g\left(\frac{\nu}{T}\right)$. Wien calculated with some simplifying model assumptions the structure of g to be as:

$$g\left(\frac{\nu}{T}\right) = a \exp\left(-b\frac{\nu}{T}\right) . \tag{1.14}$$

This theoretically not very well reasoned formula, in which a and b are constants, could explain rather well some of the existing experimental data. However, very soon it turned out as being an acceptable approximation only for the high frequency region $b\nu \gg T$.

Another derivation of $g(\nu/T)$ dates back to Rayleigh (1900), which is based on strict adherence to Classical Physics and does not need any unprovable hypothesis. Starting point is the classical equipartition theorem of energy, which states that in the thermodynamic equilibrium each degree of freedom of the motion carries the same energy $\frac{1}{2}k_BT$ (k_B = Boltzmann constant). By use of this theorem Rayleigh calculated the energy of the electromagnetic field in a hollow. For this purpose the radiation field is decomposed into a system of standing waves, where to each standing electromagnetic wave the average energy k_BT is to be assigned, namely $\frac{1}{2}k_BT$ to the electric and a further $\frac{1}{2}k_BT$ to the magnetic field. The determination of the spectral energy density therefore comes down to a counting of the standing waves in the hollow with frequencies in the interval $[\nu, \nu + d\nu]$.

Let us consider a cube of the edge length a. To realize standing waves the electric field must have nodes and the magnetic field antinodes at the walls. Let us first think of standing waves with nodes at the walls, whose normal vectors build together with the x-, y-, z-axes the angles α, β, γ. For a wavelength λ the distance of two next-neighboring nodal planes projected on the axes is (Fig. 1.2):

$$\frac{1}{2}\overline{x} = \frac{\lambda/2}{\cos\alpha} ; \quad \frac{1}{2}\overline{y} = \frac{\lambda/2}{\cos\beta} ; \quad \frac{1}{2}\overline{z} = \frac{\lambda/2}{\cos\gamma} .$$

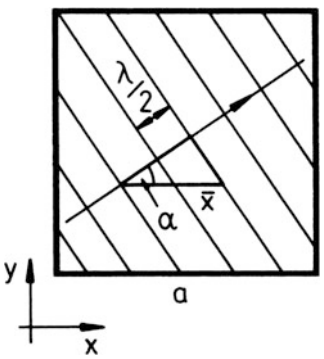

Fig. 1.2 Scheme for counting standing waves in a cube

Standing waves arise when the edge length a is an integer multiple of $\overline{x}/2, \overline{y}/2$, and $\overline{z}/2$. Angles and wave length therefore have to fulfill the conditions

$$n_1 = \frac{2a\cos\alpha}{\lambda}\ ; \quad n_2 = \frac{2a\cos\beta}{\lambda}\ ; \quad n_3 = \frac{2a\cos\gamma}{\lambda}\ ;$$
$$n_1, n_2, n_3 = 0, 1, 2, \dots\ , \tag{1.15}$$

which can be combined because of $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$ to

$$n_1^2 + n_2^2 + n_3^2 = \left(\frac{2a}{\lambda}\right)^2 = \left(\frac{2a\nu}{c}\right)^2\ . \tag{1.16}$$

$c = \nu\lambda$ is the velocity of light. Each combination of three integers n_1, n_2, n_3 yields with

$$\nu = \frac{c}{2a}\sqrt{n_1^2 + n_2^2 + n_3^2} \tag{1.17}$$

the frequency of an in principle possible standing wave in the hollow. We define the **frequency space** by a Cartesian system of coordinates, on whose axes we can mark, with $c/2a$ as unit, the integers n_1, n_2, n_3. Each point (n_1, n_2, n_3) then corresponds according to (1.17) to the frequency ν of a certain standing wave. The entirety of all these points form, in the frequency space, a simple cubic lattice. Exactly **one** point of the frequency lattice is ascribed to each elementary cube, which possesses with the chosen unit $c/2a$ just the *volume* 1. All points (n_1, n_2, n_3), belonging to a frequency between 0 and ν, are lying according to (1.16) within a sphere with its center at the origin of coordinates and a radius $R = \frac{2a\nu}{c}$. If $a \gg \lambda$ then one obtains with sufficient accuracy the number of frequencies between 0 and ν by dividing the volume of the sphere by the volume of the elementary cube. One has, however, to bear in mind that for the standing waves in the hollow only non-negative integers n_i, $i = 1, 2, 3$, come into question. The restriction to the respective octant provides a factor $1/8$:

$$N(\nu) = \frac{1}{8}\frac{4\pi}{3}\left(\frac{2a\nu}{c}\right)^3\ . \tag{1.18}$$

For the determination of the spectral energy density we need the number of frequencies in the spherical shell ν, $\nu + d\nu$:

$$dN(\nu) = 4\pi a^3\frac{\nu^2}{c^3}d\nu\ . \tag{1.19}$$

According to the equipartition theorem the energy k_BT is allotted to each of these waves. If we still consider the fact that **two** waves belong to each frequency ν with mutually perpendicular polarization planes, then we eventually obtain the required

spatial spectral energy density when we divide by $V = a^3$:

$$w_\nu d\nu = 8\pi \frac{\nu^2}{c^3} k_B T d\nu \ . \tag{1.20}$$

From this equation we read off the universal function

$$g\left(\frac{\nu}{T}\right) = \left(8\pi \frac{k_B}{c^3}\right) \frac{T}{\nu} \ , \tag{1.21}$$

which obviously fulfills *Wien's law* (1.10). One denotes (1.20) and (1.21), respectively, as the **Rayleigh-Jeans formula**. One should stress once more that its derivation is exact within the framework of Classical Physics, i.e., it does not need any hypotheses.

For practical purposes, it appears more convenient and more common, to rewrite the spectral energy density in terms of wavelengths λ. With

$$w_\nu d\nu \longrightarrow w_{\nu(\lambda)} \left|\frac{d\nu}{d\lambda}\right| d\lambda \equiv w_\lambda d\lambda$$

equation (1.20) reads:

$$w_\lambda d\lambda = \frac{8\pi k_B T}{\lambda^4} d\lambda \ . \tag{1.22}$$

For large wavelengths λ (small frequencies ν) this formula has proven to be correct. The experimental curves for the energy distribution in the spectrum of *black-body radiation* typically have a distinct maximum in the small wavelength region and then drop down very steeply to zero for $\lambda \to 0$ (Fig. 1.3). With increasing temperature, the maximum shifts to smaller wavelengths in conformity with (1.13). We recognize that the Rayleigh-Jeans formula (1.22), even though derived classically correctly, except for the region of very large wavelengths, stays in complete contradiction to experimental findings. The fact that the classical result (1.20) can indeed not be correct one recognizes clearly when one use it to

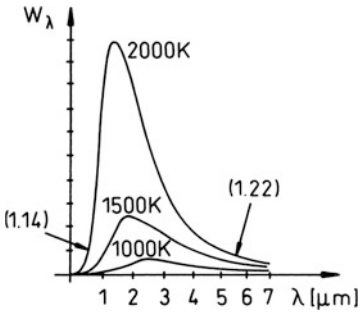

Fig. 1.3 Spectral energy density of the black-body radiator as function of the wavelength λ

calculate the total spatial energy density:

$$w = \int_0^\infty w_\nu d\nu = \frac{8\pi}{c^3} k_B T \int_0^\infty \nu^2 d\nu = \infty \,. \tag{1.23}$$

This so-called *ultraviolet catastrophe* as well as the general comparison of theory and experiment point out uniquely the *failure of Classical Physics* as regards the interpretation of the heat radiation of a *black body*.

At the turn of the century ($\approx$ 1900) there thus existed two formulas for the heat radiation, namely that of Wien (1.14) and that of Rayleigh-Jeans (1.21). Both represented good approximations for different special regions, namely (1.14) for very large ν and (1.21) for very small ν, , but turned out to be completely invalid over the full spectral region. Therefore one was searching for something like an interpolation formula, which for small ν (big λ) agreed with the Rayleigh-Jeans formula (1.21) and for big ν (small λ) with the Wien formula (1.14). Such a formula was published in the year 1900 for the first time ever by Max Planck.

1.2.3 Planck's Formula

For the derivation of his formula Planck was obliged to use a hypothesis, that blatantly ran counter to the world of ideas of Classical Physics. In a first step he replaced the actual emitting and absorbing atoms of the walls by electrically charged linear harmonic oscillators. That could be justified by the fact that the universal function $g(\nu/T)$ should actually be the same for all *thermodynamically correct* models of the hollow radiation. Each of these oscillators has a definite eigen-frequency with which the electric charge performs oscillations around its equilibrium position. As a consequence of these oscillations the oscillator can exchange energy with the electromagnetic field inside the hollow. It comes to an equilibrium state which can be calculated with the methods of Statistical Mechanics and Electrodynamics. Classical Physics allows for a *continuous* energy spectrum to each of these oscillators, so that the oscillator can in turn exchange any arbitrary radiation energy with the electromagnetic field in the hollow. The result of a calculation performed on that basis, however, is in complete contradiction to experimental experience. The problem is solved only by the

Planck's Hypothesis

The oscillators exist only in such states, whose energies are integral multiples of an elementary energy quantum ε_0:

$$E_n = n\varepsilon_0 \,; \quad n = 0, 1, 2, \ldots \tag{1.24}$$

Consequently, an oscillator can absorb or emit only such energies which correspond to integer multiples of ε_0:

$$\Delta E = m\varepsilon_0 \; ; \quad m = 0, \pm 1, \pm 2, \ldots \tag{1.25}$$

The *blatant violation* of the laws of Classical Physics consisted in the assumption that the energies of *microscopic* entities, such as the atoms of the hollow walls, can take up only **discrete** values. Energies can be absorbed and emitted, respectively, only in *'quantized packages'*.

Let the total number of the wall-oscillators be N. From these, $N(n)$ may be in a state of energy $E_n = n\varepsilon_0$:

$$N = \sum_{n=0}^{\infty} N(n) \; ; \quad E = \sum_{n=0}^{\infty} N(n) n\varepsilon_0 \; .$$

The average energy per oscillator then amounts to:

$$\hat{\varepsilon} = \frac{\sum\limits_{n=0}^{\infty} N(n) n\varepsilon_0}{\sum\limits_{n=0}^{\infty} N(n)} \; . \tag{1.26}$$

According to the classical Boltzmann statistics it holds that

$$N(n) \sim \exp(-\beta n\varepsilon_0) \; ,$$

where we have abbreviated, as it is usual, $\beta = 1/k_B T$. The unspecified proportionality factor is cancelled out after insertion into (1.26):

$$\hat{\varepsilon} = \frac{\sum\limits_{n=0}^{\infty} n\varepsilon_0 \exp(-\beta n\varepsilon_0)}{\sum\limits_{n=0}^{\infty} \exp(-\beta n\varepsilon_0)} = -\frac{d}{d\beta} \ln \left[\sum_{n=0}^{\infty} \exp(-\beta n\varepsilon_0) \right] \; . \tag{1.27}$$

β and ε_0 are positive quantities. The sum is therefore just the geometric series:

$$\sum_{n=0}^{\infty} \exp(-\beta n\varepsilon_0) = \frac{1}{1 - \exp(-\beta\varepsilon_0)} \; .$$

The average energy per oscillator amounts therewith not to $k_B T$, but to:

$$\hat{\varepsilon} = \frac{\varepsilon_0}{\exp(\beta\varepsilon_0) - 1} \; . \tag{1.28}$$

Each *wall-oscillator* is *in resonance* with one of the standing electromagnetic waves of the hollow. For the derivation of the spatial spectral energy density we can therefore adopt the considerations of Rayleigh, presented in the last section. We have only to replace the energy $k_B T$ of the classical equipartition theorem by $\hat{\varepsilon}$:

$$w_\nu = \frac{8\pi\nu^2}{c^3} \frac{\varepsilon_0}{\exp(\beta\varepsilon_0) - 1} \,.$$

If we now additionally demand that the radiation formula obeys the thermodynamically exact Wien's law (1.10), then it follows imperatively that ε_0 must be proportional to the frequency ν of the oscillator:

$$\varepsilon_0 \longrightarrow h\nu \,. \tag{1.29}$$

The universal constant h has the dimension of an *action*, i.e., 'energy · time':

Planck's Radiation Formula

$$w_\nu = \frac{8\pi}{c^3}\nu^3 \frac{h}{\exp(\beta h\nu) - 1} \,. \tag{1.30}$$

Several methods for the determination of the proportionality constant h have been developed in the aftermath. They have led for *Planck's quantum of action* h to the numerical value (1.3). It is therefore an extremely small quantity of approximately 10^{-33} Js. That explains why the microscopically necessary energy quantization (1.24) does not play any role for macroscopic phenomena and was therefore hitherto *missed* by the Classical Physics. Because of

$$\frac{h\nu}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \approx \begin{cases} k_B T & \text{for } h\nu \ll k_B T \,, \\ h\nu \exp\left(-\frac{h\nu}{k_B T}\right) & \text{for } h\nu \gg k_B T \end{cases} \tag{1.31}$$

Planck's formula incorporates Wien's formula (1.14) and Rayleigh-Jeans formula (1.21) as limiting cases.

Finally, it is easy to figure out (Exercise 1.2.1) that the total spatial energy density calculated with (1.30) does fulfill the Stefan-Boltzmann law (1.12). The T^4-proportionality follows already, as shown before, from the Wien's law (1.10), which is of course also correctly reproduced by (1.30):

$$w(T) = \left(\frac{8}{15}\pi^5 \frac{k_B^4}{c^3 h^3}\right) T^4 \,. \tag{1.32}$$

One does not need much imagination in order to comprehend the *shock* for the Classical Physics caused by Planck's ideas about the quantization of the energy. After all, not less than the equipartition theorem of the energy—among others—was therewith overruled. The average energy $\hat{\varepsilon}$ for the standing waves of the black-body radiation with different frequencies,

$$\hat{\varepsilon} = \frac{h\nu}{\exp(\beta h\nu) - 1} \ , \tag{1.33}$$

is not at all constant equal to $k_B T$, but rapidly decreases for high frequencies ν, which helps to avoid the ultraviolet catastrophe (1.23) of the Rayleigh-Jeans theory. The exact confirmation of Planck's formula by the experiment forced the physicists to accept as physical reality the

energy quantization ,

introduced by Planck at first hypothetically, with the central role of

Planck's quantum of action h .

The effort to convert Planck's hypotheses into rigorously provable physical laws initiated a new era of Theoretical Physics. One has therefore to consider the year 1900 as the year of the birth of

Quantum Mechanics .

1.2.4 Exercises

Exercise 1.2.1 Calculate with Planck's radiation formula the temperature-dependence of the total spatial energy density of the black-body (cavity) radiation!

Exercise 1.2.2 Write down the spectral energy density of the heat radiation as function of the wave length, for Planck's formula as well as for Wien's formula. Demonstrate the equivalence of the two formulas for small λ and derive therewith concrete expressions for the empirical constants a and b of Wien's formula (1.14). Compare Planck's formula for big λ with that of Rayleigh-Jeans (1.22).

1.3 Atoms, Electrons and Atomic Nuclei

The necessity of quantum-mechanical concepts became particularly mandatory after the discovery of the atomistic structure of matter. This was first recognized and included in the scientific discussion by chemistry. As we have convinced ourselves in the last section, the probability of typical quantum phenomena is higher at atomic dimensions.

1.3.1 Divisibility of Matter

If the material properties of matter are to be retained, then matter is not divisible to arbitrarily small parts. The smallest building block of matter, which still exhibits the typical physical features of the respective element, is called **atom**. It is meant therewith that with a further dissection the resulting *fragments* will differ basically from the actual atom. If, for instance, Ni atoms are arranged in a particular manner then we get the Ni-*crystal* with its typical Ni-*properties*. If one performs the same procedure with any *fragments* of the Ni atom then the resulting formation will have nothing in common with the Ni-crystal. In this sense we consider matter as not arbitrarily divisible.

First decisive indications of the atomistic structure of matter arose by Dalton's investigations (1808–1810) on the composition of chemical compounds.

1. In a chemical compound the relative weights of the elementary constituents are always constant (*law of the constancy of the compounding weights*).
2. If the same two elements build different chemical compounds and each is characterized by a certain mass proportion, then the mass proportions of the different compounds are related to one another by simple rational ratios (*law of multiple proportions*). Example: In the nitrogen-oxygen compounds N_2O, NO, N_2O_3, NO_2, N_2O_5 the oxygen masses, related to a fixed nitrogen mass, behave like 1 : 2 : 3 : 4 : 5.

With the present day knowledge of the atomic structure of matter Dalton's laws are of course easily explainable. Under the assumption of an arbitrarily divisible matter, though, they would create serious difficulties for the understanding.

Further convincing indications of the atomistic structure of matter is provided by the **kinetic theory of gases**, the basic ideas of which date back to Bernoulli (1738), Waterstone (1845), Krönig (1856) and Clausius (1857). The final formulation, however, is due to Maxwell and Boltzmann.

The *gas* is understood as a collection of small particles, which move in a straight line with constant velocity during the time between two collisions. Qualitative proofs of the correctness of this visualization can be read off from simple diffusion experiments. When one evaporates, for instance, sodium in a highly evacuated chamber, then the vapor, which reaches a screen after running through a system of blinds, creates there a sharp edge (Fig. 1.4). The latter documents the rectilinear motion of the particles of the gas. In the case of a not so good vacuum the sharpness of the edge decreases because of the then more frequently occurring collisions

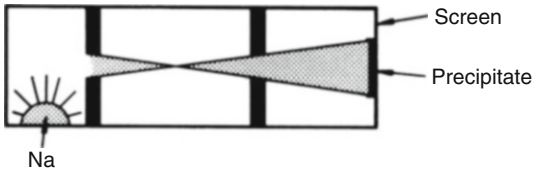

Fig. 1.4 Schematic experimental arrangement for the demonstration of the straight-line motion of the particles of a gas

between the particles. The **kinetic theory of gas** interprets the pressure of the gas on a wall of the vessel as the momentum transfer of the gas particles on the wall per unit area and unit time. Therewith one understands the **basic equation of the kinetic theory of gases** (Exercise 1.3.1):

$$p = \frac{1}{3}\frac{N}{V} m\langle \mathbf{v}^2 \rangle \ . \tag{1.34}$$

p is the pressure, V the volume, N the number of particles, m the mass of a particle, and $\langle \mathbf{v}^2 \rangle$ the average of the square of the particle velocity. Although derived from simplest model pictures, (1.34) is excellently confirmed by the experiment. Since the right-hand side of the equation contains only quantities, which at constant temperature also are constant, the Boyle-Mariotte's law $pV = \text{const}$, if $T = \text{const}$, ((1.2), Vol. 5) appears as a special case of (1.34). On the other hand, if one combines the basic equation with the equation of state of the ideal gas ((1.7), Vol. 5)

$$pV = Nk_B T \tag{1.35}$$

($k_B = 1.3805 \cdot 10^{-22}\,\mathrm{J/K}$), then one finds the internal energy of the gas consisting of noninteracting particles:

$$U(T, V) = N\frac{m}{2}\langle \mathbf{v}^2 \rangle = \frac{3}{2} N k_B T \equiv U(T) \ . \tag{1.36}$$

Its independence of the volume V agrees with the result of the Gay-Lussac experiment ((2.60), Vol. 5). Because of

$$\langle v_x^2 \rangle = \langle v_y^2 \rangle = \langle v_z^2 \rangle = \frac{1}{3}\langle \mathbf{v}^2 \rangle$$

the same thermal energy $(1/2)k_B T$ is allotted to each degree of freedom of the (linear) particle motion. That is the statement of the classical equipartition theorem.

The model picture of the kinetic theory of gases leads also to quantitative information about transport phenomena like the internal friction, the heat conduction, and the diffusion of gases. However, for that additional knowledge is needed about the particle density, the mean free path, and the *diameter* of the molecules, where, in particular, the definition of the diameter of a particle is problematic.

The successes of the *kinetic theory of gases* must be considered as a strong support of the idea of the atomistic structure of matter. Last doubts were finally removed by the novel atomic physics spectroscopies, as for instance by the *cloud chamber* first designed by Wilson, which let the tracks of atomic particles become visible, or by the X-ray diffraction on the lattice planes of crystals, which are occupied by atoms in periodic arrangements. The term

atom

as the smallest building block of matter which is not further divisible by chemical means

was therewith laid down! Analogously thereto, one defines the *molecule* as the smallest particle of a chemical compound that still possesses the typical properties of the compound.

The mass of an atom is normally not given as an absolute value, but in relative units:

(Relative) Atomic Mass A_r

$\cong$ *multiple of the atomic mass of* $1/12$ *of the mass of the pure carbon isotope* ^{12}C.

The *molecular weight* M_r is calculated, by use of the respective chemical formula, with the atomic masses of the involved atoms. The unit of mass $\left(1\mathrm{u} = 1/12m\left(^{12}\mathrm{C}\right)\right)$ is today, also absolutely, very precisely known:

Definition 1.3.1

$$1u = 1.660277 \cdot 10^{-24}\,\mathrm{g}\,. \tag{1.37}$$

The unit of the amount of material is the *mole*. By this one understands the amount of material, which consists of the same number of identical particles as atoms are contained in 12 g of pure atomic carbon of the isotope ^{12}C. According to *Avogadro's law* in equal volumes of different gases at equal pressure and equal temperature, there are the same number of atoms (molecules). Consequently, 1 mole of a gas will always take the same volume:

Definition 1.3.2

$$1\ \text{molar volume} = 22.41\,. \tag{1.38}$$

The number of particles in a mole is called *Avogadro's number* or *Loschmidt number*:

Definition 1.3.3

$$N_\mathrm{A} = 6.0222 \cdot 10^{23}\,\mathrm{mol}^{-1}\,. \tag{1.39}$$

Experimentally N_A can be fixed via the Faraday constant, via the Brownian motion of small dissolved particles (Einstein-Smoluchowski method), via the density decline, caused by gravitational force, of very small particles suspended in liquids (Perrin method), or also by measuring the coefficient of the internal friction or the heat conduction coefficient, which are both inversely proportional to N_A.

The systematics of the atomic masses has eventually led to the *periodic table of the elements* (Mendelejeff, Meyer (1869)). Firstly it is about an arrangement of the elements according to increasing atomic mass, arranged in *periods* and one below the other in *groups*. Additionally, chemically very similarly behaving elements are ascribed to the same group, thus in the periodic table they are one below the

other, as, for instance, the noble gases, the alkali metals, the alkaline earth metals, the halogens,.... This ordering principle has led to the fact that there are gaps in the periodic table since according to the chemical properties certain elements necessarily have to belong to certain groups. Just because of this fact, the sequential arrangement according to ascending atomic masses had to be interrupted at five positions (Ar-K, Co-Ni, Te-J, Th-Pa, U-Np). At the left corner of a period the electropositive character is strongest, towards the right corner the electronegative character grows. Since the atomic mass can not completely unambiguously fix the position of the element in the periodic table, one has simply numbered the elements consecutively, including the gaps present, from hydrogen up to uranium. The respective number is called the *atomic number Z*. Today we know that the atomic number has its independent physical meaning as the number of protons in the nucleus. The experiment revealed further on that chemically equivalent and therefore belonging to the same group elements can have different atomic masses. One speaks of *isotopes* marking therewith atoms with the same Z, but with different atomic masses.

The question concerning the *size of an atom*, or, if sphericity is assumed, the *atomic radius*, appears to be quite problematic. It poses in fundamental problems, the sources of which will still be a matter of discussion at a later stage. In the final analysis, the atomic radius will be defined by the range of action of forces. It is surely not a problem to determine the radius R of a billiard ball from collision processes. As soon as the distance of the centers of the spheres becomes smaller than $2R$ a deflection sets in. It is clear, though, that, e.g., for charged particles this method becomes quite problematic, since, because of the long-range Coulomb interaction, practically for arbitrarily large distances a deflection will be observable. Neutral atoms take in this connection an intermediate position. The *atomic radius* can therefore be only estimated, if one considers, at all, such a quantity as reasonably defined:

1. One could divide the mass $M = \rho V$ (ρ = mass density) of an amount of material by the atomic mass in order to get the number $N(V)$ of the atoms in the volume V:

$$N(V) = \frac{\rho V}{A_r u} \,. \tag{1.40}$$

If one assumes a closest packed *globular cluster*, then it holds approximately for the *atomic radius R*:

$$R = \left(\frac{3}{4\pi}\frac{V}{N(V)}\right)^{1/3} = \left(\frac{3}{4\pi}\frac{A_r u}{\rho}\right)^{1/3} \,. \tag{1.41}$$

One finds for instance for Cu with $\rho = 8.9\,\mathrm{g/cm^3}$ the estimation $R \approx 1.414 \cdot 10^{-8}\,\mathrm{cm}$. For a more precise calculation one has to of course take into consideration still, the actual volume filling of the *globular cluster*, and also the temperature-dependence of ρ.

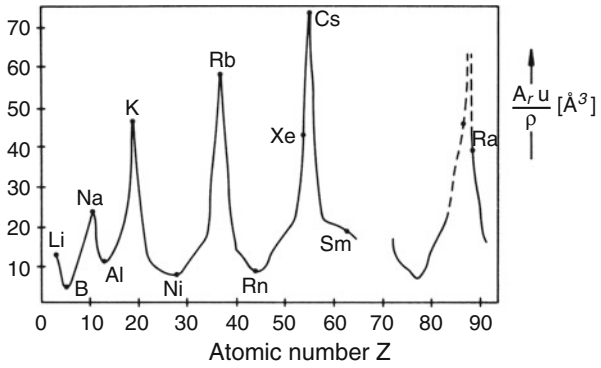

Fig. 1.5 Relative atomic volumes as functions of the atomic number

2. The constant b in the van der Waals equation for real gases ((1.14), Vol. 5) is interpreted as directly proportional to the volume of the particle. A measurement of b can therefore deliver information about R. However, one should not forget that the van der Waals model itself represents only an approximate description of reality.
3. The coefficients of viscosity (internal friction) and heat conduction, respectively, depend on the mean free path of the particles, and the latter on R.
4. When one brings an oil drop onto an expanse of water then the interfacial water–air tension pulls apart the drop to become extremely flat. From the volume of the oil drop and the effective diameter of the oil film the thickness of the monoatomic layer can be determined.

If one calculates the atomic radii by such methods, one finds for **all** atoms the same order of magnitude:

$$R = 0.8 \text{ to } 3 \cdot 10^{-8}\,\text{cm} . \tag{1.42}$$

Furthermore, there is an interesting periodicity (see Fig. 1.5). The elements of the first group of the periodic table, the alkali metals, possess the distinctly largest atomic volumes.

1.3.2 Electrons

One has considered the atoms, as is already expressed by the name derived from the Greek word *'atomos'*, at first as no further divisible building blocks of matter, and one, consequently, has thought that the total material world as build up by different atoms. Today one knows that even the atoms are further divisible, may be not by chemical, but by physical means. The first clear hint on the internal structure

of atoms and molecules, respectively, stems from experiments on gas discharges, by which, obviously, neutral atoms are fragmented into electrically charged constituents (ions, electrons). Electrically charged atoms (ions) were directly observed and investigated at first by *electrolysis*. By an *electrolyte* one understands materials, whose solution or melt conducts electricity since it is composed of ions. Today one knows that creation of ions is due to charge exchange, where electrons switch from one atom to another. If one installs in an electrolyte two electrodes and applies a voltage to them, after a certain time one finds mass precipitations for which M. Faraday (1791–1867) formulated the following rules:

1. The mass M precipitated on one of the electrodes is proportional to the transported charge Q:

$$M = AQ \,. \tag{1.43}$$

   A is called the *electrochemical equivalent* with the unit $\mathrm{kg(As)}^{-1}$.
2. A *gram equivalent* transports for **all** materials the same amount of electric charge, given by the *Faraday constant*:

$$F = 96{,}487 \frac{\mathrm{As}}{\mathrm{mol}} \,. \tag{1.44}$$

One defines thereby:

$$1 \text{ gram equivalent} = 1 \text{ mole/valence} \,.$$

One mole of each material always contains N_A atoms or molecules, respectively, (1.39). A monovalent ion therefore transports the charge

$$e = \frac{F}{N_\mathrm{A}} = 1.6021 \cdot 10^{-19}\,\mathrm{As} \,, \tag{1.45}$$

a multivalent ion, on the other hand, the charge ne. Ions can thus carry the charges $e, 2e, 3e, \ldots$, but, for instance, not $1.5e, 2.5e, \ldots$. That was a clear-cut hint for the discrete structure of the electric charge.

Millikan (1911) was the first who succeeded in the confirmation and the direct measuring of the *elementary charge* e by investigating the motion of smallest electrically charged oil drops in electric fields. A homogeneous medium with the viscosity η is prepared between the plates of a capacitor (Fig. 1.6). In this medium there act then on a spherule of the radius r and the velocity v the Stokes's frictional force

$$F_\mathrm{S} = 6\pi\eta r v \,,$$

the gravitational force mg and the electric force $qE = \frac{qU}{d}$. As soon as the total force is zero, the drop is no longer accelerated, moving thus with constant velocity. In

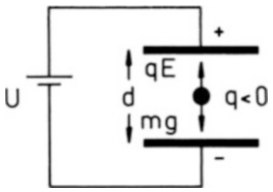

Fig. 1.6 Schematic set up of the Millikan-experiment for the measurement of the elementary electric charge

order to bring, at all, the three force components into the same order of magnitude, Millikan had to work with extremely small droplets (see the Exercises 1.3.3–1.3.5), as a result of which, he could not measure directly their radii. He needed therefore **two** conditional equations. In the case of a switched off electric field ($E = 0$) it holds in the equilibrium:

$$6\pi r\eta v_0 = m^* g = \frac{4\pi}{3} r^3 (\rho - \rho_{\text{air}}) g \ .$$

One has to take the buoyant force in the air into consideration, i.e., one has to subtract from the mass m of the droplet the mass of the displaced air. ρ and ρ_{air} are the known mass densities of the oil droplet and the air, respectively. The radius of the droplet r is thus determinable by measuring v_0.

When one now switches on the electric field then the drop gets another equilibrium-velocity v_1:

$$6\pi r\eta v_1 = m^* g + qE \ .$$

From the last two equations the charge q can be determined:

$$q = \frac{18\pi \eta^{3/2}}{E\sqrt{2(\rho - \rho_{\text{air}})g}} \sqrt{v_0}(v_1 - v_0) \ . \tag{1.46}$$

Millikan could observe, by ionization of the air between the plates of the capacitor, droplets in different charge states. The measurement of the charge q yielded always an integer multiple of an *elementary charge*, which agreed excellently with the value in (1.45), provided one used correct numbers for the material constants in (1.46). The discrete structure of the charge was therewith uniquely proven.

A first clear hint that the elementary charge occurs also *freely*, and not only in states **bound** to atoms or molecules, was found by the investigation of the electric discharge in diluted gases. For the electric gas discharge, neutral atoms are obviously fragmented into positively charged ions and negatively charged *'elementary quanta of electricity'*. For the latter, one had agreed upon the nomenclature *'electrons'*. By that the phenomena observed for the electrolysis find a simple explanation. If one applies, e.g., an electric field to a common salt solution, Na^+ ions will travel to the cathode, Cl^- ions to the anode. What has happened is obviously a charge exchange, where one electron has gone from the sodium to the chlorine.

For the determination of characteristic properties of the electron it is at first necessary to create **free** electrons. For that there are several possibilities:

1. Electron liberation by *ionization by collision* of gas atoms. For this purpose one accelerates charged particles to high velocities in an electric field or one exploits the high kinetic energies of the particles of a *very hot* gas (*thermal ionization*).
2. *Thermionic emission* from strongly heated metal surfaces. The maximal current, which can be achieved by sucking off the electrons from the thermally emitting surface by an electric field as given by *Richardson' equation*,

$$I_s \sim T^2 \exp\left(-\frac{W_\mathrm{w}}{k_B T}\right) , \tag{1.47}$$

   depends, exponentially on the temperature and the so-called *(electronic) work function* W_w. W_w is a property of the electron emitting substance.
3. *Photoeffect*. Sufficiently short-wavelength light can free electrons from solids by an energy exchange, which exceeds the value of W_w. This effect will be discussed in more detail in the next section.
4. *Field emission*. Electrons can be extracted from metal surfaces by extremely high electric fields, as they arise, for instance, at sharp metal tips.
5. *β-rays*. Certain radioactive substances spontaneously emit electrons.

After one has generated free electrons in such or similar manner one can manipulate their motions in the electromagnetic field, in order to gain further experimental information. In the framework of Classical Physics the motion of the electron is describable by the mass m_e and the charge $q = -e$, while the spatial extension of the electron can be neglected to a good approximation (charged mass point, point charge). The investigation of the electron trajectories in the electromagnetic field, though, permits only the determination of the *specific charge* q/m_e.

a) Longitudinal electric field

If the electrons, emitted by a hot cathode, are sucked off by a potential gradient U, they gain kinetic energy in the electric field, which corresponds to the work done by the field on the electrons:

$$2U = \frac{v^2}{q/m_\mathrm{e}} . \tag{1.48}$$

This equation contains with v and q/m_e two unknowns.

b) Transverse electric field

A sharply bunched cathode beam (electrons) traverses the electric field of a plane-parallel capacitor with the velocity $v_x = v$ in x-direction. Transversally to that, in y-direction, the electric field of the capacitor acts, by which the electron gets an acceleration $a_y = qE/m_\mathrm{e}$ in y-direction (Fig. 1.7). The time spent within the capacitor amounts to $\Delta t = L/v_x = L/v$. After the exit from the capacitor, i.e., after the re-entry into the field-free space, where the beam moves rectilinearly, the beam

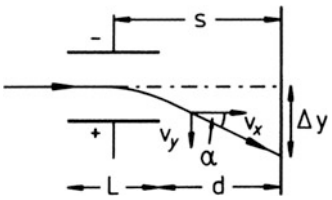

Fig. 1.7 Schematic plot concerning the measurement of the deflection of an electron beam in the transverse electric field

would have reached the velocity

$$v_y = a_y \Delta t = \frac{q}{m_e} E \frac{L}{v}$$

in y-direction. The original direction of motion is therefore deflected by the angle α:

$$\tan \alpha = \frac{v_y}{v_x} = \frac{q}{m_e} E \frac{L}{v^2} .$$

At the distance $s \gg L$ a luminescent screen is installed, on which the deflection Δy of the electron beam is recorded:

$$\Delta y \approx s \tan \alpha = \frac{L(2d + L)}{2v^2} \frac{q}{m_e} E . \tag{1.49}$$

The deflection Δy, which of course can easily be measured, is thus directly proportional to the voltage at the capacitor and inversely proportional to the kinetic energy of the electrons.

We have in both cases, (1.48) for the longitudinal and (1.49) for the transverse field, the two unknowns v^2 and q/m_e. Howsoever one combines the electric fields, one will always be able to measure only the variable

$$\frac{v^2}{q/m_e} = \frac{m_e v^2}{q} .$$

The electric field therefore sorts according to the kinetic energy and represents therewith an energy spectrometer.

c) Transverse magnetic field

The anode, which is located close to and before the cathode, has a small hole, through which the electrons can pass as a bunched beam (Fig. 1.8). Outside the capacitor only the homogeneous magnetic field **B** acts, which is oriented perpendicular to the direction of the motion of the electrons forcing them onto a circular path due to the Lorentz force

$$\mathbf{F}_L = q[\mathbf{v} \times \mathbf{B}] .$$

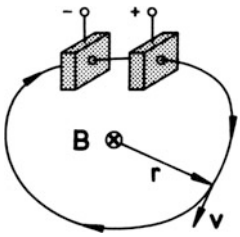

Fig. 1.8 Deflection of an electron beam in the transverse magnetic field

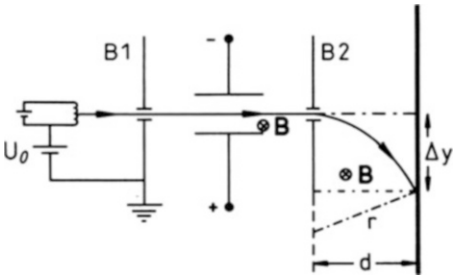

Fig. 1.9 Schematic representation of a combination of electric and magnetic fields for the determination of the ratio charge to mass of the electron (specific charge)

The radius r of the path can be determined from the equality of Lorentz force and centrifugal force ((2.80), Vol. 1):

$$\frac{m_e v^2}{r} = qvB \Longleftrightarrow \frac{v}{q/m_e} = rB \,. \tag{1.50}$$

We recognize that the magnetic spectrometer sorts according to the momentum mv.

d) Combined magnetic and electric fields

If we want to separately measure v and q/m_e for the electrons we have to obviously combine magnetic and electric fields.

One of the several possibilities is schematically plotted in Fig. 1.9. The electron leaves the thermionic cathode and travels up to the first blind B1 which is at a voltage of U_0, gaining therewith a kinetic energy qU_0. Within the capacitor a homogeneous electric field in y-direction is realized and, perpendicular to that (in the plane of the paper), a homogeneous magnetic field **B** is applied. Until it reaches the second blind B2 the electron **should not** experience, any net deflection within the capacitor:

$$q\mathbf{E} \stackrel{!}{=} q[\mathbf{v} \times \mathbf{B}] \Longrightarrow v = E/B \,.$$

The electromagnetic field thus sorts according to the velocity (*Wien filter*). By a suitable choice of E and B one can therefore adjust a desired velocity v. Outside the capacitor, only the magnetic field **B** works, which forces the electron to travel on a circular path, whose radius is given by Eq. (1.50). The deflection Δy is then

measured on a luminescent screen:

$$r^2 = d^2 + (r - \Delta y)^2 \Longrightarrow r = \frac{d^2 + \Delta y^2}{2\Delta y} \, .$$

This expression for r is inserted into (1.50):

$$\frac{q}{m_e} = \frac{E}{B^2} \left(\frac{2\Delta y}{d^2 + \Delta y^2} \right) \, . \tag{1.51}$$

The specific charge q/m_e of the electron is therewith indeed fixed only by Δy. Experiments of this kind led to:

1. For the cathode beams (electrons) q/m_e and therewith q is always negative.
2. Because of the sharp slit image q/m_e must be the same for **all** electrons.

Definition 1.3.4

$$\frac{q}{m_e} \text{ (electron)} \; = -1.75890 \cdot 10^{11} \frac{\text{As}}{\text{kg}} \, . \tag{1.52}$$

Since only q/m_e is measurable, it must be considered as a postulate, even though consistent so far, to ascribe to the electron the elementary charge e (1.45) detected by the Millikan experiment:

Definition 1.3.5

$$q \text{ (electron)} \; = -e \, . \tag{1.53}$$

so that the electron mass m_e is also determined:

Definition 1.3.6

$$m_e = 9.1096 \cdot 10^{-31} \text{kg} \, . \tag{1.54}$$

If one replaces the source of the thermionic electrons by a machine, as for instance the electron synchrotron, which can emit high-energy electrons, then one observes that the electron mass seems to be not a constant, but rather depends on the velocity v. Already several years before the development of the Special Theory of Relativity the 'proof' of the velocity dependence of the mass was thus experimentally provided. (See, however, to this point the comment given after Eq. (2.61) in Vol. 4). Einstein gave for this point the exact theoretical reasoning ((2.59), Vol. 4):

$$m(v) = \frac{m_e}{\sqrt{1 - \frac{v^2}{c^2}}} \, . \tag{1.55}$$

m_e must therefore be considered as *'rest mass'* of the electron. By modern accelerators electrons can reach such high velocities that their masses can come to many thousands times m_e.

A result of the Special Theory of Relativity which is of well-known immense consequences is the equivalence relation between mass and energy ((2.66), Vol. 4):

$$E = mc^2 \,. \tag{1.56}$$

It follows therewith for the kinetic energy of the electrons:

$$T = mc^2 - m_e c^2 = m_e c^2 \left(\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right) = m_e c^2 \left(\frac{1}{2} \frac{v^2}{c^2} + \dots \right) \,.$$

For $v \ll c$ we get the familiar non-relativistic expression

$$T = \frac{m_e}{2} v^2 \,.$$

Since $T = qU$ yields the same kinetic energy for all particles of arbitrarily different masses, provided they have the same charge q, one defines as energy unit the *electron-volt eV* which is appropriate to atom physics. It is the work, which must be done to move the elementary charge e between two points which have a potential difference of just 1 V:

$$1\,\mathrm{eV} = 1.6021 \cdot 10^{-19}\,\mathrm{J} \,. \tag{1.57}$$

For the rest mass of the electron, we get therewith the energy equivalent

Definition 1.3.7

$$m_e c^2 = 0.5110\,\mathrm{MeV} \,. \tag{1.58}$$

Besides the mass and the charge the electron possesses a further property, namely, the *spin*, which can be interpreted as intrinsic angular momentum. It manifests itself spectroscopically in the so-called *fine structure* of the spectral lines, for instance by the anomalous Zeeman effect. The latter got an explanation in 1925 by G.E. Uhlenbeck and S. Goudsmit with the bold hypothesis that the electron itself is a carrier of a magnetic moment of one *Bohr magneton*,

Definition 1.3.8

$$\mu = 1\,\mu_B = 0.927 \cdot 10^{-23}\,\mathrm{Am}^2 \,, \tag{1.59}$$

and a mechanical angular momentum of $\frac{1}{2}\hbar$.

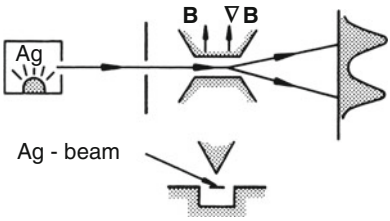

Fig. 1.10 Schematic arrangement of the Stern-Gerlach experiment

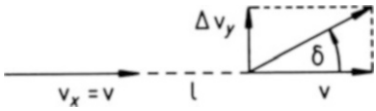

Fig. 1.11 For the calculation of the deflection of an Ag beam in the magnetic field region of the Stern-Gerlach apparatus

The first experimental hint to the electron spin came from the *Stern-Gerlach experiment* (1921/1922) (Fig. 1.10).

Ag-atoms are *vaporized* in an oven. A sharply masked out ribbon of a beam of atoms of equal velocities passes through a strongly inhomogeneous magnetic field. Each of the silver atoms carries a magnetic moment $\boldsymbol{\mu}$. The following force acts on it between the pole pieces:

$$\mathbf{F} = \nabla(\boldsymbol{\mu}\cdot\mathbf{B}) = \mu\frac{\partial B}{\partial y}\cos\alpha \; ; \quad \alpha = \sphericalangle(\boldsymbol{\mu}, \mathbf{B}) \; .$$

Before entering into the magnetic field the direction of the moments is randomly distributed, i.e., practically all angles α between field $\mathbf{B}$ and moment $\boldsymbol{\mu}$ are present. If the carrier of the magnetic moment were a stationary body, the moment would orient itself in the magnetic field parallel to the field direction. If, however, it is a rotating body, then the moment retains its initial angle with respect to the field direction, but performs instead a precessional motion around the field direction with the α-independent Larmor frequency,

$$\omega_{\mathrm{L}} = \frac{\mu}{L}B = \gamma B$$

(L: angular momentum, γ: gyromagnetic ratio). The to be expected deflection of the beam is easily calculable (see Fig. 1.11). Let l be the length of the region of the magnetic field. Then it is:

$$\tan\delta = \frac{\Delta v_y}{v} = \frac{1}{v}\frac{F}{m}\frac{l}{v} = \frac{l}{mv^2}\frac{\partial B}{\partial y}\mu\cos\alpha \; .$$

Classically, a uniformly spread out image is thus to be expected on the screen. However, the experiment exhibits two tracks of equal intensity of the beam which are deflected by the same angle:

$$\mu \cos\alpha = \frac{mv^2 \tan\delta}{l\left(\frac{\partial B}{\partial y}\right)} = \pm\frac{e\hbar}{2m} = \pm\mu_B \ . \tag{1.60}$$

Contrary to classical theories, a directional quantization has thus taken place ($\cos\alpha = \pm 1 \Longleftrightarrow \alpha = 0, \pi$).

The splitting is observed for alkaline, Ag, Cu **atoms** but **not** for alkaline$^+$, Ag^+, Cu^+ **ions**. The beam splitting has thus to be ascribed to the additionally present so-called *'valence electron'*. This should therefore carry a permanent magnetic moment $\boldsymbol{\mu}$ of the magnitude 1 μ_B. Magnetic moments are closely related to angular momenta. That was already known from Classical Physics. If we anticipate the *directional quantization*, justifiable by Quantum Mechanics (Sect. 5.1.4, Vol. 7), which means that the components of the angular momentum can differ only by integer multiples of $\hbar$,

$$J_z = m_J\hbar \ ; \quad m_J = J, J-1, \ldots, -J \ ,$$

then for the electron spin, one has to conclude from the observation of two slit tracks that

$$S = \frac{\hbar}{2} \ ; \quad m_S = \pm\frac{1}{2} \ , \tag{1.61}$$

which confirms the bold hypothesis of Uhlenbeck and Goudsmit. The rigorous explanation of the electron spin is given by Dirac's theory presented in Sect. 5.3, Vol. 7.

1.3.3 Rutherford Scattering

After electrolysis and gas discharge had given clear leads that the atoms are indeed still decomposable into certain sub-structures, the actual investigation of the atomic structure began with Lenard's experiments, who shot very fast electrons onto a metal foil. The observation that fast electrons can pass through a large number of atoms without being sinificantly deflected, enforced the bottom line that atoms can not be considered as massive structures.

Lenard's investigations regarding the dependence of the scattering probability on the velocity of the electrons turned out to be especially enlightening. The number N of the electrons, which are able to permeate the metal foil, decreases exponentially with the foil-thickness x:

$$N = N_0 \exp(-\alpha n x) \ .$$

n is the density of atoms in the foil; α has thus the dimension of an area. Assuming $\alpha = \pi r^2$ one can define an atom radius decisive for the scattering. For slow electrons ($v \leq 0.05c$) one found an effective atom radius, similar to the one deduced from the methods discussed in Sect. 1.3.1, namely, about 10^{-8} cm (see (1.42)). For high electron velocities, however, this effective radius could decrease by up to four orders of magnitude. From this observation Lenard drew the conclusion that the atom must possess a very small nucleus, in which practically the whole atomic mass is concentrated, while the rest of the space up to a radius of about 10^{-8} cm is only filled by force fields. The latter are able to influence the slow, but not the fast electrons.

In the year 1896 Becquerel discovered radioactivity. In the years 1906–1913, Rutherford could therefore perform his scattering experiments on thin layers of matter, instead of with electrons, with the about 7000 times heavier, twofold positively charged α-particles (double-ionized He atoms): A sharply focussed α-beam was shot onto a thin gold foil (thickness $\approx 10^{-3}$ mm). Possible deflections were registered by a swivelling microscope, in front of which a ZnS-scintillation spectrometer was installed, which reacted with a weak flash on each of the impinging α-particles. It was observed that almost all particles passed through the gold foil without any deviation, but that also a few of them were deflected rather strongly, sometimes by even more than 90°. Because of the rareness of such large deflection angles Rutherford concluded that the radius of the deflecting center in the atom (*atomic nucleus*) should amount to about 10^{-13} cm to 10^{-12} cm. In order to be able to deflect the heavy α-particles the center must incorporate almost the full atomic mass. From the kind of deflection it followed necessarily that the nucleus must be positively charged, as the α-particles. Charge-neutrality is guaranteed, according to Rutherford, by the almost mass-less electrons, which orbit the nucleus, where Coulomb force and centrifugal force are balancing each other. Because of the too small electron masses the heavy α-particles should be scattered only by the nucleus. These to a large extent correct, but at that time completely novel ideas are today referred to as *Rutherford atomic model*.

For a consolidation of his model image, Rutherford derived theoretically a *scattering formula*, which provides a relation between the number of α-particles, impinging the unit plane of the detector, and the angle of deflection. The formula permits to draw conclusions with respect to the spatial extension and the charge of the atomic nucleus. Because of its historical importance, we briefly sketch the derivation of the scattering formula. It is based on the following presumptions:

1) Mass of the nucleus ≫ mass of the α-particle
This assumption is surely justified because a gold foil was used as target.

2) Charge of the nucleus = Ze
The sign of the charge remains at first free. Z is an integer.

3) Coulomb's law
is valid on the whole path of the α-particle:

$$|\mathbf{F}| = \frac{1}{4\pi\varepsilon_0}\frac{(2e)(Ze)}{r^2} \,.$$

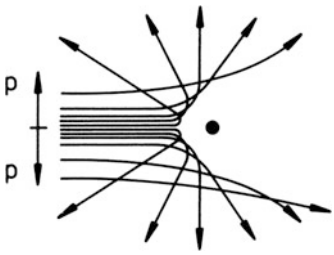

Fig. 1.12 Possible trajectories of an α-particle in the Coulomb field of an Au ion (conic sections)

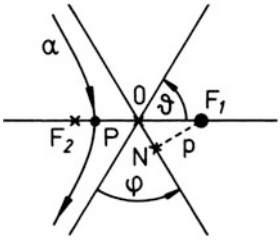

Fig. 1.13 Geometry of the path of the α-particle in the zone of influence of the positively charged nucleus

The trajectory of the α-particle is thus a conic section where the scattering nucleus is located at one of the focal points. If the nucleus is indeed positively charged then only a hyperbola comes into question because of the repulsive Coulomb interaction. In Fig. 1.12 p is the so-called *impact parameter*, which is just the distance at which the particle would pass the nucleus if there were **no** interaction. The deflection is the weaker, the larger p is.

4) No multiple scattering

The scattering by a substantial angle needs a very close approach to the nucleus and is therefore such an infrequent event that a recurrence of it by the same α-particle appears indeed highly unlikely.

In the case of a head on collision ($p = 0$) the α-particle spends its total kinetic energy and reaches the minimal distance b from the nucleus just at that moment, when the total energy consists of only potential energy (turning point!). b thus results from the energy conservation law ($T(\infty) \stackrel{!}{=} V(b)$):

$$b = \frac{4Ze^2}{4\pi\varepsilon_0 m_\alpha v_\infty^2} \,. \tag{1.62}$$

The nucleus occupies the focal point F_1. At the perihelion P the α-particle has its minimal distance from the nucleus (Fig. 1.13). We need some geometric considerations:

$$\overline{\mathrm{OP}} = \overline{\mathrm{ON}} = p \cot\vartheta \,,$$

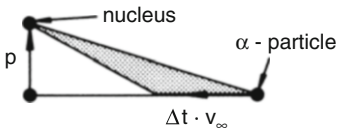

Fig. 1.14 Application of the area conservation principle to the derivation of the Rutherford scattering formula

$\overline{OP}$: *real semi-axis of the hyperbola*;

$$f = \frac{p}{\sin\vartheta} ,$$

$f = \overline{F_1 O}$: *excentricity*;

$$d = p\cot\frac{\vartheta}{2} , \tag{1.63}$$

$d = \overline{PF_1} = \overline{OP} + f$: *minimal distance from the nucleus*.

We now exploit the area conservation principle ((2.251), Vol. 1), according to which the radius vector sweeps equal areas in equal times. For large distances between the α-particle and the nucleus one finds (Fig. 1.14)

$$F_\infty = \frac{1}{2} p \Delta t v_\infty ,$$

while at the perihelion it must be:

$$F_p = \frac{1}{2} d \Delta t v .$$

For equal time intervals Δt the area conservation principle requires $F_\infty = F_p$. From that it follows:

$$v = v_\infty \frac{p}{d} . \tag{1.64}$$

Eventually we utilize the energy conservation law,

$$\frac{1}{2} m v_\infty^2 + 0 = \frac{1}{2} m v^2 + \frac{2Ze^2}{4\pi\varepsilon_0 d} ,$$

which leads with (1.62)–(1.64) to

$$b = 2p\cot\vartheta .$$

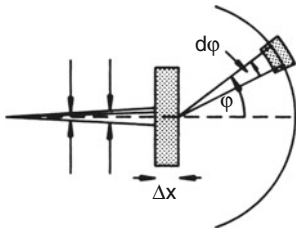

Fig. 1.15 Schematic representation concerning the statistical considerations for the Rutherford scattering formula

We still have to replace ϑ by the actual angle of deflection $\varphi = \pi - 2\vartheta$ (Fig. 1.13):

$$\cot\frac{\varphi}{2} = \frac{2p}{b} \,. \tag{1.65}$$

φ is therefore a function of p and via b also of Z and v_∞. For practical measurements, though, this formula is not yet applicable. Problems are due to the impact parameter p, which still has to be eliminated. p has namely to be of the order of magnitude of about 10^{-12} cm, in order to provide appreciable deflections. That is some orders of magnitude below usual atomic distances in solids. Hence it is illusive to plan to build a blind, which limits the α-beam so finely that one could aim at an atomic nucleus with a definite p. In addition, it is of course impossible to exactly fix the position of the nucleus. Rutherford was therefore forced to complement his so far purely mechanical considerations by a suitable statistics.

If a bunch of N α-particles penetrates a layer of matter of the thickness Δx (Fig. 1.15), then dN' particles, which enter the field of the atomic nucleus within the distance interval $[p, p + dp]$, will experience a deflection such that they are scattered into the double cone $(\varphi, \varphi - d\varphi)$ (Fig. 1.16). One can not of course target the α-particles directly into such a ring $(p, p + dp)$ and therefore is obliged to use statistical terms. Let n be the density of nuclei and F the area of the foil. The metal foil thus contains $nF\Delta x$ atomic nuclei. The probability $w(p)$ to hit a given nucleus just within the distance-ring $(p, p + dp)$, is then simply the ratio of the sum of **all** such ring areas $2\pi pdp$ to the total area F:

$$w(p) = \frac{1}{F}(nF\Delta x)(2\pi pdp) = n\Delta x 2\pi pdp \,.$$

This means for the number dN' of particles deflected by $(\varphi, \varphi - d\varphi)$:

$$dN' = Nw(p) = Nn\Delta x 2\pi pdp \,.$$

The impact parameter p, which is not directly measurable, is to be replaced by the formula (1.65). That leads to the intermediate result:

$$dN' = Nn\Delta x\pi \frac{b^2}{4} \frac{\cos\frac{\varphi}{2}}{\sin^3\frac{\varphi}{2}} d\varphi \,. \tag{1.66}$$

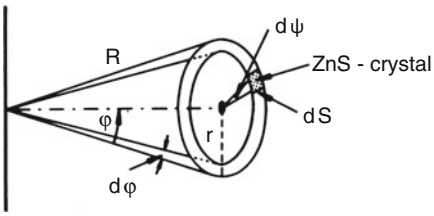

Fig. 1.16 To the determination of the actual number of particles impinging on the detector

It now remains to be considered that not the full $(\varphi, \varphi - d\varphi)$-double cone is observed but only the little sector covered by the ZnS-crystal (Fig. 1.16):

$$dF = rd\psi ds \ ,$$
$$r = R \sin\varphi \ ,$$
$$ds = Rd\varphi \ .$$

The solid angle $d\Omega$ is defined as area per square of distance:

$$d\Omega = \frac{dF}{R^2} = \sin\varphi d\varphi d\psi \ .$$

The number dN of the α-particles, which will be scattered into the solid-angle element $d\Omega$ within the double cone $(\varphi, \varphi - d\varphi)$, is related to dN' as $d\Omega$ to the total solid angle:

$$dN = dN' \frac{d\Omega}{2\pi \sin\varphi d\varphi} \ .$$

With $\sin\varphi = 2\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}$ we finally get the

Rutherford Scattering Formula

$$dN = N\frac{n\Delta x}{16}\frac{b^2}{\sin^4\frac{\varphi}{2}}d\Omega = Nn\Delta x\frac{Z^2e^4}{(4\pi\varepsilon_0)^2 m_\alpha^2 v_\infty^4 \sin^4\frac{\varphi}{2}}d\Omega \ . \tag{1.67}$$

This scattering formula illustrates in a particularly clear manner the interplay of *Mechanics* and *Statistics* typical for the whole *Quantum Mechanics*. The formula includes some very characteristic statements, which are **uniquely** confirmed by the experiment. They might therefore be used to testify the correctness of the underlying *Rutherford atomic model*:

a) $dN \sim 1/\sin^4\frac{\varphi}{2}$:
The number of the scattered α-particles exhibits a strong angle-dependence. Deflections under large angles become therewith very seldom!

b) $dN \sim \Delta x$:
The linear dependence on the thickness remains valid of course only as long as multiple scatterings can be neglected.
c) $dN \sim Z^2$
d) $dN \sim 1/v_\infty^4$
e) $dN \sim n$:
The density of the atomic nuclei in the metal foil enters the scattering formula linearly.

1.3.4 Exercises

Exercise 1.3.1 The distribution function $f(\mathbf{r}, \mathbf{v})$ determines the number of particles in the volume element d^3r at $\mathbf{r}$ of the position space and in d^3v at $\mathbf{v}$ of the velocity space. For a homogeneous ideal gas in thermal equilibrium holds:

$$f(\mathbf{r}, \mathbf{v}) \equiv f(\mathbf{v}) \equiv f(v) \ .$$

Prove the basic equation of the kinetic theory of gases:

$$p = \frac{1}{3}\frac{N}{V} m\langle \mathbf{v}^2 \rangle \ ,$$

where $\langle \mathbf{v}^2 \rangle = \frac{N}{V} \int d^3v \mathbf{v}^2 f(v)$.

Exercise 1.3.2

1. From the Boltzmann distribution

$$f(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{v}_1, \ldots \mathbf{v}_N) = f_0 e^{-\beta H}$$

(f_0 : normalizing factor, $H = T(\mathbf{v}_1, \ldots, \mathbf{v}_N) + V(\mathbf{r}_1, \ldots, \mathbf{r}_N)$: classical Hamilton function) derive the normalized Maxwell-Boltzmann velocity distribution:

$$w(\mathbf{v}_1, \ldots, \mathbf{v}_N) = \int \cdots \int d^3r_1 \cdots d^3r_N f(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{v}_1 \ldots \mathbf{v}_N) \ .$$

2. Calculate with 1. the internal energy of the ideal gas.

Exercise 1.3.3 Which voltage has to be applied to a plane-parallel capacitor with a distance between the plates of $d = 1.5\,\mathrm{cm}$, in order to keep in equilibrium an oil drop of the mass $m^* = 2.4 \cdot 10^{-13}\,\mathrm{g}$, which carries three electron charges?

Exercise 1.3.4 Calculate the fall velocity of an oil drop of the mass density $\rho = 0.98\,\mathrm{g/cm^3}$ and the radius $0.39 \cdot 10^{-4}\,\mathrm{cm}$ in the earth's gravitational field (normal pressure: η (air) $= 1.832 \cdot 10^{-5}\,\mathrm{Ns/m^2}$; $\rho_{\mathrm{air}} = 1.288\,\mathrm{kg/m^3}$).

Exercise 1.3.5 Let an oil drop of mass density $\rho = 0.98\,\mathrm{g/cm^3}$ reach the equilibrium-velocity $v_0 = 0.0029\,\mathrm{cm/s}$ in the earth's gravitational field. In a capacitor with a distance $d = 1.6\,\mathrm{cm}$ between its plates the drop is kept at equilibrium ($v_1 = 0$) by a voltage of $U = 100\,\mathrm{V}$. How many elementary charges does the drop carry? Also calculate the mass and the radius of the spherical drop (η and ρ_{air} as in Exercise 1.3.4).

Exercise 1.3.6 Give reasons for the classical electron radius

$$r_{\mathrm{e}} = \frac{e^2}{(4\pi\varepsilon_0)m_{\mathrm{e}}c^2}$$

and find its numerical value!

Exercise 1.3.7 The oldest procedure for q/m-determination is the so-called *parabola method* of Thomson. It uses electric and magnetic fields, **connected in parallel**, for the deflection of an ion or electron beam incoming in z-direction. Between the plate-shaped pole shoes of an electromagnet, a plane-parallel capacitor is installed, so that the beam there sees a magnetic as well as an electric field, which are both oriented in y-direction. The point, at which the beam would impinge the screen in the absence of fields, defines the origin of coordinates, as sketched in Fig. 1.17.

1. In the case when fields are switched on, show that the impinging points of the particles (charge q, mass m) describe a parabola on the screen.
2. Where do the high-energy particles impinge?
3. How can the slight deviations from the pure parabola shape near the apex be explained?

Exercise 1.3.8 Consider the (Rutherford) scattering of an α-particle on an Z-fold positively charged nucleus, which can be considered as *'at rest'* because of its large mass. The path of the particle is plotted in Figs. 1.18 and 1.13, respectively. It is due to the potential

$$V(\mathbf{r}) = V(r) = \frac{\alpha}{r}\,; \quad \alpha = \frac{(2e)(Ze)}{4\pi\varepsilon_0}\,.$$

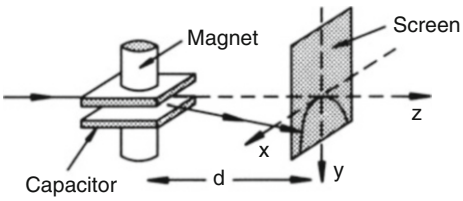

Fig. 1.17 Schematic setting for the q/m-determination according to Thomson (parabola method)

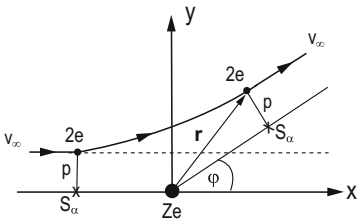

Fig. 1.18 Path of an α-particle in the force field of an Z-fold positively charged nucleus (Rutherford scattering, cf. Fig. 1.13)

It was shown in Exercise 2.5.3 of Vol. 1 that for such a potential the so-called *Lenz vector*

$$\mathbf{A} = (\dot{\mathbf{r}} \times \mathbf{L}) + V(r)\,\mathbf{r}$$

(**L**: angular momentum) represents an integral of motion. Use this fact in order to derive the Rutherford scattering formula (1.65)

$$\cot\frac{\varphi}{2} = \frac{2p}{b}\ .$$

p is the *impact parameter* (see Fig. 1.18) and b the minimal distance of the α-particle in the case of a head on collision (1.62).

1.4 Light Waves, Light Quanta

Today we know that electromagnetic waves cover a huge area of physical phenomena. The part, which is for our eyes suggestive of *light*, represents thereby only a very small portion and does not exhibit in the respective region of wavelengths any peculiarity at all. Light rays (waves) are electromagnetic transverse waves for which the electric and the magnetic field vector oscillate, periodically in space and time, perpendicular to each other and to the propagation direction. Furthermore, we also know from Classical Electrodynamics that the electromagnetic wave can continuously absorb (emit) energy. Its intensity is likewise continuously alterable. The wave theory of light, which in the middle of the nineteenth century acquired high significance by the theoretical works of J.L. Maxwell (1862) and the confirming experiments of H. Hertz (1888), is valid even today and mediates, in particular, the impression of *continuity* and *homogeneity*. At the beginning of the twentieth century, there appeared, however, first indicators for a discrete structure of the light radiation, which could not be ignored, especially in connection with the interaction of light and matter. An at first unexplainable coexistence of *wave picture* and *particle picture* was born. In order to recognize the importance of this *dualism* clearly, we will first compile in the next subsections some facts of the wave-nature of the light, disregarding the possibility that the reader may already be rather familiar with these

facts. The chapter finally ends with a consideration on some *experimental 'proofs'* for the quantum nature of light.

1.4.1 Interference and Diffraction

A decisive criterion for the concept of wave is the *'ability for interference'*. Naively formulated, this is the feature that *'light can be deleted by light'*. However, only the so-called **coherent** light waves are capable of doing that. Interfering wave trains must have a fixed phase-relation during a time span t which is large compared to the oscillation period $\tau = 1/\nu$. One learns from atomic physics that light emission is due to atoms which are in principle independent of each other. Furthermore, the act of emission takes place within a very short time span which leads to wave trains of finite length. Hence, light from two different sources can **not** be coherent. The single atom of course can not come into question as light source, either. One needs *'indirect methods'*. Let us consider here briefly two known examples: In the classical

Fresnel's mirror experiment

one replaces the light source L by the virtual images L_1 and L_2 being produced by two mirrors which are inclined relative to each other by the angle α (Fig. 1.19). The light beams B_1 and B_2 starting virtually at L_1 and L_2 are then surely coherent, so that they can interfere with each other. At a certain point P on the screen the light beams reinforce each other or extinguish each other depending on whether the path difference $\Delta = \overline{PL_1} - \overline{PL_2}$ is an even or odd multiple of half the wavelength $\lambda/2$. On the screen there appear *interference fringes* as hyperbolas since the hyperbola is defined by all points for which the difference of the distances from two fixed spots (L_1, L_2) is the same. The *bright* hyperbolas run through the intersection points of the circles around L_1 and L_2, whose differences of radii amount to $0, \lambda, 2\lambda, \ldots$ since there the coherent waves coming from L_1, L_2 mutually reinforce. On the other hand, *extinction* appears when the difference of the radii amounts to an odd multiple

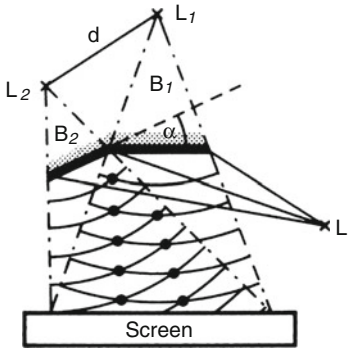

Fig. 1.19 Ray trajectory in Fresnel's mirror experiment. L is the real light source, L_1 and L_2 are its virtual images

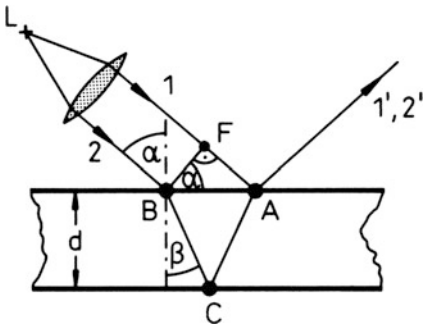

Fig. 1.20 Geometrical beam path for the reflection at two plane-parallel mirrors

of $\lambda/2$ since then a wave trough meets a wave crest. On the screen dark and bright stripes alternate.

Another method to create coherent interfering light waves exploits the

reflection on two plane-parallel mirrors .

The idea is plotted in Fig. 1.20. The ray 1 impinges at A the plane-parallel layer (index of refraction n) and is partially reflected there. The ray 2 is at B partially refracted in direction to C where it is partially reflected, in order to interfere in A with ray 1. The optical path difference amounts to (Fig. 1.20)

$$\Delta = n(\overline{\mathrm{BC}} + \overline{\mathrm{CA}}) - \overline{\mathrm{FA}} + \frac{\lambda}{2} .$$

The third term accommodates for the phase jump by π in connection with the reflection at the optically denser medium (see the Fresnel formulas (4.274)–(4.277), Vol. 3). Using further the law of refraction

$$n = \frac{\sin\alpha}{\sin\beta} .$$

we get after simple geometrical considerations

$$\Delta = 2d\sqrt{n^2 - \sin^2\alpha} + \frac{\lambda}{2} . \tag{1.68}$$

For a given thickness d of the layer the path difference Δ is determined exclusively by the **angle of inclination α**. One therefore speaks of

interference of same inclination

with

$$\begin{array}{ll} \textit{enhancement} & \Longleftrightarrow \Delta = z\lambda , \\ \textit{extinction} & \Longleftrightarrow \Delta = (2z+1)\frac{\lambda}{2} . \end{array} \quad z = 0, 1, 2, 3, \ldots \tag{1.69}$$

Both the reported examples of interference need for their analysis, unavoidably. the wave character of the light. This holds to the same extent also for the phenomenon of

diffraction

By diffraction we understand the deviation of light from the straight-lined ray path which can *not* be interpreted as refraction or reflection. It is a phenomenon which is observed for *all* wave processes. Well-known examples are:

Pinhole:

If one illuminates a small pinhole, then one observes in the center of a screen, depending on the distance of the screen from the pinhole, minima or maxima of the brightness.

Airy disk

On the other hand, behind a small disk casting shadow there is always a bright spot at the center which is called the **Poisson spot**. Light must have entered the geometrical shadow region.

Diffraction phenomena are observed only when the linear dimensions of the diffracting barriers or holes are of the same order of magnitude as the wavelength of the light or even smaller. In the optical region (small wavelengths) there are therefore not so many diffraction phenomena which belong to our *daily experience*. However, in **acoustics**, with sound-wavelengths of the order of meters, diffraction plays an important role, since it makes it possible, in the first place, e.g., hearing behind barriers. In a certain sense, sound can indeed *circumvent barriers*. The fact that light is also a wave has been recognized therefore very much later than sound.

The basis for the understanding of interference and diffraction is given by

Huygens Principle

The subsequent propagation of an arbitrarily given wavefront is determined by treating each point of the wavefront as the source of a secondary spherical wave and then obtaining the 'new' wavefront to be the envelope of all these coherent spherical waves.

With this principle the diffraction phenomena can then be understood by constructing the so-called *Fresnel zones* (Fig. 1.21). Let W be the surface of a spherical wave which originates at L. According to the Huygens principle the excitation caused by W can be traced back to the collective action of all elementary waves starting at W. Let us now put a family of spherical surfaces centered at the point of observation P whose radii differ from one another by $\lambda/2$. Let the innermost one just touch W at the point O. The spherical surfaces decompose the wavefront W into the *Fresnel zones* (Fig. 1.21). One can show that the arithmetic mean of the area-segments F_{n+1} and F_{n-1} is just equal to the enclosed area F_n. To each point from F_n one can now find another point in the upper half of the $(n-1)$-zone or in the lower half of the $(n+1)$-zone in such a way that the elementary waves starting there have at the point P a difference of their optical paths equal to just $\lambda/2$, thus mutually

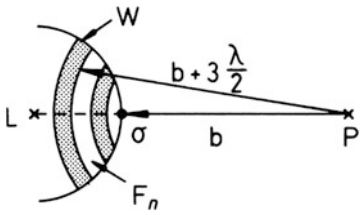

Fig. 1.21 Schematic construction of the Fresnel zones

extinguishing each other. Hence, at the point P only the contributions from half of the first zone and half of the last zone remain non-vanishing. These contributions are limited by the tangent cone which has its tip at P and its surface tangential to the wavefront W. Since the intensity decreases as $1/r^2$, the influence of the last zone can be neglected. The light excitation in P therefore stems exclusively from the half of the innermost zone.

If one puts a pinhole at the point O, which leaves open just the innermost zone only, then **all** elementary waves starting at the aperture of the blind will contribute at P without being weakened by interference. One therefore observes at and around P a higher brightness than for the case without the blind since for that case only **half** of the innermost zone contributes at P. If an even number of zones are left open by the pinhole, then we have darkness (extinction) in the middle at P. In the case of an odd number, the action of at least one zone is retained, i.e., brightness at P. If one places a disc at O instead of a pinhole (Fig. 1.21), which covers just the innermost zone, then nevertheless brightness will remain at P, because now the summation over the contributions of the second, third, ..., n-th zone will leave at P, by the same consideration as above, the action of half of the *second* zone. If the second zone, too, is shielded it remains the action of half of the third zone, etc. That explains the *Poisson spot*.

1.4.2 Fraunhofer Diffraction

One distinguishes diffraction features of the Fraunhofer-type and the Fresnel-type, depending on whether the incoming light is parallel or divergent. In the case of Fraunhofer diffraction, light from a source is converted into parallel rays by using a lense before it is incident on the diffracting object, and after diffraction light is again collected on a screen using another lense. Thus source and screen are effectively at infinite distance from the diffracting object. Let us briefly consider, as an example, the

diffraction at a slit

The slit has the width d (Fig. 1.22). We divide the broad light beam into an even number of $2n$ elements, all of the same width. For a beam *diffracted* of the angle α

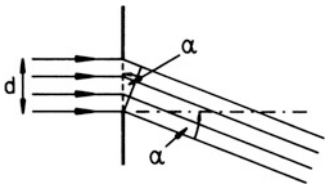

Fig. 1.22 Path of rays at a simple slit

there exists then between neighboring elements a difference in the optical paths:

$$\Delta_n = \frac{d}{2n} \sin\alpha \ .$$

If this difference just amounts to $\lambda/2$, the partial beams are mutually extinguishing each other. We therefore have as a condition for

Minima of Intensity

$$n\lambda = d \sin\alpha_n \ ; \quad n = 1, 2, 3, \ldots \ . \tag{1.70}$$

One finds the directions, at which maxima of intensity appear, if one divides the slit into an **odd** number of equally thick slit elements and requires that the contributions of adjacent elements just extinguish each other. It is then always left the light from just one element:

Maxima of Intensity

$$\left(n + \frac{1}{2}\right) \lambda = d \sin\beta_n \ ; \quad n = 1, 2, 3, \ldots \ . \tag{1.71}$$

One recognizes from (1.70) and (1.71) that diffraction phenomena can be observed only if the wavelength λ of the light is of the same order of magnitude as the linear dimensions of the diffracting object (here d).

From the rather elementary derivation presented so far one can hardly get any information about intensities; at the most, that with increasing order n of the maxima the intensity must decrease, because then the light from the element, which is **not** extinguished by interference, becomes smaller and smaller.

According to Huygens principle, a spherical wave starts at each slit-element dx which at the distance r' from dx has the amplitude

$$dW = W_0 \frac{dx}{r'} e^{i(\omega t - k' r')} \ ,$$

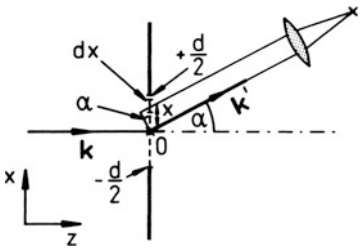

Fig. 1.23 Geometric arrangement for the calculation of the diffraction intensity at a slit

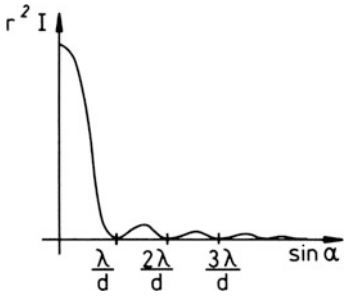

Fig. 1.24 Angle-dependence of the diffraction intensity at a slit

where of course

$$|\mathbf{k}'| = |\mathbf{k}| \ .$$

If the origin of the system of coordinates coincides with the center of the slit (Fig. 1.23) and r is the distance of the observer from the origin then it holds:

$$r' = r - x \sin\alpha \ .$$

For sufficiently large distance it can then be estimated:

$$dW \approx W_0 \frac{dx}{r} e^{i(\omega t - kr)} e^{ikx \sin\alpha} \ .$$

The absolute square of the total amplitude, which results after integrating of dW over the full slit, corresponds to the intensity of the diffracted radiation at the point of observation (Fig. 1.24):

$$I = I_0 \frac{d^2}{r^2} \frac{\sin^2\left(\frac{kd}{2}\sin\alpha\right)}{\left(\frac{kd}{2}\sin\alpha\right)^2} \ . \tag{1.72}$$

I_0 is the intensity of light falling onto the slit ($\lim_{x\to 0}(\sin^2 x)/x^2 = 1$). The diffraction pattern of the slit shows minima for the angles α_n for which it holds

$$\frac{1}{2} kd \sin\alpha_n = n\pi \ .$$

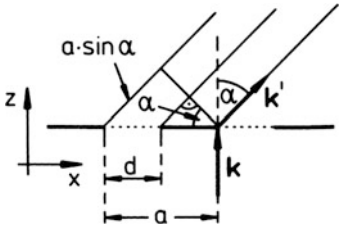

Fig. 1.25 Path of rays at the multiple slit

That agrees, because of $k = 2\pi/\lambda$, with the result (1.70) of our preceding simpler consideration. The height of the diffraction maxima is proportional to d^2, the width is proportional to d^{-1} and therewith the area under an intensity peak is proportional to the width d of the slit.

We now extend our considerations to the case of a *lattice* of N identical parallel slits, each of the width d and with the distance a between the adjacent slits (Fig. 1.25). One can, e.g., draw on a plane plate equidistant parallel grooves. The unspoiled stripes between these grooves then represent the light-transmitting slits. For normal incidence of light the Fraunhofer diffraction pattern can now be calculated completely analogously to that at the single slit. A great number N of wave trains will be brought to interference:

$$W = W_1 \sum_{n=1}^{N} e^{i(n-1)ak\sin\alpha} \; .$$

W_1 is the amplitude for the single slit of the width d. The second factor is due to the relative positions of the N slits. The sum can be easily evaluated:

$$W = W_1 \frac{1 - e^{iNak\sin\alpha}}{1 - e^{iak\sin\alpha}} \; .$$

The intensity is therewith given by:

$$I = I_1 \frac{\sin^2\left(N\frac{a\pi}{\lambda}\sin\alpha\right)}{\sin^2\left(\frac{a\pi}{\lambda}\sin\alpha\right)} \; . \tag{1.73}$$

I_1 is the intensity of the single slit for which we have found Eq. (1.72). The second factor, which is caused by the periodic arrangement of the N slits with the lattice distance a, takes care for the appearance of principal maxima and submaxima of the intensity, which are modulated by the first factor. One finds:

principal maxima:

$$\sin\alpha_n = n\frac{\lambda}{a} \; ; \quad n = 0, \pm 1, \pm 2, \ldots \; . \tag{1.74}$$

The second factor in (1.73) takes the value N^2 at these diffraction angles α_n. Between the principal maxima of orders n and $n+1$, the argument of the sine function in the numerator of (1.73) takes the value of an integer multiple of π at $(N-1)$ points fixed by:

$$\sin\overline{\alpha}_{n'} = \frac{n'}{N}\frac{\lambda}{a}\ ; \quad n' = Nn+1, Nn+2, \ldots, N(n+1)-1\ .$$

The numerator of the intensity formula is zero at these angles while the denominator in (1.73) remains finite. There are thus $(N-1)$ zeros between two principal maxima. This means, on the other hand, that there must appear also $(N-2)$ **secondary maxima**. Their intensities, however, are smaller by a factor $1/N^2$ compared to the principal maxima. In the case of many slits, i.e. largebig N, the secondary maxima are therefore unimportant.

So far we have recalled simple diffraction phenomena, which are observed for a single slit of width d or for a plane grating, artificially producible with adjustable lattice constant a. These phenomena testify uniquely to the wave character of the light and the electromagnetic radiation. It concerned thereby always scattering processes due to macroscopic bodies whose microscopic, atomic structure, however, did not play any role so far. Decisive precondition for observable diffraction patterns, though, is that a and d are of the same order of magnitude as the wavelength λ of the radiation. That means that for different regions of the wavelength one has to establish different diffraction gratings. For *radio waves, long-wave infrared* ($\lambda \geq 10^{-4}$ m) one uses wire gratings, for *short-wave infrared, visible light, ultraviolet* ($10^{-6}\,\text{m} \geq \lambda \geq 10^{-8}\,\text{m}$) the groove gratings (glass plates) discussed above are suitable, while *X-rays* ($10^{-9}\,\text{m} \geq \lambda \geq 10^{-11}\,\text{m}$) can be made to diffract and interfere by the periodic arrangement of atoms in crystal lattices. That shall be the subject of the next section.

1.4.3 Diffraction by Crystal Lattices

A plane wave impinges on a crystal, which consists of $N = N_1N_2N_3$ atoms (unit cells), with the so-called *primitive translations* $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. It is a Bravais lattice, i.e., the site of each atom (molecule) is marked by a triple $\mathbf{n} = (n_1, n_2, n_3)$ of **integers** n_i:

$$\mathbf{R^n} = \sum_{i=1}^{3} n_i \mathbf{a}_i\ . \tag{1.75}$$

Let a plane wave have the following amplitude at $\mathbf{r}$ in **free** space:

$$A(\mathbf{r}, t) = A_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\ .$$

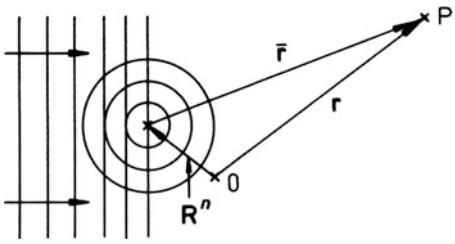

Fig. 1.26 Scattering of a plane wave at a certain lattice point

Here we are not interested in the time-dependence, which is therefore ignored. All the following considerations therefore concern a fixed point of time $t = 0$. We assume that the crystal does not disturb the incoming wave too much. Its amplitude at the lattice points $\mathbf{R^n}$ is thus:

$$A(\mathbf{R^n}) = A_0 e^{i\mathbf{k}\cdot\mathbf{R^n}} \ .$$

The atom at $\mathbf{R^n}$ scatters the wave and, according to Huygens principle, becomes the point of origin of an out-going spherical wave (Fig. 1.26). Let the point of observation be at the distance $\overline{\mathbf{r}}$ from the scattering atom. At this point the spherical wave has the amplitude

$$\left(A_0 e^{i\mathbf{k}\cdot\mathbf{R^n}}\right) \frac{e^{ik\overline{r}}}{\overline{r}} \ .$$

Thereby an elastic scattering is assumed (no absorption, ...) ($|\mathbf{k}'| = k$). The origin of the system of coordinates lies inside the crystal, while the point of observation P is far outside the crystal so that we can exploit $r \gg R^{\mathbf{n}}$:

$$\overline{r} \approx r - R^{\mathbf{n}} \cos\left(\sphericalangle(\mathbf{R^n}, \mathbf{r})\right) \ .$$

Hence we can to a good approximation replace $1/\overline{r}$ directly by $1/r$ in the above expression for the amplitude. For the argument of the exponential function, we write:

$$\mathbf{k}\cdot\mathbf{R^n} - kR^{\mathbf{n}} \cos\left(\sphericalangle(\mathbf{R^n}, \mathbf{r})\right) = (\mathbf{k} - \mathbf{k}')\cdot\mathbf{R^n} \ .$$

$\mathbf{k}'$ is the wave vector of the wave scattered in the direction of P:

$$\mathbf{k}' = k\frac{\mathbf{r}}{r} \ .$$

$k' = k$ corresponds to the assumption of an elastic scattering. The spherical wave starting at the lattice site $\mathbf{R^n}$ thus has at P the amplitude

$$A_0 \frac{e^{ikr}}{r} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R^n}} \ .$$

We have to add up this expression over all Bravais-lattice points in order to get the total amplitude in P. Its absolute square then yields the intensity of the scattered radiation:

$$I_s(\mathbf{r}) \sim \frac{1}{r^2} \prod_{i=1}^{3} \left| \sum_{n_i=1}^{N_i} e^{i(n_i-1)\mathbf{a}_i\cdot(\mathbf{k}-\mathbf{k}')} \right|^2 . \tag{1.76}$$

The evaluations of the sums on the right-hand side are performed in the same manner as shown for (1.73):

$$I_s(\mathbf{r}) \sim \frac{1}{r^2} \prod_{i=1}^{3} \left| \frac{\sin\left[\frac{1}{2}N_i\mathbf{a}_i\cdot(\mathbf{k}-\mathbf{k}')\right]}{\sin\left[\frac{1}{2}\mathbf{a}_i\cdot(\mathbf{k}-\mathbf{k}')\right]} \right|^2 . \tag{1.77}$$

Maxima of the intensity appear always when all the summands in (1.76) have the maximal value 1. This leads to the conditions which are called the

Laue Equations

$$\begin{aligned} \mathbf{a}_1\cdot(\mathbf{k}-\mathbf{k}') &= 2\pi z_1 , \\ \mathbf{a}_2\cdot(\mathbf{k}-\mathbf{k}') &= 2\pi z_2 , \quad z_{1,2,3} \in \mathbb{Z} \\ \mathbf{a}_3\cdot(\mathbf{k}-\mathbf{k}') &= 2\pi z_3 . \end{aligned} \tag{1.78}$$

For the plane grating (Sect. 1.4.2) one finds out that there are $(N_i - 1)$ zeros between two adjacent principal maxima in i-direction and therewith $(N_i - 2)$ submaxima, where, however, the intensity ratios of principal maxima to submaxima are of the order of magnitude N_i^2. A strong diffracted beam will thus arise only when all the three Laue-equations are *simultaneously* fulfilled. The Laue equations (1.78) imply that, because of (1.75), for **each** Bravais point $\mathbf{R^n}$ we must have:

$$\mathbf{R^n}\cdot(\mathbf{k}-\mathbf{k}') = 2\pi z; \quad z \in \mathbb{Z} .$$

This means:

$$\exp\left[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R^n}\right] = 1 \quad \forall\mathbf{R^n} . \tag{1.79}$$

But this is exactly the definition equation for reciprocal lattice vectors (see Sect. 4.3.16, Vol. 3 or any textbook on solid state physics), so that we come to the conclusion:

constructive interference ('Laue spot')

$$\Longleftrightarrow \mathbf{k}-\mathbf{k}' \equiv \mathbf{K} : \textbf{vector of the reciprocal lattice} . \tag{1.80}$$

The diffraction pattern, produced by the crystal lattice, is thus an effigy of the reciprocal lattice!

Let us now illuminate the Laue conditions from another side. For this purpose we have to remind the reader about some definitions and concepts of solid state physics. We begin with the term *'atomic lattice plane'* by which we understand any plane in the crystal which is occupied by at least one lattice point. According to this rather general definition, there are obviously infinitely many different lattice planes. To a given lattice plane, e.g., innumerable *parallel* lattice planes exist. Together they build a *'family of (equivalent) lattice planes'*. The orientation of a lattice plane (family of lattice planes) is described by the so-called

Miller indexes (h, k, l)

which are found as follows: One fixes the intersection points,

$$x_i \mathbf{a}_i \; ; \quad i = 1, 2, 3$$

of the considered plane with the axes defined by the primitive translations $\mathbf{a}_i$. Via

$$x_1^{-1} : x_2^{-1} : x_3^{-1} = h : k : l$$

one determines a triple of relatively prime (!) integers (h, k, l) and speaks then of the (h, k, l)-**plane** of the crystal. The triple defines uniquely the direction of the plane. Thus intercepts of the plane on the axes are:

$$x_1 = \frac{\alpha}{h} \; ; \quad x_2 = \frac{\alpha}{k} \; ; \quad x_3 = \frac{\alpha}{l}$$

with a common factor α. If an intersection point lies at infinity, i.e., if the considered plane lies parallel to one of the axes, then the respective Miller index is zero.

There exists a close relationship between the vectors of the reciprocal lattice,

$$\mathbf{K}^{\mathbf{p}} = \sum_{i=1}^{3} p_i \mathbf{b}_i \; ; \quad p_i \in \mathbb{Z} \; , \tag{1.81}$$

and the atomic lattice planes of the (direct, real) lattice. $\mathbf{b}_i$ are the *'primitive translations of the reciprocal lattice'* which are closely related to those of the real lattice being defined by

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij} \; . \tag{1.82}$$

From that one finds:

$$\mathbf{b}_i = \frac{2\pi}{V_z} (\mathbf{a}_j \times \mathbf{a}_k) \; ; \quad (i, j, k) = (1, 2, 3) \;\; \textit{and cyclic} \; , \tag{1.83}$$

$$V_z = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) : \;\; \textit{volume of the unit (elementary) cell} \; .$$

We prove the following assertions as Exercises 1.4.2 and 1.4.3:

1. The reciprocal lattice vector

$$\mathbf{K}^{\mathbf{p}} = \sum_{j=1}^{3} p_j \mathbf{b}_j$$

   is perpendicular to the (p_1, p_2, p_3)-plane of the direct lattice.
2. The distance between adjacent (p_1, p_2, p_3)-planes is given by:

$$d(p_1, p_2, p_3) = \frac{2\pi}{|\mathbf{K}^{\mathbf{p}}|} \,. \tag{1.84}$$

Let us now come back to the Laue equations (1.80). We had presumed **elastic** scattering ($k = k'$). This means:

$$k = k' = |\mathbf{k} - \mathbf{K}| \Longleftrightarrow k^2 = k^2 + K^2 - 2\mathbf{k}\cdot\mathbf{K}$$

and therewith:

$$\mathbf{k} \cdot \boldsymbol{\kappa} = \frac{1}{2} K \,; \quad \boldsymbol{\kappa} = \frac{\mathbf{K}}{|\mathbf{K}|} \,.$$

This yields a new interpretation of the Laue equations. The projection of the *incoming* wave vector $\mathbf{k}$ on the direction of a reciprocal lattice vector must be equal to half of the length of this reciprocal lattice vector. Such $\mathbf{k}$-vectors define in the reciprocal lattice a plane which is oriented perpendicular to $\mathbf{K}$ (Fig. 1.27). This plane is known as **'Bragg plane'**. Because of equal lengths ($k = k'$) the two wave vectors, which fulfill the Laue conditions, enclose the same angle ϑ with the Bragg plane (Fig. 1.28):

$$K = 2k \sin\vartheta \,. \tag{1.85}$$

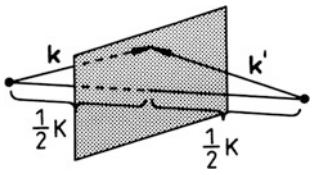

Fig. 1.27 Definition of the Bragg plane

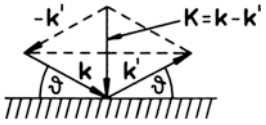

Fig. 1.28 Angle-relation between the two wave vectors which fulfill the Laue conditions

According to our preliminary considerations, **K** stands as reciprocal lattice vector perpendicular to the family of atomic lattice planes with the distance of adjacent layers

$$d = \frac{2\pi}{|\mathbf{G}^{(p_1 p_2 p_3)}|} \ .$$

Since the p_1, p_2, p_3 are relatively prime integers, $\mathbf{G}^{\mathbf{p}}$ is the shortest reciprocal vector in the direction of **K**. Furthermore, the reciprocal lattice is a Bravais lattice. Therefore it must hold:

$$K = n|\mathbf{G}^{\mathbf{p}}| = n\frac{2\pi}{d} \ ; \quad n = 1, 2, \ldots$$

If we combine this with (1.85) we get the

Bragg Law

$$2d(p_1, p_2, p_3) \sin\vartheta = n\lambda \ ; \quad n = 1, 2, \ldots \ , \tag{1.86}$$

which is completely equivalent to the Laue condition (1.80). The *order n of the Bragg reflection* hence corresponds to the length of $\mathbf{K} = \mathbf{k} - \mathbf{k}'$ divided by the length of the shortest lattice vector parallel to **K**. Relation (1.86) conveys the impression that the in-coming waves are reflected by the building blocks of an atomic lattice plane (Fig. 1.29), even though only to a small part. A diffracted beam of appreciable intensity, however, can appear only in such directions, in which the radiations, reflected at all the parallel lattice planes, constructively interfere, i.e., when they have differences of the optical paths which amount to integer multiples of the wavelength λ. This, however, comes up just by the condition (1.86). The diffraction pattern therefore provides information about the Miller indexes and therefore about the reciprocal lattice.

The essential facts about diffraction and interference phenomena discussed above can all be understood within the framework of the Maxwell's theory of Electrodynamics. Diffraction intensities, e.g. (1.77), are proportional to the intensities of the in-coming radiation. The latter, however, can be varied continuously. There are no indications whatsoever regarding quantum nature of the electromagnetic waves.

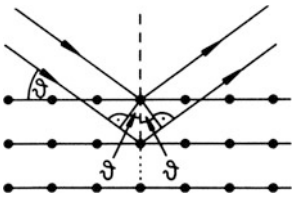

Fig. 1.29 Bragg reflection on the crystal lattice

1.4.4 Light Quanta, Photons

However, at the very beginning of the twentieth century, several phenomena were discovered which by no means could be brought into contact with the wave character of the light. In the year 1887 H. Hertz discovered the so-called *photoelectric effect (photoeffect)* by which one understands the freeing of electrons out of a metal surface when irradiated by ultraviolet light. The experimental facts can be summarized as follows:

1. The photoeffect appears only above a certain threshold frequency ν_l of the incident light. This threshold frequency is specific to the material of the metal surface.
2. The kinetic energy of the escaping *photoelectrons* is determined by the frequency of the irradiated light being, however, independent of the intensity of the light! The connection between the kinetic electron energy and the frequency of the light is linear.
3. For $\nu \geq \nu_l$ the number of emitted photoelectrons is proportional to the intensity of the incident light.
4. The photoelectric effect takes place without any time-delay ($< 10^{-9}$ s).

The analysis of the photoeffect, even in the classical wave representation, does not appear to pose any difficulties, at least at first glance. According to Classical Electrodynamics (Vol. 3) the energy of an electromagnetic wave is fixed by its intensity. The vector of the field strength of the impinging wave forces the electrons of the metal to strong co-oscillations which can occur, at resonance between the eigen-frequency of the electron oscillation and the frequency of the wave, with such a large amplitude that an escaping of the electron from the metal becomes possible. But then the energy of the freed electron must be taken from the incident electromagnetic wave. According to the classical wave-picture there should then exist a relation between the **intensity** of the incident wave and the kinetic energy of the electrons. The experimental observation 2. in the above list is in crass contradiction with that. Also point 4. is classically not understandable, since the tearing off of the electron from the metal happens only after the respective electron has absorbed sufficient amount of energy. A time delay between the incidence of the radiation and the setting free of the electron should therefore be observable being the larger the smaller the intensity.

A. Einstein (1905) succeeded in the precise analysis of the photoeffect with his famous

light quantum hypothesis

which tied in with the quantum hypothesis of M. Planck proposed 5 years earlier for an explanation of the heat radiation ((1.24) and (1.25), Sect. 1.2.2).

During the interaction with matter the radiation of the frequency ν behaves as if it were a collection of *light quanta (photons)* each with the energy

$$E = h\nu \ . \tag{1.87}$$

h is *Planck's quantum of action* with the numerical value given in Eq. (1.3), and ν is the frequency of the light.

Each electron which is freed from the metal absorbs exactly one of such light quanta which enhances its energy by $h\nu$. Out of that energy the electronic work function W_W is needed to overcome the binding forces of the metal. The remaining energy manifests itself as the kinetic energy of the photoelectron:

$$h\nu = \frac{1}{2}mv^2 + W_W \ . \tag{1.88}$$

The work function is a property of the metal used. It appears not only in connection with the photeffect, but for instance also with the thermionic emission (1.47), i.e., with the thermal freeing of electrons out of metals. One has therefore the possibility to experimentally determine W_W independently of the photoeffect. W_W is thereby always of the order of several electronvolt (eV). The lowest values are found for alkaline metals. The above mentioned limiting frequency ν_l is a direct measure of the work function:

$$h\nu_l = W_W \ . \tag{1.89}$$

For $\nu < \nu_l$ the electron cannot leave the metal. An increase of the intensity of the radiation means a greater number of in-coming light quanta and therewith more electrons have the possibility to get energy by collisions (quantum absorption!) which exceeds the work function W_W.

Einstein's formula (1.88) is uniquely confirmed by the experiment. The kinetic energy can be experimentally determined using the *'opposing field method'*. One lets the photoelectrons travel through an opposing field in a capacitor and determines the lowest countervoltage U_c (stopping potential), at which no electron is capable of reaching the collecting electrode. Obviously it must then hold:

$$\frac{1}{2}mv^2 = -eU_c \Longrightarrow U_c = \frac{h}{-e}\nu - \frac{W_A}{-e} \ . \tag{1.90}$$

$-U_c$ is thus a linear function of the frequency ν with a slope which is equal to the universal constant h/e. The intercept on the ν-axis (Fig. 1.30) represents the limiting frequency from which one can read off the work function W_W (1.89).

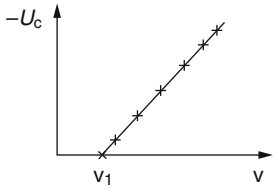

Fig. 1.30 Result of the opposing field method

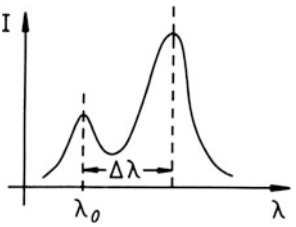

Fig. 1.31 Intensity distribution of the Compton scattering

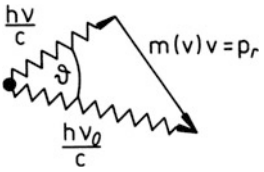

Fig. 1.32 To the momentum conservation law at the Compton scattering

The probably the most convincing experiment for the particle nature of light exploits the **Compton effect** discovered in 1922/23, which is observed when short-wavelength X-ray radiation is scattered by free or weakly bound electrons. According to elementary wave theory the electrons are excited by the incident wave to execute forced oscillations and then emit, on their part, also electromagnetic radiation. Hence, it should be expected that the frequency of the scattered radiation is the same as that of the incident radiation. In the scattered spectrum one observes, however, besides the expected wavelength λ_0 of the incident wave, another wavelength shifted to higher values (Fig. 1.31), whose shift depends on the scattering angle ϑ (Fig. 1.32) and increases with increasing ϑ. The intensity of the shifted line thereby increases with increasing scattering angle at the cost of the non-shifted one. A. Compton (1922/23) found out that the difference of the wavelengths $\Delta\lambda$ between the *Compton line* and the primary line does not depend either on the wavelength λ_0 of the primary line or on the nature of the scattering substance:

$$\Delta\lambda = \lambda_c(1 - \cos\vartheta) \,, \tag{1.91}$$

λ_c: *Compton wavelength*. The atomic number of the scattering substance, however, influences the intensities. With increasing atomic number, the intensity of the shifted line goes down, while that of the primary line goes up.

The Compton effect cannot be understood in the framework of normal wave theory, but only, if a corpuscular nature can be ascribed to the radiation, i.e., with the aid of the concept of *photons*. According to this, the scattering process is just an elastic non-head on collision between photon and electron for which the conservation laws of momentum and energy are valid. As a particle, however, the photon has rather special properties. Since it moves with the velocity of light its mass must be zero. The Theory of Special Relativity finds for the relativistic energy

of a free particle ((2.63), Vol. 4):

$$T_r = \sqrt{c^2 p_r^2 + m^2 c^4}\ . \tag{1.92}$$

This should be for the photon equal to $h\nu$. Because of $m = 0$ the relativistic momentum

$$p_r = \frac{h\nu}{c} \tag{1.93}$$

must be ascribed to the photon. We utilize the conservation laws of energy and momentum in that system of reference, in which the electron is at rest before the collision:

Photon:

before the collision: energy $= h\nu_0$; momentum $= \frac{h\nu_0}{c}$,
after the collision: energy $= h\nu$; momentum $= \frac{h\nu}{c}$,

Electron:

before the collision: energy $= m_e c^2$; momentum $= 0$,
after the collision: energy $= \sqrt{c^2 p_r^2 + m_e^2 c^4}$,
momentum $= \frac{m_e v}{\sqrt{1-\frac{v^2}{c^2}}} = p_r$.

We evaluate the momentum conservation law by use of the cosine law (Fig. 1.32):

$$p_r^2 = \frac{h^2}{c^2}\left(\nu^2 + \nu_0^2 - 2\nu\nu_0 \cos\vartheta\right)\ .$$

We square the energy conservation law,

$$\sqrt{c^2 p_r^2 + m_e^2 c^4} - m_e c^2 = h\nu_0 - h\nu\ ,$$

and subtract from it the momentum conservation law multiplied by c^2:

$$0 = h^2(-2\nu\nu_0 + 2\nu\nu_0 \cos\vartheta) + 2m_e c^2 h(\nu_0 - \nu)\ .$$

This leads with

$$\frac{\nu_0 - \nu}{\nu_0 \nu} = \frac{\frac{c}{\lambda_0} - \frac{c}{\lambda}}{\frac{c^2}{\lambda\lambda_0}} = \frac{1}{c}(\lambda - \lambda_0)$$

to the following change of the wavelength of the scattered photon:

$$\Delta\lambda = \lambda - \lambda_0 = \lambda_c(1 - \cos\vartheta) \,, \tag{1.94}$$

$$\lambda_c = \frac{h}{m_e c} = 2.4263 \cdot 10^{-2}\,\text{Å} \tag{1.95}$$

'Compton wavelength' .

λ_c is composed of three fundamental constants and has the dimension of a *length*. The change of the wavelength $\Delta\lambda$ does not depend, according to (1.94), on the wavelength λ_0 of the primary radiation. It is clear that the electrons before the collision are in reality not at rest as assumed, but exhibit initial momenta with directions, which are statistically distributed with respect to the direction of incidence of the photons. This fact causes a broadening of the Compton line, whereby, however, the statements derived above on the Compton effect are not at all contradicted.

Actually it remains only to clarify why there comes about a non-shifted line in the scattered radiation. In order to observe the Compton effect experimentally as distinctly as possible, one has to use substances with rather small electronic binding energy, which must be more or less negligible compared to the primary photon energy $h\nu_0$. This is actually the case for the weakly bound electrons in light atoms. In heavier atoms, however, in particular the inner electrons are so tightly bound that then the photon exchanges energy and momentum during the collision process not with a single electron but with the **whole** atom. Because of the comparatively large atomic mass the photon will not give away any energy at the collision with the atom, according to the laws of Classical Mechanics. $h\nu_0$ and therewith λ_0 thus remain unchanged during the scattering process. In the light atoms almost all electrons can be considered as weakly bound, while for the heavier atoms this holds only for the electrons which exist in the outer shells. This is the reason why with increasing atomic number, under otherwise identical conditions, the intensity of the shifted line decreases compared to the non-shifted one.

After we had found with interference and diffraction characteristic phenomena for light, which can be understood only in the *'wave picture'*, we see that photoeffect and Compton effect undoubtedly require the *'corpuscular nature'* of the radiation. We have to accept it as a matter of fact that light will appear to us, depending on the type of experiment, sometimes as a wave field and sometimes as a collection of point-shaped particles. We will see that the obvious

particle-wave dualism ,

which is demonstrated here for light, is valid, conversely, for matter also. There are indeed situations for which it becomes reasonable to speak of **matter waves**. We will be focused on this aspect in Sect. 2.1.

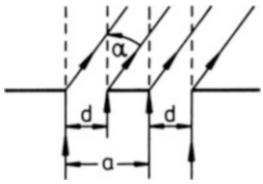

Fig. 1.33 Path of rays at the double slit

1.4.5 Exercises

Exercise 1.4.1 Discuss the diffraction of light at the double slit (slit width d, lattice constant $a = 2d$) (Fig. 1.33). Compare qualitatively the intensity distribution of the diffraction pattern with that for the single slit!

Exercise 1.4.2 Prove the assertion that the vector $\mathbf{K^p}$ of the reciprocal lattice stands perpendicularly on the (p_1, p_2, p_3)-plane of the direct lattice.

Exercise 1.4.3 Show how the distance d of the planes in the (p_1, p_2, p_3)-family of atomic lattice planes can be expressed by the reciprocal lattice vector $\mathbf{K^p}$. (Proof of (1.84)).

Exercise 1.4.4 Express the Bragg law for orthorhombic lattices by the magnitudes of the elementary translations (*lattice constants*) a_1, a_2, a_3. Which further simplification can be found for cubic lattices?

Exercise 1.4.5 The limiting wavelength λ_1 for the photoeffect on cesium is experimentally determined to be $\lambda_1 = 6400\,\mathring{\mathrm{A}}$. Calculate the work function!

Exercise 1.4.6 Calculate the relative change of the wavelength $\Delta\lambda/\lambda_0$ due to the Compton effect ($\vartheta = \pi/2$) for

1. visible light ($\lambda_0 \approx 4000\,\mathring{\mathrm{A}}$),
2. X-ray radiation ($\lambda_0 \approx 0.5\,\mathring{\mathrm{A}}$),
3. γ-radiation ($\lambda_0 \approx 0.02\,\mathring{\mathrm{A}}$).

How does the energy of the electron change thereby (*recoil energy*)?

Exercise 1.4.7 Estimate the time delay, which is to be expected classically for the photoeffect. Let the intensity of the incident radiation be $0.01\frac{\mathrm{W}}{\mathrm{m}^2}$ and the cross-section area of the atom $1\,\mathring{\mathrm{A}}^2$. How long will it take for the energy of 2 eV to be absorbed by the atom, which corresponds to the work function?

Exercise 1.4.8 X-rays of the wavelength $\lambda = 1\,\mathring{\mathrm{A}}$ are falling on a carbon block. One observes the radiation which is scattered perpendicular to the incident beam.

1. Calculate the Compton shift $\Delta\lambda$.
2. How much kinetic energy is transferred to the electron?
3. How large is the percentage energy loss of the photon?

1.5 Semi-Classical Atomic Structure Model Concepts

The interpretation of the *Rutherford scattering* (Sect. 1.3.3) has led to a very illustrative atomic model, which is based exclusively on the principles of Classical Mechanics and Electrodynamics:

The atom consists of a very small nucleus (radius $\leq 10^{-4}$ Å*), which is positively charged (charge* $+Ze$*) and in which almost all the mass of the atom is concentrated, and* Z *electrons which go round the nucleus at relatively large distances (orbit radii* ≥ 1 Å*). The Coulomb and centrifugal forces together are responsible for the electron orbits to be ellipses.*

1.5.1 Failure of the Classical Rutherford Model

A more careful inspection of the Rutherford model reveals, however, some fatal contradictions:

1. The precise shape of the elliptical orbit of an electron is classically fixed by the initial conditions for position and momentum. The latter, however, are actually completely arbitrary so that, in turn, one is allowed to assume elliptical orbits of arbitrary energy. Depending on the manner of generation, the electron shells would then be different from atom to atom and could give rise to different behavior even for atoms with the same Z. That, however, has experimentally never been observed!
2. The electrons in their elliptical orbits represent accelerated charges and consequently must radiate electromagnetic energy. This causes a decrease of energy of the electron and should inevitably lead to an approach towards the nucleus. One can estimate that the time, after which the radius of the orbit drops from about 1 Å to the nucleus radius of about 10^{-4} Å, may amount to hardly more than 10^{-10} s. For this fact, also, there does not exist any experimental evidence.
3. In the framework of Classical Physics *continuous* changes of electron energies as a consequence of the emission of *continuous* electromagnetic radiation energy should be possible in the atom. Instead of this, *discrete line spectra* are observed.

Let us take up point 3. and investigate in more detail which experimental facts were to be explained at the turn of the century by improved atom models. The most serious observation is concerned with the discrete spectral lines of an element which could be formally grouped together as a series of always the same structure. They begin with a line of lowest frequency (largest wavelength), which is followed with increasing frequency by further discrete lines, where the energetic distance of the adjacent lines becomes smaller and smaller in order to, eventually, accumulate at the so-called *series limit*. Above this limit, the spectrum becomes continuous.

Long before the discovery of the discrete energy levels in the atom, J. Balmer (1885) already concluded from the first few spectral lines of the hydrogen atom (H_α

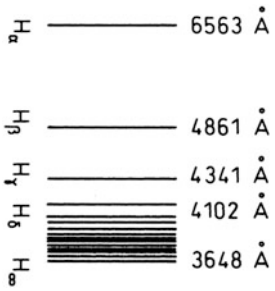

Fig. 1.34 Balmer line series of the hydrogen atom

to H_δ) (Fig. 1.34) that there is a series formula of the type

$$\lambda = B\frac{n^2}{n^2-4}\,; \quad n = 3, 4, \ldots\,,$$

which with $B^{-1} = R_\mathrm{H}/4$,

Rydberg Constant

$$R_\mathrm{H} = 109677.6\,\mathrm{cm}^{-1}\,, \tag{1.96}$$

reproduces quantitatively correctly the actual experimental observation. Balmer himself further provided the generalization of this formula for all

Rydberg Series

$$\frac{1}{\lambda} = R_\mathrm{H}\left(\frac{1}{n^2} - \frac{1}{m^2}\right) \tag{1.97}$$
$$(n \text{ fixed};\ m \geq n+1)$$

of the hydrogen atom. In principle n can be any integer so that there should exist theoretically arbitrarily many spectral series. However, only the following are actually observed:

1. Lyman series (Lyman 1906):

$$\frac{1}{\lambda} = R_\mathrm{H}\left(1 - \frac{1}{m^2}\right)\,; \quad m = 2, 3, \ldots \tag{1.98}$$
$$\text{series start: } \lambda_0 = 1216\,\mathring{\mathrm{A}}$$
$$\text{series end: } \lambda_\infty = 911\,\mathring{\mathrm{A}}\,.$$

2. Balmer series (Balmer 1885):

$$\frac{1}{\lambda} = R_{\mathrm{H}} \left(\frac{1}{4} - \frac{1}{m^2} \right) \; ; \quad m = 3, 4, \ldots \tag{1.99}$$

$$\text{series start: } \lambda_0 = 6563\,\mathring{\mathrm{A}},$$

$$\text{series end: } \lambda_\infty = 3648\,\mathring{\mathrm{A}}.$$

3. Paschen series (Paschen 1908):

$$\frac{1}{\lambda} = R_{\mathrm{H}} \left(\frac{1}{9} - \frac{1}{m^2} \right) \; ; \quad m = 4, 5, \ldots \tag{1.100}$$

$$\text{series start: } \lambda_0 = 18751\,\mathring{\mathrm{A}}$$

$$\text{series end: } \lambda_\infty = 8208\,\mathring{\mathrm{A}}.$$

4. Brackett series (Brackett 1922):

$$\frac{1}{\lambda} = R_{\mathrm{H}} \left(\frac{1}{16} - \frac{1}{m^2} \right) \; ; \quad m = 5, 6, \ldots \tag{1.101}$$

$$\text{series start: } \lambda_0 = 4.05\,\mu\mathrm{m}\,,$$

$$\text{series end: } \lambda_\infty = 1.46\,\mu\mathrm{m}.$$

One also knows of some more lines of a fifth series, the so-called Pfund series ($n = 5$ and $m \geq 6$ in (1.97)). The Lyman series is observed in the ultraviolet region and the Balmer series in the visible region. All the other series appear in the infrared region.

Very similar series formulas as that in (1.97) can be formulated also for hydrogen-like ions (He^+, Li^{++}, ...) with a somewhat changed constant in front of the bracket and for alkaline and alkaline earth metals with simple correction terms (*Rydberg corrections*).

The series formulas (1.98)–(1.101) suggest to interpret the inverse wave length of the emitted radiation as the difference of two *energy terms*:

$$\frac{1}{\lambda} = T_n - T_m \; ; \quad T_\nu = \frac{R_{\mathrm{H}}}{\nu^2} \; . \tag{1.102}$$

The *combination principle*, formulated by W. Ritz in 1908, is an immediate consequence of the above formulas:

If the inverse wavelength of two spectral lines of one and the same series are known, then their difference is the inverse wavelength of a third spectral line which belongs to the same atom (Fig. 1.35)

If one now multiplies the terms by the fundamental constant hc, then they become energies. The experimentally observed series formulas therefore indicate that in

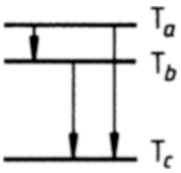

Fig. 1.35 Schematic representation of Ritz's combination principle

reality they are the energy conditions of the form

$$h\nu = E_n - E_m\,; \quad E_n = -\frac{R_{\mathrm{H}} hc}{n^2}\,. \tag{1.103}$$

It looks as if the atoms are able to accept only certain energy amounts, which are specific to them. By such an energy absorption they are brought into *excited* states of the energy E_n. A transition from the energy level E_n to E_m leads to the emission of a light quantum, whose frequency ν has to obey the condition (1.103). The above Ritz condition expresses therewith that by additive or subtractive combination of the frequencies of already known spectral lines, new spectral lines can be found. Certain level combinations are, however, forbidden, i.e., do not lead to an observable spectral line. There indeed exist certain selection rules. The goal of experimental spectroscopy must therefore be to determine the level system of an atom (or a molecule, or a solid) and the corresponding selection rules. The need for this program was reinforced by the pioneering theory of atom of Bohr and Sommerfeld.

1.5.2 Bohr Atom Model

For N. Bohr (1913) the decisive question was how to modify the Rutherford model in order to remove the radiation instability of the electron shell. He did not succeed in finding the mathematically rigorous answer to this question. He replaced it by a postulate, whose exact proof later by the modern Quantum Theory underlines impressively Bohr's ingenious physical intuition. It was obviously clear to him that the stability of the shell is probably explainable only by the assumption that the continuous energy behavior of the atomic electrons has to be replaced by an energy quantization of some sort; a concept which was already successfully used by M. Planck for his explanation of the heat radiation (Sect. 1.2.3) and by A. Einstein for the interpretation of the photoeffect (Sect. 1.4.4). It was conceivable that here also Planck's quantum of action h would play a central role. The energetic discreteness of the atomic electron motion would of course also explain the experimentally observed series line spectra which we discussed in the last section.

Bohr extended the Rutherford theory by two hypotheses which he could not prove and which are today denoted as

Bohr's postulates :

1. *Periodic motions of physical systems take place in stationary states with discrete energies* $(E_n, E_m, \ldots)$ ***without*** *radiation of energy.*
2. *Transitions between the stationary states are accompanied by electromagnetic emission (or absorption) with a frequency according to (1.103).*

As an immediate consequence of the discreteness of the energy states one has to assume the existence of an energetically lowest state, the **ground state**. In this state the system is stable, i.e., the system will not leave this state without being forced by an external influence.

Let us recapitulate Bohr's considerations in connection with the simplest element of the periodic table, the hydrogen atom. It consists of a positively charged nucleus (proton) ($q_{\mathbf{P}} = +e$), around which a single electron moves. Between the two particles the attractive *Coulomb potential* acts:

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\varepsilon_0 r} = -\frac{k}{r}; \quad k = \frac{e^2}{4\pi\varepsilon_0} \,. \tag{1.104}$$

This is centrally symmetric and therewith a special realization of the general **Kepler problem** which has been extensively discussed in Sect. 3.5.3, Vol. 2. We therefore repeat here only those aspects which appear to be vital for the following. The Hamilton function H of the system reads:

$$H = \frac{1}{2m}\left(p_r^2 + \frac{1}{r^2}p_\vartheta^2 + \frac{1}{r^2\sin^2\vartheta}p_\varphi^2\right) - \frac{k}{r} \,. \tag{1.105}$$

The coordinate φ is cyclic, the corresponding canonical momentum p_φ is therewith an integral of motion:

$$p_\varphi = mr^2\sin^2\vartheta\dot{\varphi} = \text{const} \,. \tag{1.106}$$

As to the constant, it is obviously just the z-component L_z of the orbital angular momentum. The motion therefore takes place in a fixed orbital plane. It holds for the two other generalized momenta ((2.44), Vol. 2):

$$p_r = m\dot{r} \,; \quad p_\vartheta = mr^2\dot{\vartheta} \,. \tag{1.107}$$

The most elegant approach to the solution of the Kepler problem is provided by the Hamilton-Jacobi method, which we developed in Sect. 3 of Vol. 2. This method exploits the fact that one can by a suitable canonical transformation make the Hamilton equations of motion invariant while the *old* variables $\mathbf{q} = (r, \vartheta, \varphi)$, $\mathbf{p} = (p_r, p_\vartheta, p_\varphi)$ can be transformed into *new* variables $\overline{\mathbf{q}}, \overline{\mathbf{p}}$ in such a way that all $\overline{q}_j$ are cyclic so that all $\overline{p}_j$ become constants. The transformation is mediated by the *generating function* $W(\mathbf{q}, \overline{\mathbf{p}})$ (see Sect. 2.5.3, Vol. 2):

$$p_j = \frac{\partial W}{\partial q_j} \,; \quad \overline{q}_j = \frac{\partial W}{\partial \overline{p}_j} \,; \quad \overline{H} = H + \frac{\partial W}{\partial t} = H(\overline{\mathbf{q}}, \overline{\mathbf{p}}) \equiv E \,. \tag{1.108}$$

$\overline{H} = \overline{H}(\overline{\mathbf{q}}, \overline{\mathbf{p}})$ must be constant since the $\overline{q}_j$ are all cyclic after the transformation, i.e., they do no longer appear in $\overline{H}$, and the $\overline{p}_j$ are therewith themselves already constants. That leads to the

Hamilton-Jacobi Differential Equation (HJD)

$$H\left(q_1, \ldots, q_s, \frac{\partial W}{\partial q_1}, \ldots, \frac{\partial W}{\partial q_s}\right) = E = \text{const}\,, \tag{1.109}$$

which determines the $\mathbf{q}$-dependence of the generating function, while, however, nothing saying about the *new* momenta $\overline{p}_j$. The latter can be fixed according to need or expedience. The HJD contains s derivatives (s: number of degrees of freedom) of the generating function W. That means, there are correspondingly many constants of integration $\alpha_1, \ldots, \alpha_s$, one of which, however, must be trivially additive, because with W, $W + \alpha$ is always also a solution of (1.109). We choose for this constant $\alpha_1 = E$. After solving the HJD it then follows formally:

$$W = W(\mathbf{q}, \boldsymbol{\alpha})\,.$$

The HJD of the Kepler problem reads with (1.105):

$$\frac{1}{2m}\left[\left(\frac{\partial W}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial W}{\partial \vartheta}\right)^2 + \frac{1}{r^2 \sin^2 \vartheta}\left(\frac{\partial W}{\partial \varphi}\right)^2\right] - \frac{k}{r} = E\,. \tag{1.110}$$

A separation ansatz for W appears to be reasonable:

$$W = W_r(r, \boldsymbol{\alpha}) + W_\vartheta(\vartheta, \boldsymbol{\alpha}) + W_\varphi(\varphi, \boldsymbol{\alpha})\,.$$

Since φ is cyclic we immediately get a further constant of integration,

$$p_\varphi = \frac{\partial W}{\partial \varphi} = \frac{\partial W_\varphi}{\partial \varphi} = \alpha_\varphi = \text{const}\,,$$

which is identical to L_z. The HJD can therewith be rearranged as follows:

$$\frac{r^2}{2m}\left(\frac{\partial W_r}{\partial r}\right)^2 - kr - Er^2 = -\frac{1}{2m}\left[\left(\frac{\partial W_\vartheta}{\partial \vartheta}\right)^2 + \frac{\alpha_\varphi^2}{\sin^2 \vartheta}\right].$$

Since the left-hand side depends only on r and the right-hand side only on ϑ, both sides must separately be already constant:

$$\left(\frac{\partial W_\vartheta}{\partial \vartheta}\right)^2 + \frac{\alpha_\varphi^2}{\sin^2 \vartheta} \equiv \alpha_\vartheta^2\,.$$

One easily realizes (see Sect. 3.5.3, Vol. 2) that α_ϑ^2 is just the square of the magnitude of the angular momentum $|\mathbf{L}|^2$. We have to still solve:

$$\left(\frac{\partial W_r}{\partial r}\right)^2 + \frac{\alpha_\vartheta^2}{r^2} = 2m\left(E + \frac{k}{r}\right) .$$

We did not yet fix so far the *new* momenta $\overline{p}_j$ which, according to the original aim, have to be each constant. It would be plausible to identify the momenta with the integration constants α_j. One can, however, also think of special combinations of these constants, as for instance the so-called

action variables

$$J_j = \oint p_j dq_j = \oint \frac{\partial W_j(q_j, \boldsymbol{\alpha})}{\partial q_j} dq_j = J_j(\boldsymbol{\alpha}) . \tag{1.111}$$

It is integrated here over a full period of the motion. In principle this equation should be invertible:

$$\alpha_j = \alpha_j(\mathbf{J}) \longrightarrow W = W(\mathbf{q}, \mathbf{J}); \quad \overline{H} = \overline{H}(\mathbf{J}) . \tag{1.112}$$

The coordinates, which are canonically conjugated to the action variables, are the so-called **angle variables**:

$$\omega_j \equiv \frac{\partial W}{\partial J_j} . \tag{1.113}$$

The action variables for the Kepler problem are fixed by the following integrals:

$$\begin{aligned} J_\varphi &= \oint \frac{\partial W_\varphi}{\partial \varphi} d\varphi = 2\pi\alpha_\varphi , \\ J_\vartheta &= \oint \frac{\partial W_\vartheta}{\partial \vartheta} d\vartheta = \oint \sqrt{\alpha_\vartheta^2 - \frac{\alpha_\varphi^2}{\sin^2\vartheta}} d\vartheta , \\ J_r &= \oint \frac{\partial W_r}{\partial r} dr = \oint \sqrt{2m\left(E + \frac{k}{r}\right) - \frac{\alpha_\vartheta^2}{r^2}} dr . \end{aligned} \tag{1.114}$$

The somewhat tedious evaluation of the integrals (Sect. 3.5.3, Vol. 2) leads to relatively simple expressions:

$$J_\vartheta = 2\pi\left(\alpha_\vartheta - \alpha_\varphi\right) , \tag{1.115}$$

$$J_r = -2\pi\alpha_\vartheta + \pi k\sqrt{\frac{2m}{-E}} . \tag{1.116}$$

The system of Eqs. (1.114)–(1.116) can be solved for E:

$$\overline{H} = E = -\frac{h^2 E_{\mathrm{R}}}{\left(J_r + J_\vartheta + J_\varphi\right)^2} \,. \tag{1.117}$$

The physical meaning of the so-called

Rydberg Energy

$$E_{\mathrm{R}} = \frac{2\pi^2 m e^4}{(4\pi\varepsilon_0)^2 h^2} = 13.60\,\mathrm{eV} \tag{1.118}$$

will become clear in the following. The three frequencies of the periodic motion,

$$\nu_j = \dot{\omega}_j = \frac{\partial \overline{H}}{\partial J_j} \equiv \nu \,,$$

are obviously degenerate:

$$\nu = \frac{2h^2 E_{\mathrm{R}}}{\left(J_r + J_\vartheta + J_\varphi\right)^3} \,. \tag{1.119}$$

This degeneracy can be removed by a further canonical transformation

$$(\boldsymbol{\omega}, \mathbf{J}) \underset{F_2}{\longrightarrow} (\overline{\boldsymbol{\omega}}, \overline{\mathbf{J}}) \,.$$

That succeeds with the generating function:

$$F_2(\boldsymbol{\omega}, \overline{\mathbf{J}}) = (\omega_\varphi - \omega_\vartheta)\overline{J}_1 + (\omega_\vartheta - \omega_r)\overline{J}_2 + \omega_r \overline{J}_3 \,.$$

One obtains new angle variables,

$$\overline{\omega}_1 = \tfrac{\partial F_2}{\partial \overline{J}_1} = \omega_\varphi - \omega_\vartheta \,; \quad \overline{\omega}_2 = \tfrac{\partial F_2}{\partial \overline{J}_2} = \omega_\vartheta - \omega_r \,; \quad \overline{\omega}_3 = \tfrac{\partial F_2}{\partial \overline{J}_3} = \omega_r \,,$$

with the new frequencies:

$$\overline{\nu}_1 = \nu_\varphi - \nu_\vartheta = 0 \,; \quad \overline{\nu}_2 = \nu_\vartheta - \nu_r = 0 \,; \quad \overline{\nu}_3 = \nu \,. \tag{1.120}$$

We still need the *new* Hamilton function $\overline{H}$ as function of the *new* action variables $\overline{J}_j$:

$$J_\varphi = \frac{\partial F_2}{\partial \omega_\varphi} = \overline{J}_1 \; ; \quad J_\vartheta = \frac{\partial F_2}{\partial \omega_\vartheta} = -\overline{J}_1 + \overline{J}_2 \; ; \quad J_r = \frac{\partial F_2}{\partial \omega_r} = -\overline{J}_2 + \overline{J}_3 \; .$$

Equation (1.117) then obviously reads:

$$\overline{H} = -\frac{h^2 E_\mathrm{R}}{\overline{J}_3^2} \equiv E \; . \tag{1.121}$$

The degeneracy of the frequency is thus lifted:

$$\overline{\nu}_1 = \overline{\nu}_2 = 0 \; ; \quad \overline{\nu}_3 = \frac{2h^2 E_\mathrm{R}}{\overline{J}_3^3} \; . \tag{1.122}$$

One calls $\overline{J}_3$ an **eigen-action variable**, since the associated frequency is unequal zero and **not** degenerate. $\overline{J}_3$ has the dimension of action and can take in principle, according to Classical Mechanics, unrestrictedly any arbitrary value. The experimental observation, as analyzed in the last section, requires the at first not provable

Quantum Hypothesis

For the eigen-action variable J, the motion of the system is allowed only on such paths, for which J is an integral multiple of Planck's quantum of action:

$$J = nh \; ; \quad n = 1, 2, 3, \ldots \tag{1.123}$$

This quantum hypothesis means, for the hydrogen atom, the energy of the orbital electron can not assume any arbitrary value. In fact, it is *quantized* according to :

$$E_n = -\frac{E_\mathrm{R}}{n^2} \; ; \quad n = 1, 2, 3, \ldots \tag{1.124}$$

The Rydberg energy E_R therefore is just the energy of the **ground state** of the electron. With the quantum condition (1.124) the experimentally observed Rydberg series ((1.97) to (1.101)) are explainable in a rather simple manner. They are represented in Fig. 1.36 qualitatively, but not fully true to scale. The so-called *principal quantum numbers n* of the respective terms are also indicated in the figure along with the excitation energies with respect to the ground state.

The Rydberg energy E_R can be brought into connection with the Rydberg constant in Eq. (1.96). Obviously:

$$R_\infty = \frac{E_\mathrm{R}}{hc} = \frac{2\pi^2 m e^4}{(4\pi\varepsilon_0)^2 h^3 c} = 109737.3\,\mathrm{cm}^{-1} \; . \tag{1.125}$$

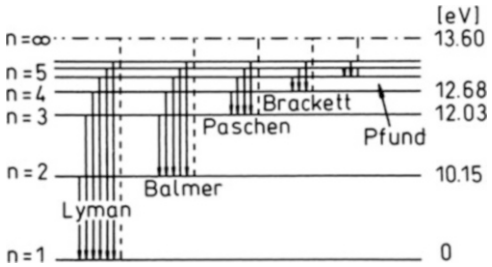

Fig. 1.36 Spectral series of the hydrogen atom

The numerical value does not exactly agree with that in (1.96). Our calculation so far is namely not yet completely exact inasmuch as we have started from the limiting case of infinite mass of the nucleus (therefore the index ∞). Implicitly, we have presumed that the electron moves around a **stationary** nucleus. Actually, however, it is about a two-body problem, in which the motion of nucleus and electron take place around a common center of gravity, which does not exactly coincide with the center of the nucleus. The two-body problem becomes an effective one-body problem if one replaces in the above formulas the electron mass m by the reduced mass μ (see Sect. 3.2, Vol. 1),

$$\mu = \frac{mM}{m+M}\,; \quad M: \text{ mass of the hydrogen nucleus}\,,$$

which because of $m/M \approx 1/1836$ does not of course differ very significantly from m. With μ for m the above theory remains valid. This means according to (1.125)

$$R_{\mathrm{H}} = \frac{\mu}{m} R_\infty \approx \frac{1836}{1837} R_\infty \tag{1.126}$$

and yields the numerical value in (1.96) which differs slightly but measurably from that in (1.125).

Because of this *two-body effect* the heavy hydrogen isotope *deuterium* was discovered by Urey (1932). For the frequency of a spectral line it namely holds $\nu_{\mathrm{H(D)}} \sim R_{\mathrm{H(D)}}$, where the index 'D' stands for deuterium. From that it follows:

$$\frac{\nu_{\mathrm{D}}}{\nu_{\mathrm{H}}} = \frac{\mu_{\mathrm{D}}}{\mu_{\mathrm{H}}} = \frac{1+m/M_{\mathrm{H}}}{1+m/M_{\mathrm{D}}} \approx 1 + m\frac{M_{\mathrm{D}}-M_{\mathrm{H}}}{M_{\mathrm{D}}M_{\mathrm{H}}}\,.$$

We neglect the relativistic mass defect ((2.66), Vol. 4) and put $M_{\mathrm{D}} \approx 2M_{\mathrm{H}}$:

$$\frac{\nu_{\mathrm{D}}}{\nu_{\mathrm{H}}} \approx 1 + \frac{1}{2\cdot 1836} \approx 1 + 2.74\cdot 10^{-4}\,.$$

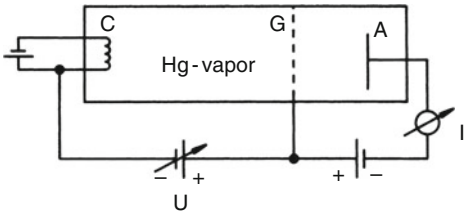

Fig. 1.37 Schematic set-up of the Franck-Hertz experiment

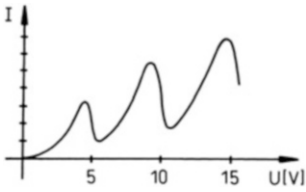

Fig. 1.38 Typical course of the voltage-current curve in the Franck-Hertz experiment

With a spectrometer of good resolving power the relative shift of the wavelength

$$\left|\frac{\Delta\lambda}{\lambda}\right| \approx 2.74 \cdot 10^{-4}$$

is easily measurable.

The experimental confirmation of Bohr's ideas was accomplished impressively by J. Franck and G. Hertz in the year 1914. Electrons come from a thermionic cathode and are accelerated by a variable voltage between a gate and the cathode (Fig. 1.37). On their way from the cathode to the gate the electrons suffer collisions with the atoms of a gas, for instance the atoms of a Hg-vapor. The electrons, which pass through the gate have then to overcome an opposing field of about 0,5 V in order to reach the electrode A. They succeed only if their kinetic energy at G is greater than 0.5 eV. Failing this, they can not reach A and therefore can not contribute to the current I. When the voltage U between C and G is increased the current I will at first increase substantially because the electrons will perform only elastic collisions with the gas atoms. At $U \approx 4.9$ V, however, the current registered at A decreases abruptly. It must be that the electrons have lost a large part of their kinetic energy by inelastic collisions with the Hg-atoms. According to *Bohr's idea* the energy, which is transferred at the collision onto the gas atom, will be used to lift an orbiting electron onto a *higher* energy level. With a further increase of the voltage, the number of electrons, which reach A, strongly increases again, and drops down distinctly once more at about 9.8 V. Obviously the accelerated electrons are now capable of exciting even **two** atoms between C and G (Fig. 1.38).

The frequency condition (1.103) offers another criterion for the correctness of *Bohr's ideas*. After a short time the excited atoms should return to the ground state, and that, too, by emission of electromagnetic radiation (photons) of exactly the frequency fixed by (1.103). The excitation energy of 4.9 eV corresponds to a wavelength of $\lambda = hc/h\nu \approx 2537$ Å. This spectral line in the UV-region could

uniquely be established by Franck and Hertz. The energy transferred to the Hg-atom by electron collision of 4.9 eV thus corresponds to the energy difference between two stationary states, which is emitted in the form of a photon with $\lambda = 2537\,\mathring{\text{A}}$ when the Hg-orbital electron *'jumps back'* into its ground state. That was the convincing experimental proof of Bohr's frequency condition and therewith, in the end, the proof of the whole Bohr's theory.

1.5.3 Principle of Correspondence

After the enterprising considerations of Bohr, which had also found impressive support by the experiment (J. Franck, G. Hertz), the setting of the task for Classical Physics was clearly predetermined. An **'atomic mechanics'** had to be developed, which can explain the existence of stable, stationary electron states with discrete energy values. This task has been accomplished convincingly, however, only after the development of the *'new'* Quantum Theory. The *'older'* Quantum Theory (1913–1924) had still to be content with *'plausibility explanations'* regarding mainly the discretization. The experimental facts on hand could be summarized and focused in such a way that the main cause for the discretization must be seen in the existence of a quantum of action $h = 6.624 \cdot 10^{-34}$ Js. The action appears to be *'quantized'* in elementary packets. If the dimensions of a physical system are such that the action has the order of magnitude of h, then the quantum character of the phenomena becomes dominant. If, however, the action is so large that the unit h is to be considered as tiny ($'h \to 0'$), then the laws and concepts of Classical Physics remain valid. Such considerations are collected together by the **principle of correspondence**:

There should exist a correspondence between Classical Physics and Quantum Physics, in such a sense that the latter converges asymptotically for $'h \to 0'$ to the 'continuous' Classical Physics

It brings out the correct perception that the Quantum Theory represents something like a super-ordinate theory which incorporates the Classical Physics as the limiting case, for which *quantum jumps* are unimportant. We already got to know a similar *correspondence* previously for the *Special Theory of Relativity* (Vol. 4), which, in the region $v \ll c$, i.e., for relative velocities v which can be considered as tiny compared to the velocity of light c ('$c \to \infty$'), is in accordance with the Classical Newton Mechanics.

Let us once more briefly reconstruct Bohr's original considerations. Our derivation in the last section is historically, strictly speaking, not fully correct, because it has already been *touched up* by some aspects of the principle of correspondence. Actually, only the frequency condition (1.103) was really experimentally assured at that time:

$$\nu_{nm} \sim \left(\frac{1}{n^2} - \frac{1}{m^2} \right) ,$$

where the proportionality constant was at first *analytically unknown*. In the classical picture, the electron performs an accelerated motion around the nucleus, emits thereby electromagnetic waves which should lead to an energy loss and therewith actually to a spiraled trajectory of the electron towards the nucleus. On the contrary, in the *quantum picture*, the electron can approach the nucleus only stepwise where energy is emitted only in connection with *jumps*. For large quantum numbers, though, the steps are very small, so that the *'abrupt'* descent will differ only slightly from a continuous sliding. In this limit ($n \gg 1$), or for $h \to 0$, which ultimately means the same, the quantum-theoretical frequencies should turn into the classical ones. According to Classical Electrodynamics the frequency of the emitted radiation corresponds to the rotational frequency ν_{kl} of the electron:

$$\begin{aligned} \nu_{n,n+1} &\Longrightarrow \nu_{\mathrm{kl}} \ , \\ \nu_{n,n+\Delta n} &\Longrightarrow \Delta n \nu_{\mathrm{kl}} \quad (\textit{harmonics}) \ . \end{aligned} \tag{1.127}$$

The *quantum-theoretical* frequency condition (1.103) can be expressed for $\Delta n \ll n$ approximately as follows:

$$\nu_{n,n+\Delta n} = \frac{1}{h}\left(E_{n+\Delta n} - E_n\right) \approx \frac{1}{h}\frac{dE_n}{dn}\Delta n \ .$$

The comparison with (1.127) yields the

basic equation of the 'older' Quantum Theory

$$\nu_{\mathrm{kl}} \Longleftrightarrow \frac{1}{h}\frac{dE_n}{dn} \ . \tag{1.128}$$

In the *'correspondence-like'* Quantum Mechanics, at first, the classical frequency ν_{kl} of the periodic motion is calculated and E_n is identified with E. That is then inserted into (1.128). The formal solution of the resulting differential equation leads to

Hasenöhrl's Quantum Condition

$$\int \frac{dE}{\nu_{\mathrm{kl}}} \stackrel{!}{=} h(n+\alpha) \ . \tag{1.129}$$

The left-hand side is calculated classically and n is interpreted as an integer quantum number. The integration constant α represents in a certain sense a *'blemish'*, which must be eliminated by respective experimental findings.

We consider, as an example, the motion of the atomic electron in the region of influence of the positively charged nucleus (H-atom!). The Bohr orbits are classically the solutions of the Kepler problem for the attractive central-force field

between electron and nucleus. They are ellipses, where the nucleus is located in one of the focal points and is *at rest*, at least as far as the *'co-moving correction'* is disregarded. The classical problem we already solved with (3.154) in Vol. 2:

$$\pi \frac{e^2}{4\pi\varepsilon_0} \nu_{\mathrm{kl}} = \sqrt{\frac{-2E^3}{m}} \ .$$

In the case that the electron moves on an ellipse its total energy is $E < 0$. We obtain therewith via (1.129) the quantum condition,

$$h^2(n+\alpha)^2 = \frac{me^4}{8\varepsilon_0^2} \frac{1}{-E} \ ,$$

or after introduction of the Rydberg energy E_{R}:

$$E \longrightarrow E_n = -\frac{E_{\mathrm{R}}}{(n+\alpha)^2} \ ; \quad n = 1, 2, \ldots \tag{1.130}$$

That is, as we know, the correct result provided we choose $\alpha = 0$.

Let us once more recall the action variables,

$$J_i = \oint p_i dq_i \ ,$$

by which one can fix the frequencies of periodic motions ((3.119), Vol. 2):

$$\nu_i = \frac{\partial \overline{H}}{\partial J_i} = \frac{\partial E}{\partial J_i} \ .$$

From that we get with the Hasenöhrl condition (1.129) an equivalent

phase-integral quantization

$$J_i = J_i(E) = h(n_i + \alpha_i) \ . \tag{1.131}$$

In order to get the quantized energies, one has to solve this expression for E. Except for the constant α_i, (1.131) agrees with the previous quantum condition (1.123). This phase-integral quantization was first brought into the discussion by A. Sommerfeld (1916). W. Heisenberg later used the relation,

$$\frac{1}{2\pi} \frac{dJ_i}{dn_i} = \frac{h}{2\pi} = \hbar \ , \tag{1.132}$$

which follows from (1.131), for the development of his consistent matrix mechanics.

The quantization prescription (1.131), when applied to the Kepler problem, holds for each of the three action variables:

$$J_r = h\big(n_r + \alpha_r\big)\ ; \quad J_\vartheta = h\big(n_\vartheta + \alpha_\vartheta\big)\ ; \quad J_\varphi = h\big(n_\varphi + \alpha_\varphi\big)\ .$$

That defines, according to (1.117), the

principal quantum number

$$n = n_r + n_\vartheta + n_\varphi\ , \tag{1.133}$$

which, as in (1.130), fixes the discrete energy steps, if one chooses for the constant $\alpha = \alpha_r + \alpha_\vartheta + \alpha_\varphi = 0$. The Kepler-motion is degenerate since its energy is determined by n, only. Classically that means that the electron energy on the elliptical orbit is exclusively given by the semi-major axis, while the semi-minor axis is fixed by other quantum numbers. To these it belongs the

azimuthal (secondary) quantum number

$$l = n_\vartheta + n_\varphi - 1\ . \tag{1.134}$$

The energy levels split in a homogeneous magnetic field (Zeeman effect). That corresponds to different orientations of the orbital plane relative to the field direction which are also *quantized*. The *orientation quantization* is described by the

magnetic (projection) quantum number

$$m_l = n_\varphi\ . \tag{1.135}$$

We know from Vol. 2 of this basic course in Theoretical Physics that J_ϑ is related to the square of the angular momentum $|\mathbf{L}|^2$ and J_φ to the z-component of the angular momentum L_z. This is transferred to the quantum numbers l and m_l, what is impressively confirmed by the *consistent* Quantum Theory, which will be presented in the next chapters. This theory will also justify the following relations, which, at that time, were only experimentally verified:

$$n = 1, 2, 3, \ldots\ ; \quad 0 \le l \le n-1\ ; \quad -l \le m_l \le l\ , \tag{1.136}$$

The theory, being based on the principle of correspondence, was the precursor of the *consistent* Quantum Mechanics. It uncovered with full decisiveness the shortcomings of the Classical Physics with respect to the description of intra-atomic processes and stressed the necessity of novel quantum laws. It *provoked* therewith a wealth of correspondingly targeted experiments. On the other hand, it goes without saying that such a semi-empirical ansatz can not, in the last analysis, be fully convincing. The 'older' Quantum Theory was by no means a closed consistent theory. It contained a series of fatal deficiencies which of course were recognized from the beginning by the then-protagonists. So some simple one-particle problems

(hydrogen atom, harmonic oscillator, ...) could be solved to a large extent, whereas the theory already failed for elementary two-particle problems (He-atom, hydrogen-molecule ion H_2^+, ...).

1.5.4 Exercises

Exercise 1.5.1 A rigid body possesses a moment of inertia J with respect to a pre-given rotational axis. On the basis of the principle of correspondence calculate the possible energy levels!

Exercise 1.5.2 Calculate by the use of the principle of correspondence the energy levels of the harmonic oscillator!

Exercise 1.5.3 Assume that the electron in the hydrogen atom moves on a stationary circular path ($\vartheta \equiv \pi/2; L_z = \text{const}$) around the singly-positively charged nucleus. Exploit the equality of Coulomb-attraction and centrifugal force together with Bohr's quantization prescription,

$$\int p dq \stackrel{!}{=} nh\,; \quad n = 1, 2, \ldots\,,$$

in order to determine the radius of the first Bohr orbit ($n = 1$). What is the rotational frequency?

1.6 Self-Examination Questions

To Section 1.1

1. By which physical quantities is the *state* of a system defined in *Classical Mechanics*?
2. What must be known about a mechanical system in order to be able to calculate its state at arbitrary times?
3. Which year can be considered as the year of the birth of Quantum Mechanics?
4. When does one speak of *quantum phenomena*?
5. Why is *Classical Mechanics* called deterministic?
6. What is expressed by the Heisenberg uncertainty principle?

To Section 1.2

1. What do we understand by *heat radiation*?
2. Which property defines the *black body*? How can it be realized?
3. How is the spatial spectral energy density defined?
4. Formulate the Kirchhoff law!
5. What is the statement about heat radiation that is given by Wien's law?
6. How does the total spatial energy density of the hollow depend on temperature? What is the name of the corresponding law?
7. How does the frequency $\nu_{\max}$, which is the frequency of the maximal spectral energy density of the *black-body radiation*, shift with the temperature?
8. Which laws of *Classical Physics* on heat radiation are uniquely confirmed by the experiment?
9. Sketch the main steps of the proof of the Rayleigh-Jeans formula. Which theorem of *Classical Physics* is decisively used in the derivation?
10. Plot typical isotherms of heat radiation! In which part does the Rayleigh-Jeans formula reasonably reproduce them?
11. Which model has been used by M. Planck for his calculation of the spectral energy density of the heat radiation?
12. Formulate *Planck's hypothesis*.
13. In what way does Wien's law enter the derivation of *Planck's radiation formula*?
14. Interpret Planck's radiation formula!

To Section 1.3

1. Historically, by which investigations did the first indications of an atomistic structure of the matter appear?
2. What is the basic equation of the kinetic theory of gases?
3. To what extent does the kinetic theory of gases support the idea of an atomistic structure of the matter?
4. Define the term *atom*!
5. What is to be understood by the term *relative atomic mass*?
6. What is the connection between the terms mole and *Avogadro's number*?
7. What are the difficulties that arise with the definition of an *atomic radius*?
8. Which methods do you know for the estimation of the atomic radius? What is the order of magnitude of the atomic radii?
9. Formulate Faraday's laws of electrolysis!
10. Describe the Millikan-experiment! How far do its results prove the discrete structure of electric charge?
11. Which methods for the creation of **free** electrons do you know?

12. Why does an electric field represent an energy spectrometer? According to what does a magnetic field *sort*?
13. How does the electron mass depend on its velocity?
14. How is the unit *electron-volt* defined?
15. Describe the Stern-Gerlach experiment!
16. Which splitting happens to an Ag-**atom** beam in the Stern-Gerlach apparatus? What happens if one takes Ag^+-ions instead of Ag-**atoms**?
17. What is the spin of an electron?
18. Describe the Rutherford atom model! Sketch the ideas and conclusions which led to this model picture!
19. What do we understand by an *impact parameter*?

To Section 1.4

1. What does one understand by the term *interference*?
2. Why does one need coherent light waves for observing interference?
3. Describe Fresnel's mirror experiment!
4. Under which conditions do enhancement and extinction, respectively, for the *interference stripes of same inclination* appear?
5. What is called a *Poisson spot*?
6. Define the term *diffraction*.
7. Formulate the Huygens principle!
8. Explain using the concept of Fresnel zones the appearance of the Poisson spot!
9. What is the difference between Fraunhofer and Fresnel diffraction?
10. Which are the conditions for, respectively, minima and maxima of the intensity in the diffraction at a single slit?
11. By which factors is the intensity of the radiation, which is diffracted at the single slit at the angle α, mainly determined?
12. Which condition is to be fulfilled for the principal maxima in the diffraction at a lattice of N slits of width d and the separation a?
13. Which type of *lattice* is needed to get diffraction phenomena by X-ray radiation?
14. What is a Bravais lattice?
15. Illustrate the meaning of the Laue equations!
16. What has the diffraction pattern of a real crystal lattice to do with the respective reciprocal lattice?
17. Express the distance d of equivalent lattice-planes by a suitable reciprocal lattice vector!
18. What is a Bragg plane?
19. What is the content of the Bragg law?
20. Which experimental facts prevent a classical interpretation of the photoeffect?
21. Describe Einstein's light quantum hypothesis!

22. Why does the photoeffect take place only above a certain threshold frequency ν_l?
23. Does an increase of the radiation intensity mean an increase of the kinetic energy of the photoelectrons?
24. Describe the Compton effect!
25. What is the rest mass of the photon? Which momentum is to be ascribed to the photon?
26. What change of the wavelength $\Delta\lambda$ arises for the scattering of X-ray radiation at weakly bound electrons? By what is it influenced?
27. How can one understand, in the Compton effect, the non-shifted line in the scattered radiation?
28. What is understood as the *particle-wave dualism* in connection with light?

To Section 1.5

1. Comment on the most weighty contradictions between the Rutherford model and the respective experimental findings!
2. Which Rydberg series of the hydrogen atom are experimentally observable?
3. What do we understand by the *series end* of a Rydberg series?
4. Which of the Rydberg series of the H-atom lies in the visible spectral region?
5. What is the statement of the Ritz's combination principle?
6. Formulate and interpret Bohr's postulates!
7. What defines the *ground state* of an atom?
8. Recall the meaning and accomplishment of the Hamilton-Jacobi differential equation.
9. What are action and angle variables?
10. Which meaning does the Rydberg energy have?
11. What is an *eigen-action variable*?
12. Formulate the Bohr-Sommerfeld quantum hypothesis!
13. How is the *principal quantum number n* defined?
14. How was the heavy hydrogen isotope deuterium detected?
15. Describe the Franck-Hertz experiment!
16. Comment on the principle of correspondence!
17. What is considered as the basic equation of the 'older' Quantum Theory?
18. Which consideration leads to Hasenöhrl's quantum condition?
19. How does the phase-integral quantization follow from the Hasenöhrl condition?
20. How can one explain in the framework of the 'older' Quantum Theory the azimuthal quantum number l and the magnetic quantum number m_l?

Chapter 2
Schrödinger Equation

The central equation of motion of Quantum Mechanics is the Schrödinger equation, which, however, can not be derived, in a strict mathematical sense, from first principles, but must be introduced more or less approximately, may be even somewhat speculatively. For its justification, one can be led by the idea that Quantum Mechanics is to be understood as a super-ordinate theory which contains the macroscopically correct Classical Mechanics as a corresponding limiting case. From the *classical side*, in particular, the Hamilton-Jacobi theory (Sect. 3, Vol. 2) reveals such a correspondence. Mechanical-optical analogy observations assign to Classical Mechanics, within the framework of Quantum Mechanics, the same role as is played by geometrical optics in relation to the general theory of light waves. Let us therefore call to mind once more at the beginning of this chapter, how the classical Hamilton-Jacobi theory with its concept of waves of action let the Schrödinger equation become *plausible* and provides first hints to the particle-wave dualism of matter.

The experimental exploitation of the wave nature of matter, e.g. electron microscope, structure investigations by neutron diffraction, etc., is today part of the day-to-day work of the physicist and is therefore no longer spectacular. But nevertheless, it does not change the fact that the realization that in certain situations wave character has to be ascribed even to matter, must be counted as one of the most decisive achievements of physics in the last century.

The wave character of matter is the reason why the *state* of a physical system is described by a *'wave function'* $\psi(\mathbf{r}, t)$ (Sect. 2.2). This function is a solution of the Schrödinger equation, but does not itself represent a measurable particle property. By the interpretation of a *gedanken-experiment* (double slit) we will illustrate the statistical character of the wave function, which permits Quantum Mechanics, in contrast to Classical Mechanics, only probability statements. Typical determinants are therefore probability densities, averages, and fluctuations (Sects. 2.2.1, 2.2.6). The statistical character of the wave function is also responsible for two important peculiarities of Quantum Mechanics, namely, for the Heisenberg uncertainty principle (Sect. 1.5) and for the *'spreading out'* of wave packets (Sect. 2.2.3).

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Quantum Mechanics assigns operators to the observables, i.e., to the measurable variables. This we will recognize first for the example of the momentum operator (Sect. 2.3), which is then subsequently verified for all other dynamical variables. The non-commutability of these operators has to be considered as an important characteristic, with far-reaching consequences. The sequence, in which we let two or more operators act on the wave function is, in general, not arbitrary, since each operator can change the state of the system in a specific manner (Sect. 2.3.2)

The last part of this chapter deals with the attempt to find a practicable prescription of translation by which one can infer the correct formulation of the Schrödinger equation from the *familiar* Classical Physics.

2.1 Matter Waves

In Sect. 1.4 we were concerned with the *'strange'* particle-wave dualism of the electromagnetic radiation. Besides unambiguous wave properties (interference, diffraction), the electromagnetic radiation also possesses unambiguously particle character (photoeffect, Compton effect). We have no other choice but to use for the interpretation of electromagnetic phenomena at one time the one picture, and at another time the other picture, although the two pictures actually exclude each other, at least in the framework of our world of experience. On the other hand, based on experimental facts, the particle-wave dualism of the electromagnetic radiation appears so convincing that the conclusion that it should also be valid *in opposite direction*, represents a plausible thesis. Nevertheless, the realization that this dualism holds also for those objects, which one would normally denote as *particles (corpuscles)*, must be accepted as one of the greatest achievements of physics in the twentieth century. The bold speculations of the French physicist L. de Broglie (dissertation 1924) represented the historical starting point for the wave theory of matter, which shortly afterwards inspired E. Schrödinger (1925/1926) for the development of his *wave mechanics*, although experimental confirmations of the wave aspect of matter, postulated by de Broglie, were not available before 1927 (C.J. Davisson, L.H. Germer).

The idea to ascribe wave properties to matter (to particles) is, though, pretty much older. It traces back to Hamilton, who already in the first half of the nineteenth century, pointed to an interesting analogy between geometrical optics and classical Newton mechanics, which consists in the fact that both can be treated by an identical mathematical formalism. By the use of the Hamilton-Jacobi theory (see Sect. 3.6, Vol. 2), a wave equation can indeed be derived for Classical Mechanics, which turns out to be mathematically equivalent to the so-called *eikonal equation of geometrical optics*. This *'drives'* to the following speculation: We know that geometrical optics represents only a limiting case with rather restricted region of validity, which, for instance, can **not** explain important phenomena such as interference and diffraction. It has therefore to be generalized to a *wave optics*, where, however, geometrical optics remains to be exact in its restricted region of validity. The situation is very

similar to that of Classical Mechanics. This theory, too, possesses obviously only a restricted applicability, being not able, e.g., to explain the stationary energy states of the atom. It might be, however, that Classical Mechanics, too, is to be understood only as a limiting case of a super-ordinate *Wave Mechanics*, in the same manner as geometrical optics is with respect to the general wave theory of light. But if this is really true, then it should be possible to derive hints for the wave mechanics, by analogy-conclusions to the known transition *geometrical optics* $\Longrightarrow$ *wave theory of light*. That this indeed is possible, we could demonstrate already in detail in Sect. 3.6 of Vol. 2. Because of its fundamental importance, in the next section, we briefly recall once more the essential steps of thoughts.

2.1.1 Waves of Action in the Hamilton-Jacobi Theory

The Hamilton-Jacobi theory of Classical Mechanics (see Chap. 3, Vol. 2), which we already recalled in Sect. 1.5.2 in connection with the Bohr atom model, is based on the concept of canonical transformations (see Sect. 2.5, Vol. 2). By this one understands a change of variables from *old* to *new* coordinates $\bar{\mathbf{q}}$ and momenta $\bar{\mathbf{p}}$,

$$(\mathbf{q}, \mathbf{p}) \quad \underset{S(\mathbf{q}, \bar{\mathbf{p}}, t)}{\longrightarrow} \quad (\bar{\mathbf{q}}, \bar{\mathbf{p}}) \,,$$

which keeps the Hamilton equations of motion invariant, being therefore *'allowed'*. If the transformation is properly chosen, the solution of a physical problem can become very much simpler in the *new* variables than it was in the *old* ones. In this sense, the Hamilton-Jacobi theory upgrades the method of canonical transformation to a general method of solution.

The *generating function* S of the transformation, which is also called *action function*, must be a function of the *old* coordinates $\mathbf{q} = (q_1, q_2, \ldots, q_s)$ and the *new* momenta $\bar{\mathbf{p}} = (\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_s)$ with the transformation formulas,

$$p_j = \frac{\partial S}{\partial q_j} \,; \quad \bar{q}_j = \frac{\partial S}{\partial \bar{p}_j} \,; \quad \overline{H} = H + \frac{\partial S}{\partial t} \qquad (j = 1, 2, \ldots, s) \,,$$

which are presented here without explicit derivation. The reader, who is interested in details, may be referred to Sect. 2.5.3, Vol. 2. In the Hamilton-Jacobi procedure, the transformation, i.e. in particular, its generating function, is chosen in such a way that all $\bar{q}_j$ are cyclic, and therewith automatically, all $\bar{p}_j$ are constant (see Sect. 1.5.2), or that **all** *new* variables $(\bar{\mathbf{q}}, \bar{\mathbf{p}})$ come out as time-independent constants. In the latter case, the mechanical problem is then trivially solved, since the constants are fixed by correspondingly many initial conditions. We certainly get such a transformation when the *new* Hamilton function $\overline{H}$ is already constant, for instance equal to zero:

$$H\left(q_1, q_2, \ldots, q_s, \frac{\partial S}{\partial q_1}, \frac{\partial S}{\partial q_2}, \ldots, \frac{\partial S}{\partial q_s}, t\right) + \frac{\partial S}{\partial t} = 0 \,. \tag{2.1}$$

For simplicity, we restrict the following considerations to the case of a single particle ($\mathbf{q} = \mathbf{r}$) in a conservative force field:

$$H = T + V = E = \text{const} . \tag{2.2}$$

Then the time-dependence of the action function can be separated:

$$S(\mathbf{r}, \bar{\mathbf{p}}, t) = W(\mathbf{r}, \bar{\mathbf{p}}) - E\,t . \tag{2.3}$$

Because of $\bar{\mathbf{p}} = \text{const}$, the condition $W = \text{const}$ defines a fixed plane in the configuration space, which is spanned by the coordinates q_j. The planes $S = \text{const}$, on the other hand, shift themselves in the course of time over the fixed W planes. They build within the configuration space, propagating wave fronts of the so-called *action waves*. One can ascribe to them a velocity, the wave or phase velocity $\mathbf{u}$. This is defined as the velocity of a given point on the wave front. We get from

$$dS \stackrel{!}{=} 0 = \nabla_r W \cdot d\mathbf{r} - E\,dt$$

the simple expression:

$$\nabla_r W \cdot \mathbf{u} = E . \tag{2.4}$$

$\mathbf{u}$ is oriented, by definition, perpendicular to the action wave fronts. Since $\nabla_r W$, too, lies orthogonal to the planes $W = \text{const}$ and is identical to the momentum of the particle

$$\mathbf{p} = \nabla_r W , \tag{2.5}$$

wave velocity $\mathbf{u}$ and particle velocity $\mathbf{v}$ must be parallel. Then it follows from (2.4):

$$u = \frac{E}{p} = \frac{E}{m\,v} \Longrightarrow u\,v = \text{const} . \tag{2.6}$$

Because of $E^2 = u^2(\nabla_r W)^2$ and (2.1)–(2.3), we have found the

wave equation of Classical Mechanics

$$(\nabla_r S)^2 = \frac{1}{u^2}\left(\frac{\partial S}{\partial t}\right)^2 . \tag{2.7}$$

Although action wave propagation and particle motion are alien to each other, they are, nevertheless, equivalent solutions of the mechanical problem. This is indeed an indication of a

particle-wave dualism

of matter.

Let us now, as announced, look for further analogies in the theory of light waves, which is known in great detail. An electromagnetic process such as that for *light* is described by the wave equation for the scalar electromagnetic potential $\varphi(\mathbf{r}, t)$

$$\nabla^2\varphi - \frac{n^2}{c^2}\frac{\partial^2\varphi}{\partial t^2} = 0 \,, \tag{2.8}$$

where $n = n(\mathbf{r})$ is the index of refraction of the medium and c is the vacuum velocity of light. $u = c/n$ is then the velocity of light in the medium. One easily recognizes that for $n = \text{const}$ the plane wave ((4.134), Vol. 3)

$$\varphi(\mathbf{r}, t) = \varphi_0\, e^{i\,(\mathbf{k}\cdot\mathbf{r} - \omega t)} \tag{2.9}$$

is a solution of the wave equation, if:

$$k = \omega\frac{n}{c} = \frac{\omega}{u} = \frac{2\pi\,\nu}{\lambda\,\nu} = \frac{2\pi}{\lambda} \,. \tag{2.10}$$

If, however, $n = n(\mathbf{r}) \neq \text{const}$, then the space-dependence of the index of refraction gives rise to diffraction phenomena. The following ansatz turns out to be convenient

$$\varphi(\mathbf{r}, t) = \varphi_0(\mathbf{r}) \exp\left[i\,\frac{k}{n}(L(\mathbf{r}) - c\,t)\right] \,, \tag{2.11}$$

where $L(\mathbf{r})$ is denoted as the *optical path* or *eikonal*. The insertion of (2.11) into the wave equation (2.8) yields a rather complicated expression, which, however, simplifies, under the assumptions of geometrical optics,

$$\begin{aligned} &\varphi_0(\mathbf{r}) \text{ weakly space-dependent,} \\ &\lambda = \frac{2\pi}{k} \;\ll\; \text{changes in the optical medium,} \end{aligned}$$

to the so-called *'eikonal equation'* ((3.198), Vol. 2):

$$\big(\nabla L(\mathbf{r})\big)^2 = n^2 = \frac{c^2}{u^2} \,. \tag{2.12}$$

According to (2.11), the solutions $L = \text{const}$ define areas of constant phase and therewith wavefronts. Their orthogonal trajectories are just the *light rays* of the geometrical optics.

The eikonal equation resembles, to a certain formal degree, the wave equation (2.7) of Classical Mechanics. That may *provoke* the conclusion by analogy, to consider Classical Mechanics as the *'geometrical-optical limiting case'* of a superordinate Wave Mechanics. This conclusion by analogy is of course not at all a scientific proof, but is rather based essentially on plausibility. Its justification can

be found, only retroactively, by comparison of theoretical results with experimental data. We will *have to accept* this point of view still several times in the next sections.

If we now presume an analogy between the action wave, which is to be ascribed to the particle and which fulfills the wave equation (2.7), and the light wave (2.11), then the action wavefronts $S = W - E\,t$ should correspond to the phase $k/n(L - c\,t)$. Thus it should be:

$$E \sim \frac{k}{n}\,c = k\,u \sim \frac{u}{\lambda} = \nu\ .$$

When we write

$$E = h\,\nu\ , \tag{2.13}$$

it further follows: $\lambda = u/\nu = E/(p\,\nu) = h/p$. This means:

$$p = \frac{h}{\lambda}\ . \tag{2.14}$$

Energy E and momentum p of the particle therewith fix the frequency ν and the wavelength λ of the associated action wave. Equations (2.13) and (2.14) are excellently confirmed by experiment, provided one identifies h with the Planck quantum of action. The above conclusions by analogy are ultimately to be traced back to L. de Broglie. One therefore calls λ the *de Broglie wavelength* of the particle.

If we eliminate by the ansatz (2.11) the differentiations with respect to time in the wave equation (2.8), it remains to be solved:

$$\nabla_r^2\varphi + k^2\varphi = \Delta_r\varphi + \frac{4\pi^2}{\lambda^2}\,\varphi = 0\ .$$

In the sense of our conclusion by analogy, the particle wave should now also be characterized by a corresponding

$$\textbf{wave function}\ \psi(\mathbf{r}, t)\ \ ,$$

which because of

$$\frac{4\pi^2}{\lambda^2} = \frac{1}{\hbar^2}\,\mathbf{p}^2 = \frac{1}{\hbar^2}\,2\,m\,(E - V)\ ; \quad \hbar = \frac{h}{2\pi}$$

solves a differential equation, which represents as

time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2\,m}\,\Delta_r + V(\mathbf{r})\right)\,\psi(\mathbf{r}, t) = E\,\psi(\mathbf{r}, t) \tag{2.15}$$

the basic equation of the whole field of wave mechanics. Thereby, it turns out to be, as we will later analyze in detail, a so-called eigen-value equation of the

Hamilton operator

$$\widehat{H} = -\frac{\hbar^2}{2\,m}\,\Delta_r + V(\mathbf{r})\ . \tag{2.16}$$

Although the Schrödinger equation (2.15) cannot be derived in a mathematically strict manner, but rather needs plausibility-considerations and conclusions by analogy, it has, nevertheless, proven its worth consistently. It marks, as a milestone, the break-through of Classical Physics to modern Quantum Physics.

If we once more exploit the analogy between the wave function $\psi(\mathbf{r}, t)$ and the solution (2.11) of the wave equation (2.8), we can, because of the special time-dependence, obviously assume, with (2.13) and (2.14), the following assignment:

$$E \implies i\,\hbar\,\frac{\partial}{\partial t}\ . \tag{2.17}$$

Since on the left-hand side there appears a variable (number!) and on the right-hand side there stands a differential **operator**, this assignment can be reasonable only if we always interpret it as applied to a wave function $\psi(\mathbf{r}, t)$, whose properties will be investigated in Sect. 2.2. In this sense we get from (2.15) the

time-dependent Schrödinger equation

$$\widehat{H}\,\psi(\mathbf{r}, t) = i\,\hbar\,\frac{\partial}{\partial t}\,\psi(\mathbf{r}, t)\ . \tag{2.18}$$

2.1.2 The de Broglie Waves

The wave-picture of matter gives rise to a highly interesting possibility of interpreting the Bohr postulate concerning stationary electron paths in the atom. If the electron can really be seen as a wave, then stationary electron paths are obviously characterized by the fact that they correspond to **standing** electron waves. If not, they would extinguish themselves by destructive interference after only a few electron cycles. The orbital circumference must therefore be an integer multiple of the wavelength λ of the electron. This consideration is indeed compatible with Bohr's quantum condition. For, if we formulate this condition as in Exercise 1.5.3 for stationary circular paths (radius r, rotational speed $v = r\,\dot{\varphi}$),

$$\int p\,dr = 2\pi\,r\,m\,v = n\,h\ ; \qquad n = 1, 2, 3, \dots\ ,$$

and insert here the de Broglie-relation (2.14) for $p = m\,v$, then it follows:

$$2\pi\,r = n\,\lambda\ ; \qquad n = 1, 2, 3, \dots\ . \tag{2.19}$$

That comes almost as a *proof* of Bohr's quantum condition. And what's more, even the problem of the energy radiation seems to be removed. A circulating electron represents an oscillating dipole, while a standing wave, as an object that does not vary in time, will not, even according to the laws of Classical Electrodynamics, require to radiate energy.

The wave nature of matter manifests itself in diffraction and interference phenomena. Davisson und Germer (1927) were the first, who succeeded in making that visible, with experiments on electron reflection at Ni-(111) planes. The intensity distribution of the reflected electrons corresponded to a Laue-back-reflection picture, as it was known at that time from experiments with X-ray radiation. In particular, the maxima of brightness were determinable by the basic Laue equations (1.78) and (1.80), respectively. All the conclusions, drawn from X-ray diffraction phenomena, could be redrawn also for the diffraction of electron waves. In 1928, Davisson und Germer directly provided evidence that the electron diffraction obeys the Bragg law (1.86), so that, in a converse way, with a known lattice constant of the crystal, one could estimate the wavelength of the matter waves, which are ascribed to the electrons. One found that, in complete agreement with (2.14), these are inversely proportional to the electron momentum.

Diffraction phenomena have been observed in subsequent times not only with electrons, but also with other particle radiations, if only the de Broglie wavelength λ has the order of magnitude of the atomic distances of the crystal lattice. In this connection the following rules of thumb are useful (e^-: electron; p: proton; n: neutron; X: roentgen):

$$\lambda(e^-)\left[\mathring{A}\right] = \frac{h}{\sqrt{2\,m_e\,E}} \approx \frac{12.25}{\sqrt{E[eV]}}\,, \tag{2.20}$$

$$\lambda(n,p)\left[\mathring{A}\right] = \frac{h}{\sqrt{2\,M_{n,p}E}} \approx \frac{0.28}{\sqrt{E[eV]}}\,, \tag{2.21}$$

$$\lambda(X)\left[\mathring{A}\right] = \frac{h\,c}{E} \approx \frac{12.4}{E[keV]}\,. \tag{2.22}$$

The energy unit eV (electron-volt) is defined in (1.57). Electrons, which pass through an accelerating voltage of 10^4 V, have therefore a wavelength of about 0.12 Å, which corresponds to that of hard X-ray radiation. As charged particles, electrons of course interact strongly with matter, what allows them only very small penetration depths into a solid. On the other hand, this *sensitivity* of the electron motion can be successfully exploited for structural analyses of surfaces and thin layers (films). The interference of electron waves, which are reflected at a crystal surface, leads eventually to a mapping of the structure of the diffracting object. The electron microscope, whose mode of action is based on this principle, has a substantially higher resolving power than the light microscope, because of the distinctly smaller de Broglie wavelength compared to light. In the meantime, even atomic and molecular structures can be made visible by the electron microscope.

A special advantage thereby is that, by variation of the acceleration voltage, the electron wavelength can be adjusted almost arbitrarily, where, however, at very high voltages the relativistic mass variation has to be taken into consideration.

Neutron diffraction has achieved a special significance because it has some special advantages. According to (2.21), in order to get wavelengths of neutrons of the order of magnitude of 1 Å, one has to decelerate them down to *thermal* velocities, e.g., by letting them traverse a paraffin block. Today one gets efficient beams of neutrons with suitable kinetic energy from nuclear reactors. The neutron is uncharged and is therefore able to penetrate the crystal much less disturbed than the electron. On the other hand, it possesses a magnetic moment, which can interact with the moments of the solid to be investigated, if there are any. Neutron diffraction is thus an excellent means for making magnetic structures observable.

In Sect. 2.1.1 we have introduced the matter waves via conclusions drawn by analogy and have just reported on their experimental confirmation. We have to now exert ourselves for an in-depth understanding of the physical meaning of the phenomenon *matter wave*.

At first, in spite of possibly comparable wave lengths, one should not at all consider matter waves as being of similar physical nature as the electromagnetic radiation. They are basically different! In a certain sense, one has to even deny the matter waves the actual *measurability*. Let us recall, which characteristic parameters mark out a *'normal'* wave process. First there are the properties *amplitude* and *phase*. The amplitude characterizes the physical process realized by the wave and is therefore different from wave type to wave type. The phase, on the other hand, is a common feature of all wave processes and indicates therewith very generally the *wave nature* of the physical process. It determines the totality of all points with identical deviations of the physical quantity from its equilibrium value. In the case of continuously changing amplitude, such points define equiphase surfaces. The distance of two surfaces of equal phases defines the wavelength. The displacement velocity of a point on such a phase area is called the *phase velocity* of the wave.

Direction of propagation, direction of oscillation (longitudinal, transverse *polarization*), and wavelength are in general easily measurable parameters of a *'normal'* wave. The measurement of the phase velocity, sometimes also that of the amplitude, however, is not so easily done, but nevertheless possible.

For matter waves, the direction of their propagation coincides with the direction of motion of the matter itself and is therewith known. The wavelength results from the de Broglie relation (2.14) and can be measured, as already discussed, by the use of diffraction experiments on lattice planes of suitable crystal lattices. However, nobody succeeded so far to measure **directly** the phase velocity or the amplitude of a matter wave! Matter waves and electromagnetic waves, familiar to us from Classical Physics, behave obviously, from many points of view, very similar, but appear, though, to be basically different with respect to their deep physical meaning.

In order to really understand the nature of matter waves, we should inspect once more, from a basic point of view, the *particle-wave dualism*. The observation is undisputed that the electron behaves in some experiments like a particle, and in

others like a wave. Does that mean that we have to understand the electron, or any other *suitable* particle, in certain situations directly as a real wave? That seems to be too simple! For instance, if one inspects carefully the diffraction phenomena, typical for waves, one encounters already serious difficulties in understanding. Elementary particles like electrons possess the peculiar property of *indivisibility*, which, on the other hand, can by no means be ascribed to a wave. We know that a wave, which is incident on the interface of two media, in which it has different phase velocities, is decomposed into a reflected and a refracted partial wave, being thus divided. For the indivisible electron, in contrast, we have to assume that it is either reflected at the interfaces or it enters the second medium as a whole. Both scenarios can not simultaneously be valid. We meet very similar difficulties with the interpretation of the diffraction patterns with their maxima and minima of the wave intensity. It is of course absurd to assume that at some spots of the photographic plate *'more electron'* and at others *'less electron'* arrives. The formulation already appears ridiculous! But what then is actually going on with the *wave nature of the particle*? We encountered therewith obviously a very fundamental question, so that it appears to be reasonable to recall the full problematic concern once more with the aid of a typical *gedanken-experiment*.

2.1.3 Double-Slit Experiment

A wave (matter, electromagnetic, ...) falls onto an impenetrable screen S, on which a double-slit (S_1, S_2) is placed (Fig. 2.1). The arriving radiation intensity is registered on a photographic plate (detector D), in the xy-plane behind the screen. We now perform the following gedanken-experiment:

a) The source emits classical particles (balls, pellets, ...)!

It is definitely possible that the particles are influenced in some manner by the slits S_1 and S_2, where it is, however, important that the actions due to the slits S_1 and S_2 are independent of each other. If $I^{(a)}_{1,2}(x, y)$ are the intensities of the two single splits, one gets for the total intensity the classically self-evident result:

$$I^{(a)}(x, y) = I^{(a)}_1(x, y) + I^{(a)}_2(x, y) \ . \tag{2.23}$$

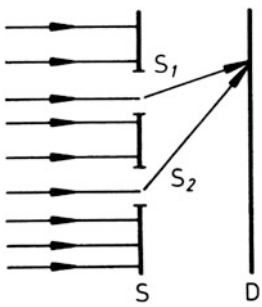

Fig. 2.1 Arrangement of the double-slit experiment

The same picture comes out for the case that the two slits are simultaneously opened, as for the case that the slits are opened for the same period of time, but one after the other, so that in each moment only one of them is opened.

b) The source emits electromagnetic waves (light, X-rays,...)!

That is the situation, which we discussed extensively already in Sect. 1.4. When we open the slits one after the other, the intensities $I^{(b)}_{1,2}(x, y)$ simply add up, where the pattern, though, has the same form as that for the diffraction at the single slit (1.71). If we, however, open both the slits at the same time, then an additional interference term $I^{(b)}_{12}(x, y)$ appears, which can be either positive or negative:

$$I^{(b)}(x, y) = I^{(b)}_1(x, y) + I^{(b)}_2(x, y) + I^{(b)}_{12}(x, y) \ . \tag{2.24}$$

When A_1 and A_2 are the amplitudes of the secondary waves, which, according to Huygens principle (Sect. 1.4.1) are to be ascribed to both the slits, then the intensity is determined by the absolute square of the **sum** of the amplitudes:

$$I^{(b)} \sim |A_1 + A_2|^2 \neq |A_1|^2 + |A_2|^2 \ . \tag{2.25}$$

The detailed intensity formulas can be read off from (1.72) and (1.73), respectively, for $N = 2$. That refers also to the labeling in Fig. 2.2.

c) The source emits electromagnetic radiation of extremely weak intensity, i.e., single photons!

The detector registers particles as in a). Energy is absorbed only in form of quanta $h\nu$. The points of incidence of the photons are, however, not predictable! The points are distributed at first rather randomly over the photographic plate. If one, however, allows sufficiently many single processes to take place, then eventually an overall picture results which corresponds to $I^{(b)}$. This appears to be paradoxical. In

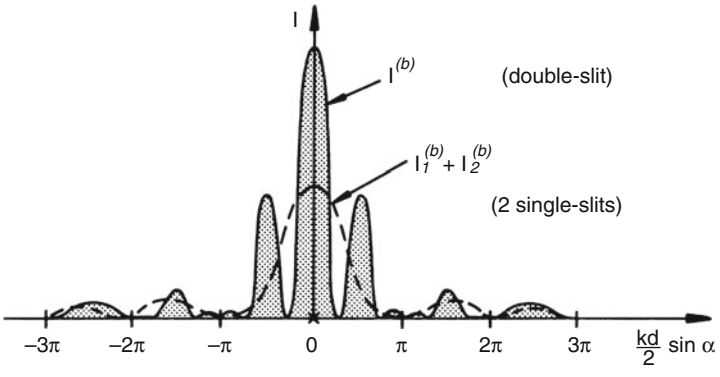

Fig. 2.2 Intensity distribution due to the double-split experiment

a gedanken-experiment we can indeed let the photons arrive one after the other at the detector. Nevertheless, it finally results an effect of interference. It looks as if the single photon would *'interfere with itself'*. Could that be true?

d) The source emits particles (electrons)!

These are individually registered as particles by the detector. Like for the photons, the arrival of the electrons is random, i.e., not predictable. The first spots, localized on the plate and produced by electrons, are distributed seemingly chaotically over the plate, in order to correspond, however, for a sufficiently great number of events to an intensity distribution like $I^{(b)}$. The differences between the intensities for the case of single-slits, which are opened one after another, and for the case of the simultaneously opened double-slit, are the same as in b) for the electromagnetic radiation. If we succeed, however, to follow exactly the path of the electron, i.e., to precisely state through which of the two slits the electron moves, then immediately the effect of interference disappears.

What is the electron now really, is it a particle, a wave or both? Let us try in Sect. 2.2 to find an answer to this question by an analysis of the reported double-split gedanken-experiment.

2.1.4 Exercises

Exercise 2.1.1 Calculate the de Broglie wavelength

1. of an electron with the energy $E = 1\,\text{eV}$,
2. of an electron with the energy $E = 100\,\text{MeV}$,
3. of a thermal neutron with the energy $E \approx k_B T\ ;\ T = 300\,\text{K}$.

Exercise 2.1.2 Show that the 'rule of thumb' (2.20) for the de Broglie wavelength of an electron must be replaced by

$$\lambda(e^-)\,[\text{Å}] \approx \frac{12.25}{\sqrt{E\,[\text{eV}]}}\,\frac{1}{\sqrt{1 + 0.978 \cdot 10^{-6} E\,[\text{eV}]}}$$

if relativistic effects are fully taken into account.

Exercise 2.1.3 Let a beam of thermal neutrons be reflected at the lattice planes of a crystal. Calculate the angle of deflection, for which intensity maxima in the Bragg reflection appear, if the distance of adjacent layers is 3.5 Å.

2.2 The Wave Function

2.2.1 Statistical Interpretation

The randomness of the elementary process turned out to be decisive for the interpretation of the double-slit experiment (see Sect. 2.1.3), i.e., the impossibility to predict exactly the time and the position of the absorption of a photon or an electron. Why this is so, we can not explain. We have to accept it as a matter of experience. But if we accept this, then we have to also consider *statistics* and therewith the term *probability* as the proper concept for the description of such random events. We cannot but

interpret 'statistically' the relation between particle and wave!

Actually, we had a similar situation with the Rutherford scattering of α-particles (see Sect. 1.2.3), for which the impact parameter p could not be absolutely fixed, so that necessarily statistical elements had to be used for the scattering formula (1.67). It provides therefore *only* probability statements. The exact course of the scattering process of a single α-particle is not predictable.

If we now agree upon the assignment

matter waves $\Longleftrightarrow$ probability waves

and let these probability waves experience interference and diffraction like *normal* waves, then, as we will develop step by step in the following sections, the in principle astonishing, sometimes even appearing paradoxical, experimental findings will be described quantitatively correctly. If we characterize the wave, as suggested by the considerations of Sect. 2.1.1, by a wave function $\psi(\mathbf{r}, t)$, then

$$|\psi(\mathbf{r}, t)|^2 \, d^3r$$

is to be interpreted as the probability to find the particle at the time t in the volume element d^3r around the position $\mathbf{r}$. Since probabilities are positive-definite quantities, it is not the wave function ψ itself, but the square of the absolute value which is decisive. Later we will see that the probability amplitude $\psi(\mathbf{r}, t)$ is in general complex. For a large number of identical particles then the intensity distribution is given by the square of the absolute value of the amplitude $|\psi(\mathbf{r}, t)|^2$. In regions, where this is large, many particles would have been landed at the time t, and in regions, where this quantity is equal to zero, no particle would be found. Diffraction maxima and minima automatically mean therefore enhanced and diminished particle density, respectively.

Matter waves thus are not a special physical property of a single particle. They owe their existence to the special **statistical** behavior of the particles. In contrast, in a **single process** only the **particle aspect** appears! In this sense, matter waves do not possess a physical reality as, for instance, electromagnetic waves. That was what was meant in Sect. 2.1.2 when it was warned to consider matter waves

and electromagnetic waves as being physically of the same type, only because of comparable wavelengths.

We thus interpret

$$\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 \tag{2.26}$$

as the *probability density* for the time-dependent location of the particle. Differing from Classical Mechanics, only probability statements are possible about its actual path. If we differentiate $\rho(\mathbf{r},t)$ with respect to time, we can write by using the Schrödinger equation (2.18):

$$\frac{\partial}{\partial t}\psi^*\psi = \left(\frac{\partial}{\partial t}\psi^*\right)\psi + \psi^*\left(\frac{\partial}{\partial t}\psi\right) = \frac{\hbar}{2mi}(\Delta\psi^*\psi - \psi^*\Delta\psi) \ .$$

This equation suggests the definition of a

probability-current density

$$\mathbf{j}(\mathbf{r},t) = \frac{\hbar}{2mi}\left\{\psi^*(\mathbf{r},t)\nabla_r\psi(\mathbf{r},t) - \psi(\mathbf{r},t)\nabla_r\psi^*(\mathbf{r},t)\right\} \ , \tag{2.27}$$

by which we can formulate a

continuity equation

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) + \mathrm{div}\mathbf{j}(\mathbf{r},t) = 0 \ . \tag{2.28}$$

It expresses the fact that the temporal change of the probability of finding a particle in a certain volume is determined by the probability current through the surface which encloses the volume. *No probability is lost*. In the last analysis, (2.28) expresses particle-number conservation. Between ρ and $\mathbf{j}$ there exists the same relationship, as in Electrodynamics ((3.5), Vol. 3), between charge density and current density.

The actual measurable quantity is the probability density $\rho(\mathbf{r},t)$, a real quantity. The wave function $\psi(\mathbf{r},t)$ itself is not directly accessible, but fixes uniquely $\rho(\mathbf{r},t)$ and is, in addition, calculable by the Schrödinger equations (2.16) and (2.18), respectively. If one combines (2.16) and (2.18),

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\Delta_r + V(\mathbf{r})\right)\psi(\mathbf{r},t) \ , \tag{2.29}$$

then there results a differential equation of first order with respect to time. That means, if the wave function is known at any point of time t_0, then it is already *uniquely* determined for *all* times. About the path of the particle, we can indeed provide only *'imprecise'* probability statements, the probability itself, however, is

exactly fixed by the Schrödinger equation. No additional *'uncertainty'* is therefore brought into play by the equation of motion (2.29) of the wave function.

For the solution of (2.29) let us, at first, keep on thinking of such quantum-mechanical systems which consist of a single particle only. The real potential $V(\mathbf{r})$ then incorporates all *external forces* which act on this particle. The generalization to many-particle systems will be presented in a forthcoming chapter. We should, however, remind ourselves once more that the decisive Schrödinger equation was, in the last analysis, only the result of *plausibility-considerations*:

The Schrödinger equation can not be derived from first principles!
It has rather the status of an axiom!

In order to get a certain confidence in it, one can inductively *'rationalize'* it by arguments of analogy, as we have tried to do in Sect. 2.1. With the same justification, however, one might *postulate* the Schrödinger equation as the basic law of wave mechanics, just like we dealt with the Newton axioms in Classical Mechanics. In any case, the theoretical statements, derived from (2.29), have to be confronted with experimental facts. Only a resulting agreement will justify the ansatz.

The probability-interpretation of the wave function of course strongly restricts the type of mathematical functions which can come into question. If one normalizes the probability, as is usually done, to one, then one has to require for the integral over the whole space

$$\int d^3r\,|\psi(\mathbf{r},t)|^2 = 1\ . \tag{2.30}$$

since the particle is definitely somewhere in the space. Since a solution of the linear differential equation (2.29) remains to be a solution even when it is multiplied by a constant, we have to require, a bit less strongly than (2.30)

$$\int d^3r\,|\psi(\mathbf{r},t)|^2 < \infty\ . \tag{2.31}$$

In particular, $\psi(\mathbf{r},t)$ has to vanish *'sufficiently fast'* at infinity. Therefore, only

square-integrable functions

can serve as wave functions.

The normalization condition (2.30) implicitly includes the assumption that the norm is time-independent. That can be demonstrated by the use of the continuity equation (2.28). It first follows, after application of the Gauss theorem ((1.53), Vol. 3), for a finite volume V with the surface $S(V)$:

$$\int\limits_V d^3r\frac{\partial\rho}{\partial t} + \oint\limits_{S(V)} \mathbf{j}\cdot d\mathbf{f} = 0\ .$$

If the volume V grows beyond all limits, then the surface integral disappears, since for square-integrable functions, the current density $\mathbf{j}$ (2.27) becomes zero on the surface S located at infinity. Because of

$$\frac{\partial}{\partial t}\int d^3r\,\rho(\mathbf{r},t) = 0\,, \tag{2.32}$$

the normalization integral (2.30) is indeed time-independent.

At the end of our quite general reflections on the wave function, let us still present an additional remark. It was already mentioned that in general the complex-valued wave function

$$\psi(\mathbf{r},t) = |\psi(\mathbf{r},t)|\,\exp\bigl(i\varphi(\mathbf{r},t)\bigr)$$

is not directly measurable. Only the square of the absolute value seems to be of physical importance. That could tempt into considering the phase $\varphi(\mathbf{r},t)$ as unimportant. From many points of view this is indeed justified; nevertheless, a bit of caution is advised. The Schrödinger equation (2.29) is linear, i.e., if $\psi_1(\mathbf{r},t)$ and $\psi_2(\mathbf{r},t)$ are solutions then the same holds for each linear combination:

$$\psi(\mathbf{r},t) = \alpha_1\psi_1(\mathbf{r},t) + \alpha_2\psi_2(\mathbf{r},t) \qquad \alpha_{1,2} \in \mathbb{C}\,. \tag{2.33}$$

It is evident that in such a case the relative phase of the two partial solutions ψ_1 and ψ_2 gets a decisive importance. We have to only think of the result of the double-slit experiment, discussed in Sect. 2.1.3.

2.2.2 *The Free Matter Wave*

Let us collect further information about the wave function $\psi(\mathbf{r},t)$, being associated with a particle, which obviously represents the central quantity for the solution of a quantum-mechanical problem. According to the considerations in Sect. 2.2.1, it is clear that the vector $\mathbf{r}$ in the argument of ψ is not at all to be identified with the position of the particle, but marks only the space point. The wave function is observable only in form of the probability density (2.26).

We start with the simplest case, the wave function of a free particle. *'Free'* means thereby that no forces whatsoever act on the particle. Therewith it does not possess any potential energy $V(\mathbf{r}) \equiv 0$. The Hamilton operator $\widehat{H}_0$ of the free particle then reads according to (2.16):

$$\widehat{H}_0 = -\frac{\hbar^2}{2m}\Delta_r\,. \tag{2.34}$$

One realizes immediately that the plane wave (see Sect. 4.3.2, Vol. 3),

$$\psi_0(\mathbf{r}, t) = \alpha e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \,, \tag{2.35}$$

solves the Schrödinger equation if only

$$E = \hbar\omega = \frac{\hbar^2 k^2}{2\,m} \Longleftrightarrow \omega = \omega(k) = \frac{\hbar k^2}{2\,m} \,. \tag{2.36}$$

Difficulties arise in connection with the normalization of the wave function (2.35). $\psi_0(\mathbf{r}, t)$ is apparently **not** square-integrable. One helps oneself here with the idea that the free particle is certainly somewhere in the in principle arbitrarily large, but nevertheless finite volume V. Thus one requires:

$$\int\limits_V d^3r\,|\psi(\mathbf{r}, t)|^2 = 1 \,. \tag{2.37}$$

Note that the integration is here not taken over the whole space, but only over the finite volume V. From (2.37) it follows then for the normalization constant α in (2.35):

$$\alpha = \frac{1}{\sqrt{V}} \tag{2.38}$$

(see also Sect. 2.2.5).

Plane waves are space-time periodical formations, whose phases,

$$\varphi = \varphi(\mathbf{r}, t) = \mathbf{k}\cdot\mathbf{r} - \omega t \,, \tag{2.39}$$

define planes at fixed times t. These consist of all the points, for which the projection of the space vector $\mathbf{r}$ onto the direction of $\mathbf{k}$ has the same value. At a fixed time $t = t_0$, planes with equal wave amplitudes $\psi_0(\mathbf{r}, t_0)$ recur periodically in space. The wavelength λ is defined as the perpendicular distance between two such adjacent planes:

$$\Delta\varphi = \Delta(\mathbf{r}\cdot\mathbf{k}) \stackrel{!}{=} 2\pi \Longleftrightarrow \lambda = \frac{\Delta(\mathbf{r}\cdot\mathbf{k})}{k} = \frac{2\pi}{k} \,. \tag{2.40}$$

With (2.14) and (2.36) it follows therefrom:

$$p = \hbar k \,; \quad E = \frac{p^2}{2\,m} \,. \tag{2.41}$$

That is the energy-momentum relation of a non-relativistic free particle, known from Classical Mechanics.

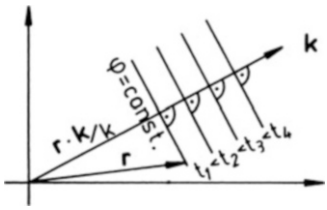

Fig. 2.3 Propagation of a plane wave

If one fixes, instead of time, now the space point, then the wave amplitude recurs with the time period:

$$\tau = \frac{2\pi}{\omega} = \frac{1}{\nu} \Longleftrightarrow \omega = 2\pi\nu \; . \tag{2.42}$$

Planes of constant phase propagate with the phase velocity u in the direction of $\mathbf{k}$ (Fig. 2.3):

$$u = \frac{d}{dt}\left(\mathbf{r}\cdot\frac{\mathbf{k}}{k}\right) = \frac{d}{dt}\left[\frac{1}{k}\big(\omega(k)\,t + \text{const}\big)\right]$$

$$\Longrightarrow u = \frac{\omega(k)}{k} = \frac{p}{2\,m} = \frac{v}{2} \; . \tag{2.43}$$

This velocity does not appear directly in the experiment with matter waves and the frequency ω, either. Soon we will see that the *group velocity* $\mathbf{v}_\mathrm{g}$ is more important, which in the special case of the plane wave is identical to the particle velocity:

$$\mathbf{v}_\mathrm{g}(\mathbf{k}) = \nabla_k\,\omega(k) = v_\mathrm{g}(k)\,\mathbf{e}_k \; ; \quad \mathbf{e}_k = \frac{\mathbf{k}}{k} \; , \tag{2.44}$$

$$v_\mathrm{g}(k) = \frac{d\omega}{dk} = \frac{\hbar\,k}{m} = v \; . \tag{2.45}$$

The plane wave $\psi_0(\mathbf{r}, t)$ is characterized, according to (2.35), (2.36), by a fixed wave vector $\mathbf{k}$, whose direction corresponds to the direction of propagation of the wave, while its magnitude uniquely determines the matter wavelength λ. Wavelengths of electromagnetic waves as well as of matter waves can be measured, in principle, arbitrarily accurately. If one ascribes a plane wave to the particle, the momentum of the particle is then exactly determined with (2.40), (2.41) by a measurement of the wavelength. In contrast to that, a statement about the position of the particle is completely impossible. As a consequence of

$$\rho_0(\mathbf{r}, t) = |\psi_0(\mathbf{r}, t)|^2 \equiv \frac{1}{V} \; , \tag{2.46}$$

the probability density is the same for all space points. For the strictly harmonic plane wave indeed no point of the space is different from any other point in anyway.

Fig. 2.4 Periodic space-dependence of the real part of the plane wave

We have no other choice but to accept that the possibility of an exact determination of the momentum is accompanied by a complete uncertainty concerning the *position of the particle* as the conjugate variable. That agrees, as a special case, with the Heisenberg uncertainty principle (1.5), which will engage us in the following over and over again (Fig. 2.4). On the other hand, it is surely undeniable that it is possible, under certain circumstances, to fix the position of the particle, maybe not exactly, but at least to a finite space region. But that obviously requires a wave function $\psi(\mathbf{r}, t)$, which represents a finite *wave train*. We know from the theory of Fourier transforms that one can realize wave trains of arbitrary shape by suitable superpositions of plane waves, since the plane waves build a so-called complete system of functions (see Sect. 2.3.5, Vol. 3). In addition it is clear that, because of the linearity of the wave equation (2.29), besides the plane waves also every linear combination of them represents a possible solution for the free particle. If we insert the general superposition

$$\psi(\mathbf{r}, t) = \int d\omega \int d^3k \widehat{\psi}(\mathbf{k}, \omega) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \tag{2.47}$$

into the time-dependent Schrödinger equation (2.18), so it follows with the Hamilton operator (2.34) of the free particle:

$$\int d\omega \int d^3k \widehat{\psi}(\mathbf{k}, \omega) \left(\hbar\omega - \frac{\hbar^2 k^2}{2\,m} \right) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} = 0 \,.$$

This equation requires

$$\widehat{\psi}(\mathbf{k}, \omega) = \widehat{\psi}(\mathbf{k}) \delta\big(\omega - \omega(k)\big) \tag{2.48}$$

with $\omega(k)$ as in (2.36). Hence, if we *'bunch'* plane waves to *wave packets* of the form

$$\psi(\mathbf{r}, t) = \int d^3k \widehat{\psi}(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega(k) t)} \,, \tag{2.49}$$

we are sure that they are solutions of the Schrödinger equation, where, on the other hand, the amplitude function $\widehat{\psi}(\mathbf{k})$ is still freely adjustable. We can surely ensure, by a proper choice of $\widehat{\psi}(\mathbf{k})$, that $|\psi(\mathbf{r}, t)|^2$ is distinctly different from zero only in a small spatial region. If a wave function of such a type is ascribed to the particle, then its position is no longer completely undetermined. On the other hand, however, the momentum is no longer exactly known, since for the construction of the wave

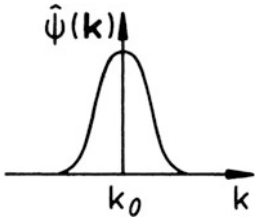

Fig. 2.5 Typical shape of the amplitude function of a wave packet

packet several plane waves of different wavelengths $\lambda = 2\pi/k$ are needed. This issue, too, confirms, at least qualitatively, the uncertainty relation (1.5).

2.2.3 Wave Packets

Let us look a bit more closely at the wave packets (2.49). We assume for the moment that the amplitude function $\widehat{\psi}(\mathbf{k})$ is concentrated essentially around the fixed vector $\mathbf{k}_0$, having there, for instance, a distinct maximum (Fig. 2.5). Then the value of the integral (2.49) will be determined, above all, by those wave numbers, which do not differ too much from $\mathbf{k}_0$. We are therefore allowed to truncate, without too big a mistake, a Taylor expansion of $\omega(k)$ around $\omega(k_0)$ after the linear term:

$$\begin{aligned}\omega(\mathbf{k}) &= \omega(k_0) + (\mathbf{k}-\mathbf{k}_0)\cdot\nabla_k\omega(k)|_{k_0} + \ldots = \\ &= \omega(k_0) + (\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{v}_\mathrm{g}(k_0) + \ldots \ .\end{aligned} \tag{2.50}$$

The wave packet (2.49) therewith takes the following form:

$$\psi(\mathbf{r},t) \approx e^{i(\mathbf{k}_0\cdot\mathbf{r}-\omega(k_0)t)}\widetilde{\psi}_{k_0}(\mathbf{r},t) \ . \tag{2.51}$$

The singling out of the wave number $\mathbf{k}_0$ should not at all be misinterpreted in such a way that a definite wavelength is to be ascribed also to the wave packet. In reality, it is of course a complicated process due to various partial waves. That manifests itself in the modulation function:

$$\widetilde{\psi}_{k_0}(\mathbf{r},t) = \int d^3q\,\widehat{\psi}(\mathbf{q}+\mathbf{k}_0)\exp\bigl(i\mathbf{q}\cdot(\mathbf{r}-\mathbf{v}_\mathrm{g}(k_0)t)\bigr) \ . \tag{2.52}$$

The by itself unimportant phase velocity of the wave packet comes out to be, exactly as in (2.43):

$$u = \frac{d}{dt}(\mathbf{r}\cdot\mathbf{e}_{k_0}) = \frac{\omega(k_0)}{k_0} \ . \tag{2.53}$$

On the other hand, the modulation function defines for

$$\mathbf{r} - \mathbf{v}_\mathrm{g}(k_0)t = \text{const} .$$

planes of constant amplitude which propagate with the velocity

$$\dot{\mathbf{r}} = \mathbf{v}_\mathrm{g}(k_0) = \nabla_k \omega(k)|_{k_0} . \tag{2.54}$$

This is simultaneously the displacement-velocity of the whole packet and therewith ultimately the velocity, at which information can be transported. According to the laws of the Theory of Special Relativity (Vol. 4) it must therefore always be $v_\mathrm{g} \leq c$; a restriction which does not affect the phase velocity u.

We want to illustrate the full issue once more by a simple *one-dimensional* example as plotted in Fig. 2.6:

Let the propagation direction of the wave packet be the z-direction and the amplitude function $\widehat{\psi}(k)$ be piecewise constant:

$$\widehat{\psi}(k) = \begin{cases} \widehat{\psi}(k_0), & \text{if } k_0 - \Delta k_0 \leq k \leq k_0 + \Delta k_0 , \\ 0 & \text{otherwise} . \end{cases} \tag{2.55}$$

Therewith the modulation function ,

$$\widetilde{\psi}_{k_0}(z,t) = \widehat{\psi}(k_0) \int_{-\Delta k_0}^{+\Delta k_0} dq \, \exp[i\, q(z - v_\mathrm{g}(k_0)\, t)] ,$$

can easily be calculated:

$$\widetilde{\psi}_{k_0}(z,t) = 2\, \widehat{\psi}(k_0)\, \Delta k_0 \, \frac{\sin[\Delta k_0 (z - v_\mathrm{g}\, t)]}{\Delta k_0 (z - v_\mathrm{g}\, t)} . \tag{2.56}$$

Hence, it is a function of the type $\sin x/x$. According to our considerations in Sect. 2.2.1 only the square of the absolute value $|\widetilde{\psi}_{k_0}|^2 \sim (\sin x/x)^2$ is of physical importance. It consists of a principal maximum at $x = 0$ with the value 1 and zeros at $x = \pm n\,\pi$; $n = 1, 2, \ldots$ (Fig. 2.7). Submaxima lie between these zeros at the x-values for which $\tan x = x$. These are found between $n\,\pi$ and $(n + 1/2)\pi$, with increasing n closer and closer to $(n + 1/2)\pi$. The first submaximum, though, just

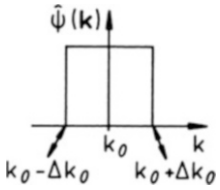

Fig. 2.6 Simple example of an amplitude function of a one-dimensional wave packet

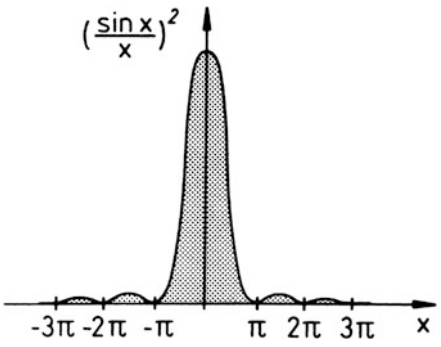

Fig. 2.7 Qualitative behavior of $(\sin x/x)^2$ *as function of* x

exhibits a function value of about 0.047 only. With increasing $|x|$ the submaxima become rapidly still smaller compared to the principal maximum. With an error less than 5%, the area under the curve $(\sin x/x)^2$ is restricted to the interval $-\pi$ to $+\pi$. Therewith, the amplitude function $\widehat{\psi}(k)$ from (2.55) very obviously takes care for the realization of a wave packet.

The maximum of the wave packet,

$$\psi(z,t) = 2\,\widehat{\psi}(k_0)\,\Delta k_0\,\frac{\sin[\Delta k_0(z - v_g\,t)]}{\Delta k_0\,(z - v_g\,t)}\,\exp[i(k_0\,z - \omega(k_0)\,t)]\;, \tag{2.57}$$

lies at

$$z_m(t) = v_g\,t \tag{2.58}$$

and moves in the positive z-direction with the velocity v_g. Although it seems to be so, by the representation (2.57), that the wavelength $\lambda_0 = 2\pi/k_0$ and the frequency $\omega(k_0)$ are especially distinguished compared to the other wavelengths and frequencies, we have, nevertheless, in reality a process which incorporates many different wavelengths. This corresponds exactly to the result of our previous general considerations after (2.51).

It is rather instructive to think about with what accuracy the position of a particle, which is described by a wave function (2.57), can be given at a fixed time, say $t = 0$. As discussed above, the probability density $|\psi(z, t = 0)|^2$ is essentially concentrated in the interval

$$-\pi \le \Delta k_0\,z \le +\pi\;.$$

The effective width Δz of the wave packet therewith fulfills the relation

$$\Delta k_0\,\Delta z = 2\pi\;. \tag{2.59}$$

We get the momentum of the particle when we multiply the wave number by $\hbar$. The above equation then expresses the fact that the product of the uncertainty of the position and the uncertainty of the momentum can not be made arbitrarily small. In this respect, the plane wave obviously represents a limiting case. It possesses a sharply defined wave number (*monochromatic*) which corresponds to $\Delta k_0 = 0$. On the other hand, it is infinitely extended ($\Delta z \to \infty$), so that, all in all, there is no contradiction to (2.59). By (2.59), the Heisenberg uncertainty principle (1.5) is again confirmed, at least qualitatively.

The spreading out (*increase of width*) is another important peculiarity of wave packets, which will be investigated in detail for a prominent example, namely the Gaussian wave packet, in the Exercises 2.2.2 and 2.2.3. So far we have presumed that the expansion (2.50) of $\omega(k)$ around $\omega(k_0)$ can be terminated after the linear term. Indeed, for $\nabla^2\omega \equiv 0$ all hitherto existing statements remain valid. In the case that $\nabla^2\omega \not\equiv 0$, however, the various plane partial waves, with which the packet is put together, obviously possess different phase velocities:

$$u = \frac{\omega(k)}{k} = u(k) \; . \tag{2.60}$$

The wave-vector dependence of u is called *'dispersion'*. The faster partial waves run ahead, the slower ones are lag behind. The phase relations, which exist at the point of time $t = 0$, are no longer valid the very next moment. The packet thus can not retain its shape. One says: *'It melts away!'*. The phase velocity u of the free particle, according to (2.36), is in any case wave-vector dependent ($u \sim k$). Corresponding matter wave packets have to therefore melt away. In case of no dispersion, phase velocity and group velocity are identical. The whole packet then travels exactly with the same velocity as each of the individual partial waves. This situation is familiar for electromagnetic waves ($\omega = c\,k$). Wave packets, which are built up by electromagnetic waves, as they are used for radar detection, therefore do **not** melt away. If, however, dispersion is present, as for the matter waves, then the resulting, wave vector dependent group velocity,

$$v_g(k) = \frac{d\omega}{dk} = u(k) + k\frac{du}{dk} \; , \tag{2.61}$$

can be smaller (*normal dispersion*) as well as larger (*abnormal dispersion*) than u.

Although we have already made the origin of the diffluence of the wave packets plausible, we now want to derive once more, very formally, the condition for non-diffluence. For simplicity, we do that again for the one-dimensional wave packet. When the packet as a whole moves by the distance $z_0(t)$ in the time t, and that too without deforming itself, then it must obviously hold:

$$|\psi(z,t)|^2 \stackrel{!}{=} |\psi(z - z_0(t), 0)|^2 \; .$$

According to (2.49), it is therefore to require:

$$\int dk \int dk' \, \widehat{\psi}(k) \, \widehat{\psi}^*(k') \, e^{i(k-k')z} \left\{ e^{-i(\omega(k)-\omega(k'))t} - e^{-i(k-k')z_0(t)} \right\} \stackrel{!}{=} 0 \, .$$

When we substitute k' by $k + p$, then this condition reduces to:

$$\int dk \, \widehat{\psi}(k) \, \widehat{\psi}^*(k+p) \left\{ e^{-i(\omega(k)-\omega(k+p))t} - e^{ip\,z_0(t)} \right\} \stackrel{!}{=} 0 \, .$$

This condition should be valid for arbitrary weight functions $\widehat{\psi}$. Therefore it must be assumed

$$[\omega(k+p) - \omega(k)] \; t \stackrel{!}{=} p \, z_0(t) \, ,$$

and, consequently, because the left-hand side must be independent of k,

$$\omega(k) \stackrel{!}{=} \alpha \, k \, .$$

A constant which can appear in principle can be made to zero by a proper energy normalization. For the non-diffluence of the wave packet it is therefore required, as expected, that the phase velocity and the group velocity are identical:

$$\frac{\omega(k)}{k} \stackrel{!}{=} \frac{d\omega(k)}{dk} \, . \tag{2.62}$$

If this condition is not fulfilled, then the wave packet will inevitably melt away, and that the faster the closer the packet was packed at $t = 0$. Fourier-analysis tells us that for the construction of a certain wave packet the more plane partial waves are used, the stronger the spatial concentration of the packet would be. In accordance with the uncertainty relation (1.5), the indeterminacy of the momentum at $t = 0$ is therefore the greater, the sharper the position of the particle can be fixed. Because of the greater indeterminacy of the momentum, the future ($t > 0$) position of the particle will be predictable the less precisely, the more exactly it was known at $t = 0$. The diffluence, typical for wave packets, can thus be understood with the aid of the uncertainty relation. This statement is supported with (2.59) by the above calculated Example (2.55) of a wave packet.

In Exercise 2.2.2 we calculate for a special packet of matter waves, which at $t = 0$ has the shape of a *Gaussian bell*:

$$\psi(z, 0) = (\pi \, b^2)^{-\frac{1}{4}} \, \exp\left(-\frac{z^2}{2\, b^2} \right) \exp(i \, k_0 \, z) \, . \tag{2.63}$$

This evolves in the course of time, where the probability density always retains the shape of a Gaussian for all later times t:

$$\rho(z,t) = |\psi(z,t)|^2 = \frac{1}{\sqrt{\pi}\,\Delta b(t)} \exp\left[-\frac{\left(z - \frac{\hbar k_0}{m} t\right)^2}{(\Delta b(t))^2}\right] . \tag{2.64}$$

The maximum of the bell obviously lies at

$$z_{\mathrm{m}}(t) = \frac{\hbar\, k_0}{m}\, t$$

and travels with the velocity $v_{\mathrm{m}} = \hbar\, k_0/m$. The width $2\Delta b(t)$ of the bell changes thereby according to:

$$\Delta b(t) = \frac{1}{b}\sqrt{b^4 + \left(\frac{\hbar}{m} t\right)^2} . \tag{2.65}$$

By 'width' we understand here the distance between the points, for which the function value of the Gaussian bell has reduced to the e-th part of its maximum value (see Fig. 2.8),

$$\rho(z_{\mathrm{m}}, t) = \frac{1}{\sqrt{\pi}\,\Delta b(t)} . \tag{2.66}$$

Hence, height and width of the packet change with time such that the area under the ρ-curve keeps to be normalized to one for all t. After the time

$$t_{\mathrm{d}} = \sqrt{3}\,\frac{m}{\hbar}\, b^2 \tag{2.67}$$

the initial width ($2\,\Delta b(0) = 2\,b$) has just doubled. For a particle of the mass $m = 1\,\mathrm{g}$ with $b = 1\,\mathrm{mm}$ the width of the packet doubles after $1.642 \cdot 10^{25}\,\mathrm{s}$, i.e., after about $5.2 \cdot 10^{17}$ years. For an electron, however, with an initial width of $b = 0.5\,\mathring{\mathrm{A}}$, t_{d} amounts only to about $3.74 \cdot 10^{-17}\,\mathrm{s}$. After our discussion in Sect. 2.2.1 it is, however, clear that the diffluence of the electronic wave packet should not be

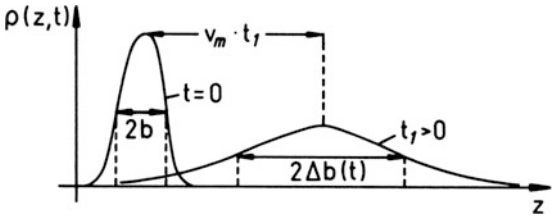

Fig. 2.8 Illustration of the diffluence with the Gaussian wave packet as example

interpreted in the sense of something like an *'exploding'* of the electron. Nothing else but the uncertainty in the determination of the particle position is spreading out in the course of time. $\rho(\mathbf{r}, t)$ of course does not make any statement about the *structure* of the particle.

2.2.4 Wave Function in the Momentum Space

In Sect. 2.2.1 we have investigated the statistical interpretation of the wave function $\psi(\mathbf{r}, t)$. The most important result was that the square of the absolute value of the wave function enables one to make probability statements about the position of the particle. It would of course be just as important and interesting to get to know the corresponding probability distribution for the conjugate variable *momentum*, too. As in (2.26) for the probability density in the position space, there should exist an analogous expression,

$$w(\mathbf{p}, t)\, d^3p = |\overline{\psi}(\mathbf{p}, t)|^2\, d^3p\ , \tag{2.68}$$

which represents the probability that the particle has at time t a momentum in the volume element d^3p around $\mathbf{p}$ in the momentum space. We want to represent this probability, too, by the square of the absolute value of a corresponding wave function $\overline{\psi}(\mathbf{p}, t)$. Necessarily, it must again be a square-integrable function in order to guarantee

$$\int d^3p |\overline{\psi}(\mathbf{p}, t)|^2 = 1\ . \tag{2.69}$$

Strictly speaking, nothing else comes out here but the trivial statement that the particle must certainly have some momentum. If we now combine (2.69) with (2.30),

$$\int d^3r |\psi(\mathbf{r}, t)|^2 = \int d^3p |\overline{\psi}(\mathbf{p}, t)|^2\ , \tag{2.70}$$

then we are reminded of the Parseval relation of the Fourier transformation, which we proved as Exercise 4.3.5 in Vol. 3. It states that the normalization of a function does not change with a Fourier transformation. It therefore seems to be obvious to identify $\overline{\psi}(\mathbf{p}, t)$ with the Fourier transform of the wave function $\psi(\mathbf{r}, t)$ (see Sect. 4.3.6, Vol. 3):

Definition 2.2.1

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi\,\hbar)^{3/2}} \int d^3p\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\, \overline{\psi}(\mathbf{p}, t)\ , \tag{2.71}$$

$$\overline{\psi}(\mathbf{p}, t) = \frac{1}{(2\pi\,\hbar)^{3/2}} \int d^3r\, e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\, \psi(\mathbf{r}, t)\ . \tag{2.72}$$

Both functions ψ and $\overline{\psi}$ are completely equivalent, one determines the other and vice versa. ψ as well as $\overline{\psi}$ are both suitable for the description of the state of the particle. We therefore denote both as *wave functions*. The ansatz (2.71) is in accordance with our considerations in Sect. 2.2.3 on the free matter waves and the wave packets built up by them. $\psi(\mathbf{r}, t)$ appears as linear combination of weighted plane waves,where the Fourier transform $\overline{\psi}(\mathbf{p}, t)$ agrees with the amplitude function, used in (2.49), except for an unimportant pre-factor and the time-dependence.

The identification of the momentum-wave function, which fulfills (2.68) and (2.69), with the Fourier transform of $\psi(\mathbf{r}, t)$ has again to be classified, though, as *plausible speculation*, which, however, has proven so far as absolutely consistent to the experiment. The probability densities $\rho(\mathbf{r}, t)$ and $w(\mathbf{p}, t)$, which are connected via (2.70), are measurable. That (2.70) is fulfilled by (2.71) and (2.72) can easily be shown by insertion and by use of the Fourier representation of the δ-function ((4.189), Vol. 3):

Definition 2.2.2

$$\delta(\mathbf{r} - \mathbf{r}') = \frac{1}{(2\pi\hbar)^3} \int d^3p \, e^{\frac{i}{\hbar}\mathbf{p}(\mathbf{r}-\mathbf{r}')} , \tag{2.73}$$

$$\delta(\mathbf{p} - \mathbf{p}') = \frac{1}{(2\pi\hbar)^3} \int d^3r \, e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} . \tag{2.74}$$

2.2.5 Periodic Boundary Conditions

Let us consider in this section, as an interlude, an incidental remark on the square-integrability (2.31) of the wave function $\psi(\mathbf{r}, t)$. We had already seen, in connection with the plane wave (2.35), that the square-integrability is not always ensured. One frequently helps oneself with the assumption that, instead of the integrability, the wave function is **periodic** in a basic volume. If this is, for instance, a cuboid with the edge lengths L_x, L_y, L_z ($V = L_x L_y L_z$), then this periodicity means:

$$\psi(x, y, z, t) = \psi(x + L_x, y, z, t) = \psi(x, y + L_y, z, t) = \psi(x, y, z + L_z, t) . \tag{2.75}$$

This implies that the events in the basic volume recur outside periodically, which of course need not necessarily correspond to reality. Otherwise, this *incorrect* assumption is without any serious consequence for events in atomic dimensions, provided L_x, L_y, L_z are chosen sufficiently large, for instance, in the region of centimeters. The conclusion, which led to (2.32), can no longer exploit the vanishing of the wave function on the surface $S(V)$, but rather the fact that non-vanishing partial contributions on the surface of the periodicity volume mutually compensate because of the periodicity (2.75).

The assumption of periodic boundary conditions (2.75) has the consequence that the momentum $\mathbf{p}$ can no longer take arbitrary continuous values, but instead

becomes discrete and therewith countable. Equation (2.75) can be fulfilled by (2.72) only for

$$p_{x,y,z} = n_{x,y,z} \frac{2\pi\,\hbar}{L_{x,y,z}} \; ; \quad n_{x,y,z} \in \mathbb{Z} \tag{2.76}$$

That yields in the momentum space a grid volume

$$\Delta^3 p = \frac{(2\pi\,\hbar)^3}{L_x L_y L_z} = \frac{(2\pi\,\hbar)^3}{V} \; , \tag{2.77}$$

in which exactly one *'allowed'* momentum value is found. Such a discretization frequently offers substantial computational advantages, so that one applies periodic boundary conditions often only because of considerations of expedience, independently of the above explained original goal. The *discretionary* assumption (2.75) represents a *surface effect*, which is the more unimportant the larger the periodicity volume (*thermodynamic limit*, see Vol. 6). The physical statements of the respective evaluation are not falsified by (2.75) if $L_{x,y,z} \to \infty$.

The Fourier integral (2.71) becomes, because of (2.76), a sum:

$$\psi(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} c_{\mathbf{p}}(t)\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} \; . \tag{2.78}$$

The square of the absolute value $|c_{\mathbf{p}}(t)|^2$ of the coefficients now adopts the role of $|\overline{\psi}(\mathbf{p}, t)|^2$:

$$c_{\mathbf{p}}(t) = \frac{1}{\sqrt{V}} \int\limits_V d^3 r\, e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} \psi(\mathbf{r}, t) \; . \tag{2.79}$$

$|c_{\mathbf{p}}(t)|^2$ is the probability that the particle possesses the momentum $\mathbf{p}$ at time t.

The δ-function $\delta(\mathbf{p} - \mathbf{p}')$ (2.74) has to switch over, for discrete momenta (2.76), to a Kronecker delta:

$$\delta_{\mathbf{p},\mathbf{p}'} = \frac{1}{V} \int\limits_V d^3 r\, e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} \; . \tag{2.80}$$

We perform the proof hereto as Exercise 2.2.9. The other δ-function (2.73), we obtain from a summation over momenta in the limiting case $V \to \infty$:

$$\begin{aligned} \frac{1}{V} \sum_{\mathbf{p}} e^{\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} &= \frac{1}{(2\pi\hbar)^3} \sum_{\mathbf{p}} \Delta^3 p\, e^{\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} \\ \longrightarrow \; \frac{1}{(2\pi\,\hbar)^3} \int d^3 p\, e^{\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} &= \delta(\mathbf{r} - \mathbf{r}') \quad (V \to \infty) \; . \end{aligned} \tag{2.81}$$

We will apply periodic boundary conditions frequently in the subsequent chapters, and we will realize thereby how useful they are.

2.2.6 Average Values, Fluctuations

The probability densities $\rho(\mathbf{r}, t)$ and $w(\mathbf{p}, t)$ represent the actually measurable statements of Quantum Mechanics with respect to position and momentum of a particle. This differs basically from the characterization of particles in Classical Mechanics, where exact values are ascribed to position and momentum. In a certain sense one can consider Classical Mechanics as that limiting case for which the probability densities ρ and w turn into sharp δ-functions, or, at least to a good approximation, can be replaced by them.

Which physical statements can further be formulated by the use of $\rho(\mathbf{r}, t)$ and $w(\mathbf{p}, t)$? We are not able to predict exactly the position of the particle, but for each *'thinkable'* experimental value of $\mathbf{r}$ we know the probability of obtaining just this value when a single measurement is made. Many single measurements, one after another, on one and the same particle, or, equivalently, many simultaneous measurements on similar particles, which are all described by the same wave function, should then deliver an *average value* $\langle \mathbf{r} \rangle$, which is determined as integral (sum) over all individual values, which are weighted by the probability of their occurrence.

$$\langle \mathbf{r} \rangle_t = \int d^3 r \, \rho(\mathbf{r}, t) \, \mathbf{r} = \int d^3 r \, \psi^*(\mathbf{r}, t) \, \mathbf{r} \, \psi(\mathbf{r}, t) \; . \tag{2.82}$$

This definition presumes that ψ is normalized. The symmetric notation on the right-hand side of the equation has been chosen intentionally in this way. The reason will become clear very soon. In Quantum Mechanics, average values are in general called *expectation values*.

We define the expectation value of a more general particle property $A(\mathbf{r})$ in a completely analogous manner

$$\langle A(\mathbf{r}) \rangle_t = \int d^3 r \, \psi^*(\mathbf{r}, t) \, A(\mathbf{r}) \psi(\mathbf{r}, t) \; , \tag{2.83}$$

which can of course change in the course of time, even if $A = A(\mathbf{r})$ itself is not explicitly time-dependent.

Besides the average value of the distribution of measured values, another important figure is the width of the distribution. In the elementary error theory such widths are marked by the *mean square fluctuation*,

$$\begin{aligned} \int d^3 r \, \rho(\mathbf{r}, t) \left(A(\mathbf{r}) - \langle A(\mathbf{r}) \rangle_t \right)^2 &= \left\langle \left(A(\mathbf{r}) - \langle A(\mathbf{r}) \rangle_t \right)^2 \right\rangle_t \\ &= \langle A^2(\mathbf{r}) \rangle_t - \langle A(\mathbf{r}) \rangle_t^2 \; , \end{aligned}$$

which indicates how strongly, on an average, the actually measured value will deviate from its average value. Since the deviation can take place *upwards* as well as *downwards*, it is possible that, when adding up the corresponding contributions, they mutually compensate each other, partially or even completely. It is therefore reasonable to consider the **quadratic** deviations. As *root mean square deviation* one defines the positive root of the square fluctuation:

$$\Delta A_t = \sqrt{\left\langle \left(A(\mathbf{r}) - \langle A(\mathbf{r})\rangle_t\right)^2 \right\rangle} = \sqrt{\langle A^2(\mathbf{r})\rangle_t - \langle A(\mathbf{r})\rangle_t^2}\ . \tag{2.84}$$

Let us now come to the expectation value of momentum:

$$\langle \mathbf{p}\rangle_t = \int d^3p\ w(\mathbf{p},t)\,\mathbf{p} = \int d^3p\,\overline{\psi}^*(\mathbf{p},t)\mathbf{p}\,\overline{\psi}(\mathbf{p},t)\ . \tag{2.85}$$

This definition is reasoned in the same manner as that for $\langle \mathbf{r}\rangle$ in (2.82), in particular, if one thinks of the completely equal status of the wave functions $\psi(\mathbf{r},t)$ and $\overline{\psi}(\mathbf{p},t)$. This transfers to the expectation values of more general particle properties $B(\mathbf{p})$:

$$\langle B(\mathbf{p})\rangle_t = \int d^3p\,\overline{\psi}^*(\mathbf{p},t)\,B(\mathbf{p})\,\overline{\psi}(\mathbf{p},t)\ . \tag{2.86}$$

However, we know from Classical Mechanics that a general measurand (*observable*) will in general depend on the position as well as on the momentum of the particle: $F = F(\mathbf{r},\mathbf{p})$. The question is how to average in such a case. This we will investigate in the next section.

2.2.7 Exercises

Exercise 2.2.1 For the wave function of an electron of the mass m one has found

$$|\psi(\mathbf{r},t)|^2 = \frac{1}{(\pi\, b^2(t))^{3/2}}\ \exp\left(-\frac{(\mathbf{r}-\mathbf{v}_0 t)^2}{b^2(t)}\right)$$

with

$$b(t) = b\sqrt{1+\frac{\hbar^2 t^2}{m^2 b^4}}\ .$$

1. Show that at each point of time the total probability of finding the electron is normalized to one.
2. Calculate the most probable position of the electron.

Exercise 2.2.2 Let the one-dimensional wave packet

$$\psi(z,t) = \int_{-\infty}^{+\infty} dk\, \widehat{\psi}(k)\, e^{i(kz-\omega(k)t)}\ ; \qquad \omega(k) = \frac{\hbar\, k^2}{2\,m}$$

have at the time $t = 0$ the shape of a Gaussian bell:

$$\psi(z,0) = A\, e^{-\frac{z^2}{2b^2}}\, e^{i\,k_0 z}\ .$$

1. Determine the (real) normalization constant A.
2. Show that the weight function (Fourier transform) $\widehat{\psi}(k)$ of the wave function $\psi(z,t)$ also has the shape of a Gaussian bell.
3. We define as *width* of the Gaussian bell the distance between the points, located symmetrically to the maximum, for which the value of the function has reduced to the e-th part of the maximum. Calculate the width Δk of $|\widehat{\psi}(k)|^2$.
4. Determine the full position- and time-dependence of the wave function $\psi(z,t)$.
5. Verify for the probability density the following expression:

$$\rho(z,t) = |\psi(z,t)|^2 = \frac{1}{\sqrt{\pi}\,\Delta b(t)}\, \exp\left\{-\frac{\left(z-\frac{\hbar\,k_0}{m}t\right)^2}{(\Delta b(t))^2}\right\}\ .$$

where:

$$\Delta b(t) = \frac{1}{b}\sqrt{b^4 + \left(\frac{\hbar}{m}\,t\right)^2}\ .$$

Exercise 2.2.3 A particle of mass m and momentum p is described by the Gaussian wave packet from Exercise 2.2.2.

1. After what time of flight does the width of the packet double?
2. After how much length of travel does the width of the packet double?
3. A free proton has the kinetic energy $T = 1$ MeV. After how much length of travel does the proton double its initial linear extension of $b = 10^{-2}$ Å?

Exercise 2.2.4 Let the wave function of an electron be described by a Gaussian wave packet.

1. How broad is the packet after 1 s, when it had at the time $t = 0$ the width $2\,b = 1$ Å?
2. The electron from part 1. has traversed a voltage difference of 100 V. Which width does it have after a length of run of 10 cm?

3. How do the results of 1. and 2. change, when the wave packet has an initial width of $2\,b = 10^{-3}$ cm?

Exercise 2.2.5 A particle of the mass m is described by the following wave function:

$$\psi(\mathbf{r},t) = A \cdot r \exp\left(-\frac{r}{2a} + i\frac{\hbar}{8ma^2} \cdot t + i\varphi\right) \sin\vartheta$$

1. Calculate the real normalization constant A!
2. Calculate the probability-current density $\mathbf{j}(\mathbf{r},t)$!
3. Find the energy-eigen value E!
4. Calculate the potential energy $V(\mathbf{r})$ of the particle! Identify the constant a with the Bohr radius:

$$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2}\ .$$

Exercise 2.2.6 A particle is described at a certain point of time by the wave function

$$\psi(x) = \begin{cases} Axe^{-\alpha x} & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases}$$

A real, $\alpha > 0$. Calculate the probability that a measurement of the momentum at the mentioned point of time yields a value between $-\hbar\alpha$ and $+\hbar\alpha$!

Exercise 2.2.7

1. As average value (expectation value) of the position z of the particle one defines the quantity:

$$\langle z\rangle_t = \frac{\int\limits_{-\infty}^{+\infty} dz|\psi(z,t)|^2 z}{\int\limits_{-\infty}^{+\infty} dz|\psi(z,t)|^2}\ .$$

   Interpret this expression!
2. Calculate $\langle z\rangle_t$ for the one-dimensional Gaussian wave packet!
3. Calculate the root mean square deviation

$$\Delta z = \sqrt{\langle (z - \langle z\rangle)^2\rangle}$$

   for the Gaussian wave packet!

4. Calculate and interpret the probability-current density $j(z,0)$ of the one-dimensional Gaussian wave packet!

Exercise 2.2.8 A particle obeys, in the position space, the Schrödinger equation

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\psi(\mathbf{r},t) = 0$$

with

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

How does the Schrödinger equation read in the momentum space, provided $V(\mathbf{r})$ possesses a Fourier transform $V(\mathbf{p})$:

$$V(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p\ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\,V(\mathbf{p})\ ?$$

Exercise 2.2.9 Periodic boundary conditions are defined on a cuboid with the edge lengths L_x, L_y, L_z. Verify the representation (2.80) of the Kronecker delta:

$$\delta_{\mathbf{p},\mathbf{p}'} = \frac{1}{V}\int\limits_V d^3r\, e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}}\ ; \qquad V = L_x L_y L_z\ .$$

Exercise 2.2.10

1. As a consequence of periodic boundary conditions for the wave function $\psi(\mathbf{r},t)$ on a cuboid with the edge lengths L_x, L_y, L_z, the momenta of the particle are discretized as given in (2.76). In particular, the delta-function $\delta(\mathbf{p}-\mathbf{p}')$ has to be replaced by the Kronecker delta $\delta_{\mathbf{p}\mathbf{p}'}$. Show that the following formal connection exists:

$$\delta(\mathbf{p}-\mathbf{p}') \to \lim_{V\to\infty}\frac{V}{(2\pi\hbar)^3}\,\delta_{\mathbf{p}\mathbf{p}'}$$

2. The wave function $\psi(\mathbf{r},t)$ can be expressed by the Fourier *sum*

$$\psi(\mathbf{r},t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} c_{\mathbf{p}}(t)\exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)\ .$$

   How does the *'reversal'* read, and what is the physical meaning of $c_{\mathbf{p}}(t)$?

Exercise 2.2.11 Consider a system of two (spin-less) particles of the masses m_1 and m_2, which interact with one another via the real potential $V(\mathbf{r}_1,\mathbf{r}_2)$. The system is described by the wave function $\psi(\mathbf{r}_1,\mathbf{r}_2,t)$. How does the continuity equation read in this case?

Exercise 2.2.12 Assume that the classical relation between position and momentum holds in Quantum Mechanics for the corresponding expectation values (Ehrenfest theorem):

$$\langle \mathbf{p} \rangle_t = m \frac{d}{dt} \langle \mathbf{r} \rangle_t \ .$$

Show by the use of the Schrödinger equation and the square-integrability of the wave function that:

$$\langle \mathbf{p} \rangle_t = \int d^3 r \ \psi^*(\mathbf{r}, t) \ \frac{\hbar}{i} \nabla_r \psi(\mathbf{r}, t)$$

Exercise 2.2.13 Let the wave function $\psi(\mathbf{r}, t)$ of a particle be real-valued. Show that then the expectation value of the momentum vanishes!

Exercise 2.2.14 Let the momentum-dependent wave function $\psi(\mathbf{p}, t)$ be real-valued. Show that then the expectation value of the position $\mathbf{r}$ is zero!

Exercise 2.2.15 Show that the expectation value

$$\langle \mathbf{r} \rangle_t = \int d^3 p \ \overline{\psi}^\star(\mathbf{p}, t) \left(-\frac{\hbar}{i} \nabla_p \right) \overline{\psi}(\mathbf{p}, t)$$

is real, where the wave function $\overline{\psi}(\mathbf{p}, t)$ is square-integrable.

2.3 The Momentum Operator

2.3.1 Momentum and Spatial Representation

We come back once more to the expectation value of the momentum (2.85), but now we try to calculate $\langle \mathbf{p} \rangle_t$ in the position space using $\psi(\mathbf{r}, t)$. However, without further ado, that is not possible, because we do not know, how we have to express $\mathbf{p}$ by $\mathbf{r}$. Otherwise we could directly apply (2.83). In a first step, though, we can replace in (2.85) $\overline{\psi}(\mathbf{p}, t)$ by $\psi(\mathbf{r}, t)$, by the use of the Fourier transformation (2.72),:

$$\begin{aligned} \langle \mathbf{p} \rangle_t &= \int d^3 p \overline{\psi}^*(\mathbf{p}, t) \mathbf{p} \overline{\psi}(\mathbf{p}, t) \qquad (2.87) \\ &= \frac{1}{(2\pi\hbar)^3} \int d^3 p \iint d^3 r d^3 r' \exp\left(\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right) \psi^*(\mathbf{r}, t) \mathbf{p} \exp\left(-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}' \right) \psi(\mathbf{r}', t) \end{aligned}$$

This can also be written as follows:

$$\langle \mathbf{p} \rangle_t = \frac{1}{(2\pi\hbar)^3} \int d^3p \iint d^3r d^3r' \exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)\psi^*(\mathbf{r},t)\left(i\hbar\nabla_{r'}\exp\left(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}'\right)\right)\psi(\mathbf{r}',t)\,.$$

With the special form of the δ-Funktion,

$$\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi\hbar)^3}\int d^3p \exp\left(\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')\right)\,,$$

we have

$$\langle \mathbf{p} \rangle_t = \iint d^3r d^3r' \psi^*(\mathbf{r},t)\left(i\hbar\nabla_{r'}\delta(\mathbf{r}-\mathbf{r}')\right)\psi(\mathbf{r}',t)\,.$$

The $\mathbf{r}'$-integration can be performed (see (1.16) in Vol. 3):

$$\int d^3r' \left(\nabla_{r'}\delta(\mathbf{r}-\mathbf{r}')\right)\psi(\mathbf{r}',t) = -\nabla_r\psi(\mathbf{r},t)\,.$$

We obtain therewith for the expectation value of the momentum in the position space the following remarkable result:

$$\langle \mathbf{p} \rangle_t = \int d^3r\, \psi^*(\mathbf{r},t)\left(\frac{\hbar}{i}\nabla_r\right)\psi(\mathbf{r},t)\,. \tag{2.88}$$

This expression is formally identical to the expectation value (2.83), but only if one ascribes to the dynamical variable *momentum* an operator in the position space:

momentum in spatial representation

$$\hat{\mathbf{p}} \longrightarrow \frac{\hbar}{i}\nabla_r\,. \tag{2.89}$$

We have encountered therewith a very fundamental characteristic of Quantum Mechanics, which assigns **operators** to the observables, i.e., to the measurable quantities. Many important considerations on this decisive feature are still to be performed in the following chapters. Unless stated otherwise, we will mark operators by a 'hat' ($\widehat{\ }$), in order to distinguish them from normal variables. Later, when confusion is no longer to be feared, we will give up on that. In the position space, the position operator $\hat{\mathbf{r}}$ is, as a special case, identical to the vector $\mathbf{r}$. It therefore behaves in the integrand of (2.82) purely multiplicatively, whereas in (2.88) the sequence of the terms must of course be strictly maintained. The gradient acts to the right on the $\mathbf{r}$-dependent wave function $\psi(\mathbf{r},t)$.

We can transfer the result (2.89) to the more general particle property $B(\mathbf{p})$, for which we assume that it can be written as a polynomial or as an absolutely convergent series with respect to p_x, p_y, p_z:

$$\langle \widehat{B}(\mathbf{p}) \rangle_t \;=\; \int d^3r\, \psi^*(\mathbf{r},t)\, B\left(\frac{\hbar}{i}\nabla_r\right) \psi(\mathbf{r},t)\;, \tag{2.90}$$

$$\widehat{B}(\mathbf{p}) \;\longrightarrow\; B\left(\frac{\hbar}{i}\nabla_r\right)\;. \tag{2.91}$$

Inspecting the average values (2.82), (2.83), (2.88) and (2.90), one recognizes always the same structure: To the physical quantity, which is to be averaged, an operator $\widehat{X}$ is ascribed with special properties, which are still to be discussed in detail. The average value is then given by the expression

$$\langle \widehat{X} \rangle_t = \int d^3r\, \psi^*(\mathbf{r},t)\, \widehat{X}\, \psi(\mathbf{r},t) \tag{2.92}$$

with the prescription of correspondence

$$\widehat{X} = \begin{cases} X(\hat{\mathbf{r}}) \;\longrightarrow\; X(\mathbf{r}), \\ X(\hat{\mathbf{p}}) \;\longrightarrow\; X\left(\frac{\hbar}{i}\nabla_r\right)\;. \end{cases} \tag{2.93}$$

One speaks in this case of the

spatial representation of the operator $\widehat{\mathbf{X}}$.

Let us now recall that we came to these results, at first by trying to represent the expectation value of the momentum $\langle \mathbf{p} \rangle_t$ in the position space. Of course, we could have started just as well with the goal to formulate the expectation value of the particle position $\langle \mathbf{r} \rangle$ in the momentum space, i.e., to express it by $\overline{\psi}(\mathbf{p},t)$. Following exactly the same chain of arguments we would have come to the conclusion that to each physical quantity, which is to be averaged, one has to ascribe an operator $\widehat{Y}$ with the prescription of correspondence

$$\widehat{Y} = \begin{cases} Y(\hat{\mathbf{r}}) \;\longrightarrow\; Y\left(-\frac{\hbar}{i}\nabla_p\right)\;, \\ Y(\hat{\mathbf{p}}) \;\longrightarrow\; Y(\mathbf{p})\;. \end{cases} \tag{2.94}$$

This one calls the

momentum representation of the operator $\widehat{\mathbf{Y}}$.

The average value is now given by the expression

$$\langle \widehat{Y} \rangle_t = \int d^3p\, \overline{\psi}^*(\mathbf{p},t)\, \widehat{Y}\, \overline{\psi}(\mathbf{p},t)\;. \tag{2.95}$$

In particular, it holds for the

position vector in momentum representation

$$\hat{\mathbf{r}} \longrightarrow -\frac{\hbar}{i}\nabla_p \,. \tag{2.96}$$

∇_p is the gradient in the momentum space:

$$\nabla_p \equiv \left(\frac{\partial}{\partial p_x}, \frac{\partial}{\partial p_y}, \frac{\partial}{\partial p_z}\right) \,. \tag{2.97}$$

We recognize once again a complete equivalence of position and momentum representations. The equivalence of the wave functions $\psi(\mathbf{r}, t)$ and $\psi(\mathbf{p}, t)$ we had already seen earlier. The strict symmetry of the two representations of the operators is documented by (2.93) and (2.94). The average values (2.92) and (2.95) are built in both the representations in a formally identical manner. The reason for these symmetries and equivalences is to be seen in the fact that the quantum-mechanical concepts can be formulated in a general and abstract way, independently of any special representation. In this sense, position representation and momentum representation are just two equivalent, concrete realizations of these general concepts, which will be developed extensively and in detail in Chap. 3.

The prescriptions (2.93) and (2.94) can be transferred in combined form to such particle properties, which depend on the position as well as on the momentum:

$$\widehat{F}(\mathbf{r}, \mathbf{p}) \longrightarrow \begin{cases} F\left(\mathbf{r}, \frac{\hbar}{i}\nabla_r\right) : & \textit{spatial representation} \,, \\ F\left(-\frac{\hbar}{i}\nabla_p, \mathbf{p}\right) : & \textit{momentum representation} \,. \end{cases} \tag{2.98}$$

Two equivalent formulations result therewith for the average value of the quantity $\widehat{F}$:

$$\begin{aligned} \langle \widehat{F} \rangle_t &= \int d^3 r \, \psi^*(\mathbf{r}, t) \, F\left(\mathbf{r}, \frac{\hbar}{i}\nabla_r\right) \psi(\mathbf{r}, t) = \\ &= \int d^3 p \, \overline{\psi}^*(\mathbf{p}, t) \, F\left(-\frac{\hbar}{i}\nabla_p, \mathbf{p}\right) \overline{\psi}(\mathbf{p}, t) \,. \end{aligned} \tag{2.99}$$

2.3.2 Non-commutability of Operators

A special peculiarity of Quantum Mechanics establishes, though, that the prescription (2.98) is in this form not yet unique. This peculiarity consists in the non-commutability of certain operators. The so-called

Definition 2.3.1

$$\textbf{commutator:} \quad \left[\widehat{A},\widehat{B}\right]_- = \widehat{A}\,\widehat{B} - \widehat{B}\,\widehat{A}\;, \tag{2.100}$$

built up by the operators $\widehat{A}$ and $\widehat{B}$, can be different from zero and, what is more, can even itself be an operator.

The sequence of operators in general is not arbitrary!

Let us demonstrate this fact by an important example. Since the commutator is built up by operators, we have to let it act on a wave function. Let $\psi(\mathbf{r},t)$ an arbitrarily given wave function:

$$[\widehat{z},\widehat{p}_z]_-\psi(\mathbf{r},t) = \frac{\hbar}{i}\left(z\frac{\partial}{\partial z} - \frac{\partial}{\partial z}z\right)\psi(\mathbf{r},t) = -\frac{\hbar}{i}\psi(\mathbf{r},t)\;.$$

Since that is valid for all ψ, we can read off from this equation the following operator-identity:

$$[\widehat{z},\widehat{p}_z]_- = -\frac{\hbar}{i} = i\hbar\;. \tag{2.101}$$

Corresponding relations can also be derived for the other components. Altogether one therefore finds:

$$\left[\widehat{p}_{x_i},\widehat{x}_j\right]_- = \frac{\hbar}{i}\delta_{ij}\;, \tag{2.102}$$

$$\left[\widehat{p}_{x_i},\widehat{p}_{x_j}\right]_- = \left[\widehat{x}_i,\widehat{x}_j\right]_- = 0 \tag{2.103}$$

$$i,j = 1,2,3\;; \quad x_1 = x, x_2 = y, x_3 = z\;.$$

Later we will see that the non-commutability of operators has something to do with the fact that the corresponding operators are not simultaneously be sharply measurable. Furthermore, we will show in Chap. 3 that (2.102) has a direct relationship to the Heisenberg uncertainty principle (1.5).

The non-commutability of position and momentum operators makes the prescription of correspondence (2.98) ambiguous. Algebraically equivalent forms of the observable $F(\mathbf{r},\mathbf{p})$ can lead indeed, according to (2.98), to different operators. The two one-dimensional examples

$$p_z^2 \longleftrightarrow \frac{1}{z^2}p_z^2z^2$$

are of course algebraically equivalent, but belong, according to the prescription of correspondence (2.98), to two different operators. One finds in spatial representation:

$$p_z^2 \longrightarrow -\hbar^2 \frac{\partial^2}{\partial z^2} ,$$
$$\frac{1}{z^2} p_z^2 z^2 \longrightarrow -\hbar^2 \left(\frac{\partial^2}{\partial z^2} + \frac{4}{z} \frac{\partial}{\partial z} + \frac{2}{z^2} \right) .$$

Such an ambiguity is of course unavoidable, when one builds Quantum Mechanics based on a correspondence to Classical Mechanics, since for the latter all the variables are commutative (interchangeable). One has to supplement (2.98) by additional prescriptions. This will be demonstrated by an important example in the next section.

2.3.3 *Rule of Correspondence*

We have already found in this chapter a series of rather decisive results, which enable us, in principle, to already start with a quantitative discussion of typical quantum-mechanical phenomena. Central scope of work will be, at least preliminarily, the solution of the Schrödinger equation. It is therefore necessary to design a unique and clearly arranged recipe for the setting up of the Schrödinger equation. The following steps are offered by our preliminary considerations:

1. We formulate the physical problem, to be solved, at first by the familiar Classical Hamilton Mechanics, i.e., we construct the corresponding classical Hamilton **function**:

   $$H = H\big(q_1, \ldots, q_s, p_1, \ldots, p_s, t\big) = H(\mathbf{q}, \mathbf{p}, t) .$$

   The q_j are generalized coordinates, the p_j the corresponding canonically conjugated momenta; s is the number of degrees of freedom. For a conservative system, H is identical to the total energy E:

   $$H\big(q_1, \ldots, p_s, t\big) = E . \tag{2.104}$$

2. We ascribe to the classical system a quantum system, whose state is described by a wave function $\psi(q_1, \ldots, q_s, t)$. This is defined in the *configuration space* spanned by the q_j (see Sect. 2.4.1, Vol. 2).
3. Special operators are ascribed to measurable physical properties of the system (*observables*), with distinct, still to be discussed properties. Classical observables

are functions in the phase space, thus are $(\mathbf{q}, \mathbf{p})$-dependent. According to the prescription of correspondence (2.98), now they are operators:

$$A(\mathbf{q}, \mathbf{p}, t) \longrightarrow \widehat{A}\left(q_1, \ldots, q_s, \frac{\hbar}{i}\frac{\partial}{\partial q_1}, \ldots, \frac{\hbar}{i}\frac{\partial}{\partial q_s}, t\right) . \tag{2.105}$$

This holds especially for the Hamilton function which in this sense becomes the Hamilton operator:

$$H(\mathbf{q}, \mathbf{p}, t) \longrightarrow \widehat{H}\left(q_1, \ldots, q_s, \frac{\hbar}{i}\frac{\partial}{\partial q_1}, \ldots, \frac{\hbar}{i}\frac{\partial}{\partial q_s}, t\right) . \tag{2.106}$$

These operators act as special differential operators on the wave function in 2..

4. The energy relation (2.104) is to be multiplied by the wave function ψ and, subsequently, the transition (2.106) is done. The result is the

   time-independent Schrödinger equation

$$\widehat{H}\left(q_1, \ldots, q_s, \frac{\hbar}{i}\frac{\partial}{\partial q_1}, \ldots, \frac{\hbar}{i}\frac{\partial}{\partial q_s}, t\right)\psi\left(q_1, \ldots, q_s, t\right) = \\ = E\psi\left(q_1, \ldots, q_s, t\right) , \tag{2.107}$$

   which we already know from (2.15), but we have *derived* it here in a completely different manner.

5. The special role of energy and time as conjugate variables will engage us further in the following sections. With the further prescription of transformation (2.17),

$$E \longrightarrow i\hbar\frac{\partial}{\partial t} , \tag{2.108}$$

   we come from (2.107) to the **time-dependent Schrödinger equation**.

The problem is therewith completely written up. The next task is to look for mathematical algorithms for solving the Schrödinger equation.

Let us comment on this concept with respect to two important points, in order to preclude sources of mistakes and misunderstandings:

A)

In Classical Hamilton-Mechanics (see Chap. 2, Vol. 2), the choice of the generalized coordinates $q_1, \ldots, q_s$ is arbitrary, only their total number s is fixed. So we find, for instance, that the Hamilton functions, respectively, in Cartesian coordinates,

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(x, y, z) , \tag{2.109}$$

and in spherical coordinates (1.104),

$$H = \frac{1}{2m}\left(p_r^2 + \frac{1}{r^2}p_\vartheta^2 + \frac{1}{r^2\sin^2\vartheta}p_\varphi^2\right) + V(r,\vartheta,\varphi)\ , \tag{2.110}$$

are formally completely different. They lead, however, to the same physical results. Therefore, we can decide ourselves in favour of the one or the other version, only according to certain points of view of expedience.

The freedom in the choice of the generalized coordinates $q_1,\ldots,q_s$ leads, however, with the prescription of correspondence (2.106), to ambiguity in the quantum-mechanical Hamilton **operator**. So it follows with (2.109),

$$\widehat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x,y,z) = -\frac{\hbar^2}{2m}\Delta + V(\mathbf{r})\ , \tag{2.111}$$

while (2.110) yields with the prescription (2.106):

$$\overline{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\vartheta^2} + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right) + V(r,\vartheta,\varphi)\ .$$

This expression is **not** equivalent to (2.111), which one recognizes if one inserts into (2.111) the Laplace operator Δ with respect to spherical coordinates ((2.145), Vol. 3):

$$\begin{aligned}\Delta &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{\vartheta,\varphi}\ ,\\ \Delta_{\vartheta,\varphi} &= \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\ .\end{aligned} \tag{2.112}$$

We overcome this obvious discrepancy by the additional prescription that the correspondence (2.106) is permitted only for Cartesian coordinates. In this sense, $\widehat{H}$ in (2.111) is correct, while $\overline{H}$ is not. After having performed the so-defined prescription of correspondence, then it is of course allowed, if it appears to be convenient, to transform the Laplace operator to any other suitable system of coordinates. We can, for instance, use (2.112) in (2.111). This prescription appears rather random, but so far it has proven to be unambiguous. It can be, by the way, more precisely reasoned, but that exceeds the limits of our ground course in Theoretical Physics.

B)

There is another source for ambiguity in the prescription of correspondence (2.106), which is due to the non-commutability of momentum and position operators, which was already discussed in the last section. In most cases, the Hamilton function, formulated with Cartesian coordinates, consists of a term, which depends only

on the squares of the momenta, and a term, which depends only on the position coordinates. For such terms of course there do not result any difficulties. In some cases, however, there can appear, in addition, expressions of the form

$$p_j f_j(q_1, \ldots, q_s) \ ,$$

which include, linearly, the momenta. According to the rule of correspondence (2.106), the two expressions $p_j f_j$ and $f_j p_j$ would not be equivalent. One therefore agrees to symmetrize such terms **before** the application of the rule of correspondence:

$$p_j f_j(\mathbf{q}) \longrightarrow \frac{1}{2}\big(p_j f_j(\mathbf{q}) + f_j(\mathbf{q}) p_j\big) \ . \tag{2.113}$$

A prominent example of application concerns the charged particle in an electromagnetic field (charge $\bar{q}$; vector potential $\mathbf{A}(\mathbf{r}, t)$; scalar potential $\varphi(\mathbf{r}, t)$). It is described by the Hamilton **function** ((2.39), Vol. 2):

$$H = \frac{1}{2m}\big(\mathbf{p} - \bar{q}\mathbf{A}(\mathbf{r}, t)\big)^2 + \bar{q}\varphi(\mathbf{r}, t) \ . \tag{2.114}$$

By expanding the bracket, the mixed term has to be handled according to (2.113). The rule of correspondence then yields the following Hamilton **operator**:

$$\widehat{H} = \frac{1}{2m}\left[-\hbar^2\Delta - \bar{q}\frac{\hbar}{i}(\mathrm{div}\mathbf{A}(\mathbf{r}, t) + 2\mathbf{A}(\mathbf{r}, t)\cdot\nabla_r) + \bar{q}^2\mathbf{A}^2(\mathbf{r}, t)\right] + \bar{q}\varphi(\mathbf{r}, t) \ . \tag{2.115}$$

2.3.4 Exercises

Exercise 2.3.1 Show that the expectation value

$$\langle \mathbf{p} \rangle_t = \int d^3 r \psi^*(\mathbf{r}, t) \frac{\hbar}{i} \nabla_r \psi(\mathbf{r}, t)$$

is real. The wave function $\psi(\mathbf{r}, t)$ is assumed to be square-integrable.

Exercise 2.3.2 The ground state wave function of the electron in hydrogen atom is:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{\pi a_\mathrm{B}^3}} \exp\left(-\frac{|\mathbf{r}|}{a_\mathrm{B}}\right) \ ; \quad a_\mathrm{B} = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \ .$$

Calculate:

1. $\int d^3r|\psi(\mathbf{r})|^2$,
2. $\langle \mathbf{r} \rangle$; $\langle \mathbf{r}^2 \rangle$; $\Delta r = \sqrt{(\langle \mathbf{r}^2 \rangle - \langle \mathbf{r} \rangle^2)}$,
3. $\langle \mathbf{p} \rangle$; $\langle \mathbf{p}^2 \rangle$; $\Delta p = \sqrt{(\langle \mathbf{p}^2 \rangle - \langle \mathbf{p} \rangle^2)}$,
4. $\Delta r \Delta p$,
5. current density $\mathbf{j}(\mathbf{r})$.

Exercise 2.3.3 Let the wave function of an electron in an excited state of the hydrogen atom be given by:

$$\psi(\mathbf{r}) = \frac{1}{4\sqrt{4\pi a_{\mathrm{B}}^3}} \frac{r}{a_{\mathrm{B}}} \exp\left(-\frac{r}{2a_{\mathrm{B}}}\right) \sin\vartheta \exp(i\varphi) \ .$$

Calculate the current density!

Exercise 2.3.4 Calculate the following commutators:

1. $[p, x^n]_-(n \geq 1)$,
2. $[x^{-1}, p]_-$,
3. $[p^n, x]_-(n \geq 1)$.

Exercise 2.3.5 Calculate the commutators:

1. $\left[x^{-1}, xp\right]_-$
2. $\left[L_x, L_y\right]_-$; $\mathbf{L} = (L_x, L_y, L_z)$ *'angular momentum'*
3. $\left[\mathbf{L}^2, L_z\right]_-$

Exercise 2.3.6

1. Let $F(x)$ be a function of the x-component of the position operator. Show that

$$[p_x, F(x)]_- = \frac{\hbar}{i} \frac{dF(x)}{dx} \ .$$

2. Let $G(p_x)$ be a function of the x-component of the momentum operator. Verify:

$$[G(p_x), x] = \frac{\hbar}{i} \frac{dG(p_x)}{dp_x} \ .$$

Exercise 2.3.7

1. The translation operator $T(\mathbf{a})$ is defined by

$$T(\mathbf{a})\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{a}) \ ,$$

where $\psi(\mathbf{r})$ is an arbitrary wave function. Express $T(\mathbf{a})$ by the momentum operator $\mathbf{p}$.

2. Prove that:

$$T(\mathbf{a})\mathbf{r}T^{-1}(\mathbf{a}) = \mathbf{r} + \mathbf{a} \, .$$

Exercise 2.3.8 The wave function of a particle of mass m is given by:

$$\psi(\mathbf{r}, t) = \frac{1}{(\pi b^2)^{3/4}} \exp\left(-\frac{r^2}{2b^2} - i\frac{\hbar}{2mb^2}t\right)$$

$b = \sqrt{\hbar/m\omega}$ is a constant with the dimension *length* and ω is a fixed frequency: Determine the potential energy $V(\mathbf{r})$ of the particle.

Exercise 2.3.9 Use the momentum representation to formulate the time-independent, one-dimensional Schrödinger equation in the potential

$$V(q) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp \, \bar{V}(p) e^{\frac{i}{\hbar}pq} \, ,$$

i.e., for the wave function $\bar{\psi}(p)$:

$$\bar{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dq \, \psi(q) e^{-\frac{i}{\hbar}pq} \, .$$

Exercise 2.3.10 Show that for a free particle the expectation values of position and momentum fulfill the 'classical' relation

$$\langle \dot{\mathbf{r}} \rangle = \frac{1}{m} \langle \mathbf{p} \rangle \, .$$

Use already at this stage the fact that the Hamilton operator of the free particle

$$H_0 = \frac{p^2}{2m}$$

is a 'Hermitean operator', which means:

$$\int dx \, \varphi^\star(x) \Big(H\psi(x) \Big) = \int dx \, \Big(H\varphi(x) \Big)^\star \psi(x) \, .$$

2.4 Self-Examination Questions

To Section 2.1

1. When, by whom, and in which connection, the idea for the first time, was conceived to ascribe wave properties to matter?
2. In which special manner does the Hamilton-Jacobi theory use the method of canonical transformations?
3. What does one understand by waves of action?
4. Which relationships exist, with respect to absolute value and direction, between particle velocity $\mathbf{v}$ and wave velocity $\mathbf{u}$?
5. Formulate the wave equation of Classical Mechanics!
6. What are the conditions, under which geometrical optics is valid?
7. How does the *eikonal equation* of geometrical optics read?
8. By which simple relations do momentum and energy of the particle fix the frequency and the wavelength of the associated wave of action?
9. Interpret the time-independent Schrödinger equation!
10. What is to be understood by the Hamilton operator of a particle?
11. Which operator is ascribed to the energy variable E when one goes from the time-independent to the time-dependent Schrödinger equation?
12. How can the Bohr postulates be motivated by the use of the wave-picture of matter?
13. How can the wavelength of an electron be experimentally determined?
14. How large must the energy of a neutron be, in order to bring its wavelength into the order of magnitude of a typical lattice constant?
15. On which principle does the electron microscope work?
16. Why is neutron diffraction especially helpful for the investigation of magnetic solids?
17. Analyze the most important differences between electromagnetic waves and matter waves!
18. Can the phase velocity of a matter wave be measured?
19. Discuss the electron diffraction at the double-slit! How does the intensity distribution change, when the two slits are not opened simultaneously, but one after the other for the same period of time?
20. Is it possible, for a single electron in the double-slit experiment, to predict the point of incidence on the detector? Which statements are actually possible?
21. Which reasons contradict a direct identification of the electron as a wave?

To Section 2.2

1. Which physical meaning has to be ascribed to matter waves?
2. Interpret the wave function $\psi(\mathbf{r}, t)$ and the square of its absolute value $|\psi(\mathbf{r}, t)|^2$!

3. Can the Schrödinger equation be mathematically proven?
4. Is the wave function $\psi(\mathbf{r}, t)$ directly measurable?
5. Which kind of mathematical function can at all come into consideration as wave function?
6. How is the probability-current density defined?
7. How does the continuity equation of the probability read? What is its physical statement?
8. Of which mathematical type is the Schrödinger equation?
9. What is a plane wave? Why is it called *'plane'*?
10. How do, in the case of a plane wave, the phase velocity and group velocity differ?
11. Which statements can be made on the position and momentum of a particle, if a plane wave as wave function is ascribed to this particle?
12. What does one understand by a wave packet?
13. With which velocity can information be transported by a wave packet?
14. Why can the phase velocity u even exceed the velocity of light?
15. Illustrate by means of the simple one-dimensional wave packet (2.55), why momentum and position of a particle, which is described by this wave packet, can not be simultaneously exactly known!
16. Does the plane wave violate the uncertainty principle?
17. Explain qualitatively the diffluence of wave packets!
18. When does one speak of *dispersion* in connection with wave packets?
19. Is the diffluence also observed for packets, which are built up by electromagnetic waves?
20. Which connection exists between the diffluence and the Heisenberg uncertainty principle?
21. How are the wave functions in the position space and the momentum space, $\psi(\mathbf{r}, t)$ and $\widehat{\psi}(\mathbf{p}, t)$, related to each other?
22. Which meaning is ascribed to $|\widehat{\psi}(\mathbf{p}, t)|^2$?
23. What do we understand by periodic-boundary conditions?
24. Which statements about position and momentum are really measurable?
25. Formulate the average value $\langle A(\mathbf{r})\rangle$ by means of the wave function $\psi(\mathbf{r}, t)$ and $\widehat{\psi}(\mathbf{p}, t)$, respectively.
26. How is the root mean square deviation defined? Which physical statement can be read off from it?

To Section 2.3

1. Which operator form does the dynamical variable *momentum* take in the spatial representation?
2. How does the momentum representation of the particle position $\mathbf{r}$ read?
3. What is the reason for the formal equivalence of momentum and spatial representation?

4. According to which prescription is the expectation value $\langle F \rangle_t$ of the observable $F(\mathbf{r}, \mathbf{p})$ built in the position space and the momentum space, respectively?
5. How is the commutator of two operators defined?
6. Which value does the commutator $[z, p_z]_-$ have?
7. By which prescription of correspondence does one obtain from a classical variable $A(q_1, \ldots, q_s, p_1, \ldots, p_s)$ the corresponding quantum-mechanical operator?
8. Which operator is attributed to the energy variable E?
9. Is the above-mentioned prescription of correspondence unique in connection with a change of coordinates?
10. Discuss the ambiguity, which results from the non-commutability of position and momentum operators. How does one cure that?
11. How does the Hamilton operator of a charged particle in the electromagnetic field read?

Chapter 3
Fundamentals of Quantum Mechanics (Dirac-Formalism)

In the last chapter it was shown, among other things, that position and momentum representations (see Sect. 2.3.1) are completely equivalent descriptions of Quantum Mechanics. According to the need or expedience we can decide in favor of the one or the other representation. We already argued that the reason for this is that there must exist a super-ordinate and general formulation of Quantum Mechanics, for which the position and momentum representation are merely two of several possible realizations. This super-ordinate structure will be in the focus of this chapter. While we have argued for Quantum Mechanics more or less qualitatively and inductively in Chap. 1, we will now choose the opposite, i.e., the deductive way. We will introduce the fundamental principles axiomatically and derive therewith statements which can be compared with experimental data. This is the so-called Dirac-formalism of Quantum Mechanics.

The task of Quantum Theory, just like the task of any other physical theory, is to predict and to interpret the results of experiments performed on certain physical systems. These results are of course influenced by the *state*, in which the system existed before the measurement. Physical measurements, in general, change the state and thus represent operations on the state. Therefore, the accompanying mathematics must be an operator theory. The possible states of the system are, in an abstract sense, considered as elements (*state vectors*) of a special linear vector space, the so-called Hilbert space (Sect. 3.2.1). In Quantum Theory, the measurable classical dynamical variables become operators (*observables*), which act, according to certain rules, on the vectors of the Hilbert space (Sect. 3.2.2).

After introducing the fundamental concepts *state* and *observable* in Sect. 3.1, we will develop the abstract mathematical structures of Quantum Mechanics (Hilbert space, linear operators, ...) in Sect. 3.2, which, however, would remain worthless without a precise physical interpretation (Sect. 3.3). In particular, the quantum-mechanical *measurement process* has to be linked to the abstract mathematics.

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The fourth section of this chapter is devoted to the dynamics of quantum systems and therefore deals with equations of motion and the time-dependences of the states and observables. With the principle of correspondence in Sect. 3.5 we establish once more the bridge to Classical Mechanics, for instance with the aid of a certain relationship between the classical Poisson bracket (see Sect. 2.4, Vol. 2) and the quantum-mechanical commutator (2.100). At the end of this chapter, we will be able to recognize Schrödinger's wave mechanics, which is already familiar to us, as a special realization of the abstract Dirac formalism (Sect. 3.5.2)

3.1 Concepts

3.1.1 State

We have already met the concept of state in Classical Mechanics (see Sect. 2.4.1, Vol. 2). There we had defined the state as a minimal but complete set of determinants (parameters) which is sufficient to derive from it all properties of the system. Since each mechanical measurand can be written as a function of the generalized coordinates $q_1,\ q_2, \ldots, q_s$ and the generalized momenta $p_1,\ p_2, \ldots, p_s$, the classical state is to be defined as a point $\boldsymbol{\pi}$ in the state space:

classical state

$$|\psi\rangle_{\mathrm{cl}} \Longleftrightarrow \boldsymbol{\pi} \equiv (\mathbf{q},\ \mathbf{p}) \ .$$

The time evolution of the state results from Hamilton's equations of motion ((2.11) and (2.12), Vol. 2):

$$\dot{q}_j = \frac{\partial H}{\partial p_j} \ ; \quad \dot{p}_j = -\frac{\partial H}{\partial q_j} \ ; \quad j = 1, \ldots s \ .$$

These are differential equations of first order, so that with a known Hamilton function $H = H(\mathbf{q}, \mathbf{p}, t)$ the classical trajectory in the phase space $\boldsymbol{\pi}(t)$ is uniquely fixed if only the state $\boldsymbol{\pi}$ is known at a single point of time t_0.

We know already that this way of describing a state of the system by coordinates and momenta can not be taken over for Quantum Mechanics, because q_j and p_j are not simultaneously sharply measurable, i.e., they are not precisely known at the same time. The quantum-mechanical description is therefore in general insufficient to predict, uniquely and precisely, the state of the system for all times. It is not so far-reaching as the classical description and must be content, essentially, to come to probability statements.

But how can we reasonably hallmark a *state* in Quantum Mechanics? That succeeds obviously only when we look for a maximal set of simultaneously sharply measurable quantities, measure them, and use the measured values for the definition of the state. One says:

The simultaneous measurement of a maximal set of 'compatible', i.e., simultaneously measurable, properties 'prepares' a 'pure' quantum-mechanical state $|\psi\rangle$.

For the identification-marking of a quantum-mechanical state we will always use the symbol $|\ldots\rangle$ introduced by Dirac. It is a fundamental assertion of Quantum Mechanics that a still more precise description of the state of the system than that by the so-defined $|\psi\rangle$ is basically impossible. There does not exist any other physical property, which is not simply a function of the aforementioned ones and still could have a sharp value in this state $|\psi\rangle$.

We add some further remarks:

1. The state $|\psi\rangle$, also called *'state vector'* in the following, has no real meaning in the sense of measurability. Together with the still to be discussed operators it *only* allows for the description of experimental processes.
2. The transition $|\psi\rangle \rightarrow \alpha|\psi\rangle$, where α is an arbitrary complex number, does not have any influence on the results of a measurement, i.e., $|\psi\rangle$ and $\alpha|\psi\rangle$ represent the same state.
3. If there are several partial systems interacting with one another, then $|\psi\rangle$ describes the total system.
4. $|\psi\rangle = |\psi(t)\rangle$ will in general change in the course of time, e.g., by external influences or even by measurements on the system.
5. The Schrödinger wave function $\psi(\mathbf{r}, t)$ of the last section is to be understood as special representation of the state of the system, with an explicit accent on the position variable $\mathbf{r}$. There are other representation, which stress the dependence on other quantities (momentum, energy, angular momentum, spin, ...). That is will be investigated in more detail later.

In the next section we want to point out, by use of a simple gedanken-experiment, the preparation of a pure state by measuring. Therewith, amongst others, the considerations in Sect. 3.3 will be set up, by which we will try to get a deeper understanding of the measurement process, which is extremely important for Quantum Mechanics.

3.1.2 Preparation of a Pure State

In Sect. 1.3.2 we have commented on the Stern-Gerlach experiment which gave the first hint on the existence of the electron spin. If one brings a beam of particles with a permanent magnetic moment $\boldsymbol{\mu}$ into a magnetic field, then the directional quantization of the angular momentum $\mathbf{j}$, intimately connected with $\boldsymbol{\mu}$, which we can understand only later, takes care for the fact that the projection j_z of $\mathbf{j}$ on the field direction can take only such discrete values which differ by integer multiples of $\hbar$. If, in addition, the beam traverses an inhomogeneous magnetic field, then the different components of the angular momentum are deflected differently strongly

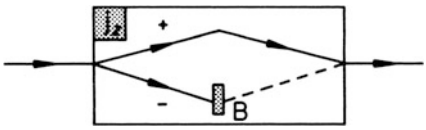

Fig. 3.1 The principle of a measurement, schematically demonstrated by the example of the Stern-Gerlach experiment

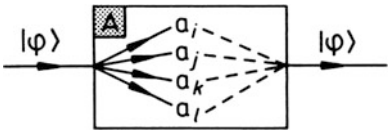

Fig. 3.2 The observable A in its function as separator $T(A)$

(see Sect. 1.3.2). The simplest case, namely the splitting into just two partial beams, is schematically plotted in Fig. 3.1. We imagine that the inhomogeneities of the field are chosen such that the beams, after having traversed the apparatus, come together again. The spatial splitting permits to block one of the two partial beams. It is important to realize that only by the insertion of the blind B a real measurement takes place, because then it is sure that a particle, which traverses the apparatus must be a $(+)$-particle (Fig. 3.1). The $(-)$-component is absorbed in B. Without the blind the sketched *paths* represent only the different possibilities of the particle.

We now want to detach ourselves a bit from the concrete imagination of a Stern-Gerlach apparatus but rather assume, in a gedanken-experiment, that there exists for the (arbitrary) physical property A an analogously working

$$\textbf{separator } T(A) \ .$$

We presume that A, like j_z in the Stern-Gerlach experiment, possesses a *discrete spectrum* $(\ldots, a_i, \ldots, a_j, \ldots)$. That means, it can assume only values a_i, which are *quantized* according to a certain physical point of view (Fig. 3.2). We anticipate here a bit, but we will very soon be able to show that this situation is a typical feature of Quantum Mechanics. The system

$$\textbf{separator } T(A) + \textbf{system of blinds} = \textbf{filter } P(a_i)$$

permits the measurement of the property A and the simultaneous preparation of the state $|a_i\rangle$ (Fig. 3.3). We definitely know that for the particle, which has passed the apparatus, the property A possesses the value a_i. With respect to A it is in a definite state, which is purposefully denoted as $|a_i\rangle$. Now it is possible, however, that by the measurement of A the state of the system is not yet sufficiently precisely determined. If the property B, which can assume the discrete values b_j, is also sharply measurable, simultaneously with A, then the state $|a_i\rangle$, prepared by the filter

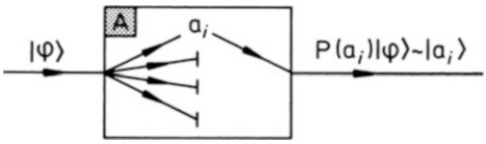

Fig. 3.3 Chematic representation of a filter

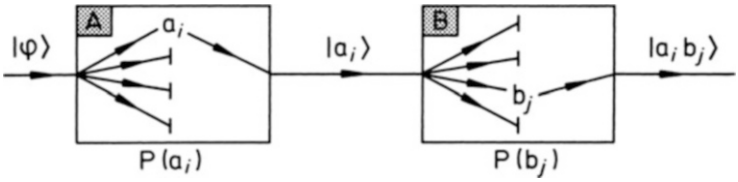

Fig. 3.4 Series connection of two filters

$P(a_i)$, will be still degenerate with respect to the b_j-values. We can remove this uncertainty by letting pass the particle beam through a further filter $P(b_j)$ (Fig. 3.4):

$$P(b_j)\, P(a_i)|\varphi\rangle \sim |a_i\, b_j\rangle \ .$$

This symbol is to be read in such a way that the particle beam in the state $|\varphi\rangle$ successively passes through the filters $P(a_i)$ and $P(b_j)$. After each partial step, in general, the state will have changed. Each filter thus executes an *operation* on the system. We will therefore later represent, abstractly, such a filter by a certain operator. After the beam has traversed both filters it will be in a state, for which the property A as well as the property B have definite values. A and B are, according to the presumption, *compatible* properties. The filters $P(a_i)$ and $P(b_j)$ therefore do not disturb each other, i.e., the partial preparation by the filter $P(a_i)$ will not be modified by the filter $P(b_j)$. This means, on the other hand, that in principle we could have applied them also in the reversed sequence. The respective operations are independent of each other and therefore permutable. Indeed, we will later be able to show explicitly and exactly the assignment:

$$\begin{array}{l} \textit{compatible} \\ \textit{measurands} \end{array} \quad \Longleftrightarrow \quad \begin{array}{l} \textit{interchangeable} \\ \textit{(commuting)} \\ \textit{operators} \ . \end{array}$$

For that, however, we still have to do some preparatory work.

The just described procedure can of course evidently be generalized from two to a maximal set of simultaneously sharply measurable properties. We connect in series correspondingly many filters preparing therewith, as above, a pure state:

pure state

$$|\psi\rangle \equiv |a_i\, b_j \ldots z_m\rangle \sim P(z_m) \cdots P(b_j)\, P(a_i)|\varphi\rangle \ . \tag{3.1}$$

Let us try to get some more information about the so prepared states. The probability that a particle in the state $|\varphi\rangle$ traverses the filter $P(a_i)$ can be expressed and measured via the corresponding intensities $I(a_i)$ and $I(\varphi)$:

$$w(a_i|\varphi) = \frac{I(a_i)}{I(\varphi)} \ . \tag{3.2}$$

$I(\varphi)$ is the intensity impinging on the filter, and $I(a_i)$ is the transmitted intensity. If we connect in series two identical filter, the state prepared by the first filter will be able to pass the second filter in an unimpeded manner (see Fig. 3.5). This means:

$$\begin{aligned} I(a_i,\, a_i) &= I(a_i) \ , \\ w(a_i|a_i) &= 1 \ , \\ P(a_i)\, P(a_i) &= P^2(a_i) = P(a_i) \ , \\ P(a_i)|a_i\rangle &= |a_i\rangle \ . \end{aligned}$$

These results are not only plausible, but correspond also exactly to the experimental observation. The results are similarly evident for the case that we connect in series two identical separators $T(A)$, however, with different blinds (Fig. 3.6). The experiment confirms uniquely that no particle can traverse this combined system of filters. Thus we have to conclude from the last two gedanken-experiments:

$$\begin{aligned} I(a_j,\, a_i) &= \delta_{ij}\, I(a_i) \ , \\ w(a_j|a_i) &= \delta_{ij} \ , \\ P(a_j)\, P(a_i) &= \delta_{ij}\, P(a_i) \ , \\ P(a_j)|a_i\rangle &= \delta_{ij}|a_i\rangle \ . \end{aligned} \tag{3.3}$$

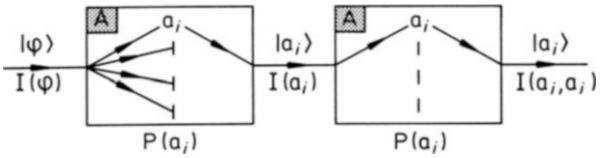

Fig. 3.5 Series connection of two identical filters

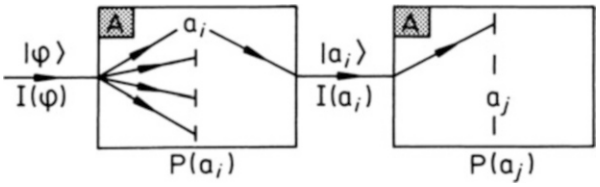

Fig. 3.6 Series connection of two non-identical filters

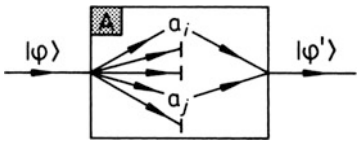

Fig. 3.7 Filter with two apertures for the properties a_i and a_j to define the sum of two filters

The states, prepared via the property A, are said to be *orthogonal*. This fact strongly delimits the type of operators which come into question for the representation of A (Sects. 3.2.6 and 3.3.1).

We have symbolized the series connection of filters as a product of *P-operators*. We still have to define the sum (Fig. 3.7):

$$P(a_i) + P(a_j) \;\Leftrightarrow\; \text{filter with } \textbf{two} \text{ apertures for } a_i \text{ and } a_j \ .$$

When we open all blinds, then nothing happens. That means not only that all particles, which enter the apparatus, will also come out again, but, what is more, the state of the system $|\varphi\rangle$ does not change at all (Fig. 3.2). Subsequent measurements will all yield the same results, independently of whether or not the beam has traversed the separator. This experimental observation, inspected carefully, turns out to be not at all trivial. Classically, the separator $T(A)$ does not absorb any particle, either, but it will change the state of the system, since the originally *disordered* state $|\varphi\rangle$ is an *ordered* one after traversing the A-apparatus. Quantum-mechanically, however, nothing happens. This means:

$$T(A)|\varphi\rangle = \left(\sum_{i=1}^{n} P(a_i)\right)|\varphi\rangle = |\varphi\rangle \ . \tag{3.4}$$

The arbitrarily given state $|\varphi\rangle$ can therefore be written as a linear combination of the states $|a_i\rangle$ ($P(a_i)|\varphi\rangle \sim |a_i\rangle$):

$$|\varphi\rangle = \sum_{i=1}^{n} c_i|a_i\rangle \quad c_i \in \mathbb{C} \ . \tag{3.5}$$

The system of state vectors $|a_i\rangle$ thus turns out to be complete, in the sense that each state $|\varphi\rangle$ can be expanded with respect to the $|a_i\rangle$ as in (3.5). The relation, resulting from (3.4),

$$\sum_{i=1}^{n} P(a_i) = \mathbf{1} \qquad (\textit{identity}) \tag{3.6}$$

will later come across again as the so-called *completeness relation*.

3.1.3 Observables

Quantum-mechanical dynamical variables are often introduced in analogy to classical dynamical variables, although they are quantities of completely different mathematical character. All the classical variables are real and can always be measured so that during the process the course of motion is not disturbed. We remember:

$$\textit{classical dynamical variable } F \iff \textit{phase function } F = F(\mathbf{q}, \mathbf{p}) \ .$$

Examples:

$$\begin{aligned} &\textit{kinetic energy:} && T = T(\mathbf{p}) = \mathbf{p}^2/2\,m \ , \\ &\textit{Hamilton function (= total energy):} && H = H(\mathbf{q}, \mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q}) \ , \\ &\textit{component of the angular-momentum:} && L_z = x\,p_y - y\,p_x \ . \end{aligned}$$

Such phase functions can be *translated* from Classical Mechanics to Quantum Mechanics by the use of the *rules of correspondence*. That we did in Sect. 2.3.3, where it was sufficient to introduce *basic transformations* for the generalized coordinates $\mathbf{q} = (q_1, \ldots, q_s)$ and for the generalized momenta $\mathbf{p} = (p_1, \ldots, p_s)$. All the phase functions $F(\mathbf{q}, \mathbf{p})$ therewith became quantum-mechanical operators $\widehat{F}$. These operators act on the elements of a special vector space, which is associated with the system, and which we will get to know in the next section as the so-called Hilbert space.

There also exist, though, quantum-mechanical dynamical variables (operators) which do not possess a classical analog. Prominent examples are the electron spin and the parity operator. In such cases the corresponding operators must be deduced from the results of respective experiments or from the symmetry properties, respectively. Internal consistency of the mathematical concepts and confirmation of the theoretical conclusions by experimental observations are, thereby, of course the criteria for reasonable definitions of such operators.

All products of non-commutable operators are without classical analogs, even if each single operator of the product has such an analog. As we have already discussed in the Sects. 2.3.2 and 2.3.3., additional prescriptions have to be introduced, *'ad hocly'*.

There exists, among the quantum-mechanical operators, an especially important class, namely, the observables. One defines:

Observable:

quantum-dynamical variable (operator)
with directly observable, real measurable values.

That needs some further explanation. It should be possible to ascribe to each observable A, a measuring equipment (*separator* $T(A)$). This apparatus interacts with the system, which may be in a certain state $|\varphi\rangle$, which, as described in

the last section, is decomposed by the *separator* into orthogonal states $|a_i\rangle$. The measurement takes place by the insertion of blinds (*filters* $P(a_i)$). The possible values a_i, measured by using filters, must be real. The real numerical values a_i as well as the orthogonal states $|a_i\rangle$ are characteristic for the observable A and fix the observable in a unique manner.

Because of these requirements (a_i real; $|a_i\rangle$ orthogonal) only very special types of operators come into question for representing observables. Which kind of operators they are, we can clarify only after we have dealt in the next section with the abstract mathematical framework of Quantum Mechanics. In the section after the next we will further deepen the quantum-mechanical concepts, which were only rudimentarly broached in this section. But that can then already be done on the basis of a complete mathematical formalism.

3.2 Mathematical Formalism

3.2.1 Hilbert Space

The mathematical framework of the Quantum theory is the theory of the Hilbert space which allows for formulating the basics of Quantum Theory generally and independently of special representations. For this purpose we postulate the following mapping:

Postulate:

$$\begin{aligned} \textit{quantum system} &\iff \textit{Hilbert space } \mathcal{H} \ , \\ \textit{pure state} &\iff \textit{Hilbert vector } |\psi\rangle \ . \end{aligned}$$

The Hilbert space $\mathcal{H}$ is defined as an ensemble of elements, which we will call states or state vectors, with the following properties:

Axiom 3.2.1

$$\mathcal{H} \textit{ is a complex, linear vector space!}$$

Two connections are defined for the elements

$$|\alpha\rangle, |\beta\rangle, \ldots, |\varphi\rangle, \ldots, |\psi\rangle, \ldots \in \mathcal{H} \ ,$$

which are closed with respect to $\mathcal{H}$, i.e., the results of these connections are again elements of $\mathcal{H}$:

Addition:

$$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle \equiv |\alpha + \beta\rangle \in \mathcal{H} \ . \tag{3.7}$$

Multiplication:

$$c \in \mathbb{C} \ : \quad c|\alpha\rangle = |\alpha\rangle\, c = |c\,\alpha\rangle \in \mathcal{H} \ . \tag{3.8}$$

The addition is commutative. Furthermore, it holds:

a) Associativity:

$$|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle \ , \tag{3.9}$$

$$c_1,\, c_2 \in \mathbb{C} : \quad (c_1\, c_2)|\alpha\rangle = c_1(c_2|\alpha\rangle) \ . \tag{3.10}$$

b) Zero vector:
There exists an element $|0\rangle \in \mathcal{H}$ with:

$$|\alpha\rangle + |0\rangle = |\alpha\rangle \qquad \forall\, |\alpha\rangle \in \mathcal{H} \ . \tag{3.11}$$

In particular:

$$0|\psi\rangle = |0\rangle \quad \forall\, |\psi\rangle \in \mathcal{H}$$

and

$$c|0\rangle = |0\rangle \quad \forall\, c \in \mathbb{C} \ .$$

c) Inverse element with respect to the addition:
For each element $|\alpha\rangle \in \mathcal{H}$ there exists an *inverse* element $|-\alpha\rangle \in \mathcal{H}$ with:

$$|\alpha\rangle + |-\alpha\rangle = |0\rangle \ . \tag{3.12}$$

We write $|\alpha\rangle + |-\beta\rangle = |\alpha\rangle - |\beta\rangle$ and define therewith the *subtraction* of Hilbert vectors.

d) Distributivity:
With $c,\, c_1,\, c_2 \in \mathbb{C}$ we have:

$$c(|\alpha\rangle + |\beta\rangle) = c|\alpha\rangle + c|\beta\rangle \ , \tag{3.13}$$

$$(c_1 + c_2)|\alpha\rangle = c_1|\alpha\rangle + c_2|\alpha\rangle \ . \tag{3.14}$$

We further list some important concepts:

α) The elements $|\varphi_1\rangle, |\varphi_2\rangle, \ldots, |\varphi_n\rangle$ are called

linearly independent,

if the relation

$$\sum_{\nu=1}^{n} c_\nu |\varphi_\nu\rangle = |0\rangle$$

can be fulfilled only for $c_1 = c_2 = \ldots = c_n = 0$.

β) As *dimension of* $\mathcal{H}$ one denotes the maximal number of linearly independent elements in $\mathcal{H}$. In this sense, $\mathcal{H}$ is infinite-dimensional if there are infinitely many linearly independent elements in $\mathcal{H}$. Infinitely many state vectors are linearly independent, if this is true for each finite subset of them.

Axiom 3.2.2

$\mathcal{H}$ is a unitary vector space!

One could also say that $\mathcal{H}$ is a complex vector space with a scalar product. To each pair of vectors $|\alpha\rangle, |\beta\rangle \in \mathcal{H}$ a

$$\textit{complex number } \langle\alpha|\beta\rangle$$

is assigned with the following properties:

$$\text{a) } \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* \tag{3.15}$$

(* means *complex conjugate*) ,

$$\text{b) } \langle\alpha|\beta_1 + \beta_2\rangle = \langle\alpha|\beta_1\rangle + \langle\alpha|\beta_2\rangle \ , \tag{3.16}$$

$$\text{c) } \langle\alpha|c\,\beta\rangle = c\langle\alpha|\beta\rangle = \langle c^*\alpha|\beta\rangle \quad c \in \mathbb{C} \ , \tag{3.17}$$

$$\text{d) } \langle\alpha|\alpha\rangle \geq 0 \quad \forall|\alpha\rangle \in \mathcal{H}$$

$$= 0 \text{ only for } |\alpha\rangle = |0\rangle \ . \tag{3.18}$$

According to these rules we can perform calculations with the symbol $\langle\alpha|\beta\rangle$, without knowing, what this number really means. The dual vector $\langle\alpha|$ will be introduced later.

Let us connect again a list of some additional remarks:

α) Orthogonality:
$|\alpha\rangle, |\beta\rangle$ are called *orthogonal* if:

$$\langle\alpha|\beta\rangle = 0 \ . \tag{3.19}$$

β) Norm:
As *norm* or *length* of the vector $|\alpha\rangle$ one denotes:

$$\| \alpha \| = \sqrt{\langle\alpha|\alpha\rangle} \ .$$

We will call a vector $|\alpha\rangle$ *normalized* if $\| \alpha \| = 1$.

γ) Schwarz's inequality:

$$|\langle\alpha|\beta\rangle| \leq \| \alpha \| \| \beta \| \ . \tag{3.20}$$

(Proof as Exercise 3.2.2)

δ) Triangle inequality:

$$\big| \| \alpha \| - \| \beta \| \big| \leq \| \alpha + \beta \| \leq \| \alpha \| + \| \beta \| \ . \tag{3.21}$$

(Proof as Exercise 3.2.3)

ε) Convergence:

The sequence $\{|\alpha_n\rangle\}$ converges *strongly* towards $|\alpha\rangle$, if

$$\lim_{n\to\infty} \| \alpha_n - \alpha \| = 0 \tag{3.22}$$

η) Cauchy sequence:

A sequence $\{|\alpha_n\rangle\}$ is called *Cauchy sequence*, if there exists for each $\varepsilon > 0$ an $N(\varepsilon) \in \mathbb{N}$ so that

$$\| \alpha_n - \alpha_m \| < \varepsilon \qquad \forall n, m > N(\varepsilon) \ . \tag{3.23}$$

Each *strongly* converging sequence is also a Cauchy sequence.

If the linear complex vector space $\mathcal{H}$ has a finite dimension n, then the so far discussed Axioms 3.2.1 and 3.2.2 are completely sufficient. Each set of n linearly independent state vectors then represents a basis of $\mathcal{H}$, i.e., each element of $\mathcal{H}$ can be written as a linear combination of these basis states. This one proves as follows:

Let $|\alpha_1\rangle, \ldots, |\alpha_n\rangle$ be linearly independent vectors and $|\beta\rangle$ an arbitrary element of $\mathcal{H}$. Then the vectors

$$|\beta\rangle, |\alpha_1\rangle, \ldots, |\alpha_n\rangle$$

are of course linearly dependent because, otherwise, $\mathcal{H}$ would be $(n+1)$-dimensional. Therefore there exists a set of coefficients

$$(b, a_1, \ldots, a_n) \neq (0, 0, \ldots, 0)$$

with

$$\sum_{j=1}^{n} a_j|\alpha_j\rangle + b|\beta\rangle = |0\rangle \ .$$

We have to further assume that $b \neq 0$ because otherwise it would be

$$\sum_{j=1}^{n} a_j |\alpha_j\rangle = |0\rangle \text{ in spite of } (a_1, \ldots, a_n) \neq (0, \ldots, 0) .$$

In contradiction to our presumption, the $|\alpha_j\rangle$ would then be linearly dependent. With $b \neq 0$ and $c_j = -a_j/b$, however, follows the assertion:

$$|\beta\rangle = \sum_{j=1}^{n} c_j |\alpha_j\rangle . \tag{3.24}$$

The system of the linearly independent basis vectors $|\alpha_j\rangle$ can always be made a complete orthonormal (CON)-system by a standard orthonormalization method (Exercise 3.2.4):

$$\langle \alpha_i | \alpha_j \rangle = \delta_{ij} . \tag{3.25}$$

Then we have in (3.24):

$$c_j = \langle \alpha_j | \beta \rangle . \tag{3.26}$$

Obviously, all the considerations so far are about generalizations of the corresponding features in the real three-dimensional space. They can therefore be illustrated by respective plots as it is demonstrated by an example in Fig. 3.8.

The dimension of $\mathcal{H}$ is of course given by the current quantum system, i.e. ultimately, by the physical assignment. Experience teaches that only seldom one gets by with finite-dimensional spaces. The transition from finite to infinite dimension, however, brings about a lot of mathematical problems, which we can not discuss here all with full accuracy. In any case, we need two additional axioms.

Axiom 3.2.3

$\mathcal{H}$ is separable.

There exists in $\mathcal{H}$ (at least) one, everywhere dense sequence of vectors $|\alpha_n\rangle$.

This axiom states that for even the smallest $\varepsilon > 0$ there exists for each vector $|\psi\rangle \in \mathcal{H}$ at least one $|\alpha_m\rangle$ with $\| \alpha_m - \psi \| < \varepsilon$. The adjective *dense* is important,

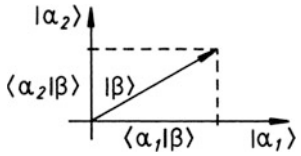

Fig. 3.8 Splitting up a state vector into components with respect to a given basis

according to which the sequence approaches each element from $\mathcal{H}$ arbitrarily closely in the sense of strong convergence. We define a

complete orthonormal system (CON)

as the set M of orthonormal vectors (3.25) of $\mathcal{H}$, for which there does not exist an element in $\mathcal{H}$, which, on the one hand, does not belong to M, but, on the other hand, is orthogonal to all elements of M. The above-mentioned sequence approaches of course also each state vector of the CON-system arbitrarily closely. The terms of a sequence are surely countable. The CON-system thus contains at most countably infinite elements. The orthonormal vectors of the CON-system are of course linearly independent. The Axiom 3.2.3 hence enforces the conclusion that the

dimension of $\mathcal{H}$ is at most countably infinite!

With some *'mathematical effort'* one can further conclude that there always exists a CON-system, which *spans* the full space $\mathcal{H}$. Each vector $|\varphi\rangle \in \mathcal{H}$ can be expanded in terms of this CON-system:

$$|\varphi\rangle = \sum_j c_j |\alpha_j\rangle \; ; \quad c_j = \langle \alpha_j | \varphi \rangle \; . \tag{3.27}$$

Necessary condition for the convergence of this so-called *expansion law* is the convergence of

$$\sum_j |c_j|^2 = \langle \varphi | \varphi \rangle = \| \varphi \|^2 \; . \tag{3.28}$$

The condition is, however, not sufficient. The convergence of (3.27) could lead to a boundary element, which does not belong to $\mathcal{H}$. We therefore need an additional axiom!

Axiom 3.2.4

$\mathcal{H}$ is complete!

Each Cauchy sequence $|\alpha_n\rangle \in \mathcal{H}$ converges to an element $|\alpha\rangle \in \mathcal{H}$.

If a linear unitary vector space still possesses separability and completeness, i.e., that the Axioms 3.2.1–3.2.4 are fulfilled, then this space is called a Hilbert space. For this the expansion law (3.27) holds in any case. For a given basis system, the *components* c_j uniquely mark the state $|\varphi\rangle$. It is, however, of great importance for the further extension of the theory that the state can be expanded in completely different basis systems. Two vectors are considered to be identical, if they, with respect to the same CON-system, agree in all components. The scalar product of two state vectors,

$$|\varphi\rangle = \sum_j c_j |\alpha_j\rangle \; ; \quad |\psi\rangle = \sum_j d_j |\alpha_j\rangle \; ,$$

can be expressed solely by the components:

$$\langle \psi | \varphi \rangle = \sum_j d_j^* \, c_j \; . \tag{3.29}$$

3.2.2 Hilbert Space of the Square-Integrable Functions ($\mathcal{H} = L^2$)

We want to squeeze in an important example of application, in order to demonstrate that the preceding considerations are not to be judged as superfluous *'mathematical playing around'*. We have learned in Chap. 2 that a quantum-mechanical state can be described by a wave function $\psi(\mathbf{r})$, whose possible time-dependence is not interesting at the moment. Because of physical reasons, at first, only

square-integrable functions

$$\int d^3r |\psi(\mathbf{r})|^2 < \infty \tag{3.30}$$

over the unrestricted three-dimensional, real space come into question. One can indeed show that these functions, under certain additional conditions, define a Hilbert space $\mathcal{H} = L^2$.

First we investigate whether they fulfill the Axioms 3.2.1 and 3.2.2, i.e., whether they build a unitary vector space, provided addition (3.7) and multiplication by a complex number (3.8) are fixed as usual for functions. Furthermore, we define the scalar product as follows:

$$\langle \varphi | \psi \rangle = \int d^3r \, \varphi^*(\mathbf{r}) \, \psi(\mathbf{r}) \tag{3.31}$$

We have first to show that the two connections are not running out of the L^2. This is surely guaranteed when with the two arbitrary elements $\psi_1(\mathbf{r})$, $\psi_2(\mathbf{r})$ of the L^2 also the function

$$c_1 \, \psi_1(\mathbf{r}) + c_2 \, \psi_2(\mathbf{r}) \; ; \quad c_1, \, c_2 \in \mathbb{C}$$

will be square-integrable. For this purpose we investigate:

$$\begin{aligned}
&\int d^3r |c_1 \, \psi_1(\mathbf{r}) + c_2 \, \psi_2(\mathbf{r})|^2 \leq \\
&\leq \int d^3r \left\{ |c_1 \, \psi_1(\mathbf{r}) + c_2 \, \psi_2(\mathbf{r})|^2 + |c_1 \, \psi_1(\mathbf{r}) - c_2 \, \psi_2(\mathbf{r})|^2 \right\} = \\
&= 2 \int d^3r \, \left\{ |c_1|^2 \, |\psi_1(\mathbf{r})|^2 + |c_2|^2 \, |\psi_2(\mathbf{r})|^2 \right\} < \infty \; .
\end{aligned}$$

Because $\int d^3r|\psi_{1,2}(\mathbf{r})|^2 < \infty$ it is also true that $|c_{1,2}|^2 \int d^3r\,|\psi_{1,2}(\mathbf{r})|^2 < \infty$. It is not a big problem to verify the Axioms (3.9)–(3.14) of the vector space. As zero element we take the *identically vanishing* function $\psi_0(\mathbf{r}) \equiv 0$, which is trivially square-integrable.

The Axioms (3.15)–(3.18) of the scalar product can also be easily checked with (3.31). However, we still have to give thought to the point, whether the scalar product in the form (3.31) does really exist for **all** elements of the space L^2. Let $\varphi(\mathbf{r})$ and $\psi(\mathbf{r})$ be two arbitrary square-integrable functions. Because of

$$\big(|\varphi(\mathbf{r})| - |\psi(\mathbf{r})|\big)^2 \geq 0 \Longleftrightarrow \big(|\varphi(\mathbf{r})|^2 + |\psi(\mathbf{r})|^2\big) \geq 2|\varphi(\mathbf{r})|\,|\psi(\mathbf{r})| \quad \forall \mathbf{r}$$

we can conclude,

$$\begin{aligned} |\langle\varphi|\psi\rangle| = \left|\int d^3r\,\varphi^*(\mathbf{r})\,\psi(\mathbf{r})\right| &\leq \int d^3r|\varphi(\mathbf{r})|\,|\psi(\mathbf{r})| \leq \\ &\leq \frac{1}{2}\left\{\int d^3r|\varphi(\mathbf{r})|^2 + \int d^3r|\psi(\mathbf{r})|^2\right\} < \infty\,, \end{aligned}$$

what proves the existence of the scalar product. The L^2 is thus indeed a unitary vector space. In particular, the norm for elements of the L^2,

$$\| \psi \| = \left(\int d^3r|\psi(\mathbf{r})|^2\right)^{1/2}\,, \tag{3.32}$$

is a finite quantity and can therefore serve to *normalize the wave function to one* (2.30), according to its probability interpretation:

$$\begin{aligned} &\psi(\mathbf{r}) \qquad \text{arbitrary from } L^2\,, \\ &\widehat{\psi}(\mathbf{r}) = \frac{1}{\| \psi \|}\,\psi(\mathbf{r})\,, \\ &\| \widehat{\psi} \| = 1\,. \end{aligned} \tag{3.33}$$

We got to know the strong convergence (3.22) of the wave functions of the L^2 in ((2.141), Vol. 3) as *convergence in the mean*:

$$\begin{aligned} &\lim_{n\to\infty} \| \psi_n - \psi \| = \lim_{n\to\infty} \int d^3r|\psi_n(\mathbf{r}) - \psi(\mathbf{r})|^2 = 0 \\ &\Longleftrightarrow \{\psi_n(\mathbf{r})\} \text{ converges strongly to } \psi(\mathbf{r})\,. \end{aligned} \tag{3.34}$$

We still have to investigate the L^2 with respect to separability and completeness, i.e., we have to check the Axioms 3.2.3 and 3.2.4. Unfortunately, this part of our investigation will come out a bit unsatisfying. Up to now, we could apply well-known properties of the integral in (3.30). For the two remaining axioms we have to make demands on the fact that the elements of the L^2 are square-integrable functions

in the Lebesgue sense. For a reasonable further discussion, we would have to first introduce precisely the concept of a Lebesgue-integral. This, however, is somewhat beyond the framework of our ground course in Theoretical Physics and does not lead to any new insight for the use-oriented Quantum Mechanics. We will *calculate*, anyway, all occurring integrals always as we have learned it for the Riemann-integral. The Lebesgue-integral is to be thought as a real extension, in order to make also certain *pathological* functions integrable, without changing anything for already Riemann-integrable situations. The in this way *newly-added* square-integrable functions appear as limiting elements of the Riemann-square integrable functions and provide the completeness of the Hilbert space L^2. Details of the proof of this completeness should be taken from the relevant special literature. We have already pointed out in Sect. 2.3.4 of Vol. 3 of the existence of CON-systems of functions of countably-infinite elements, in which square-integrable functions can be expanded ($\rightarrow$ separability). A further important example of a Hilbert space will be discussed as Exercise 3.2.6.

3.2.3 Dual (Conjugate) Space, bra- and ket-Vectors

Sometimes it appears to be convenient, without being absolutely necessary, to assign to the symbol $\langle\varphi|$ in the scalar product (3.15) a self-contained meaning. To each vector $|\varphi\rangle \in \mathcal{H}$ a *dual* vector $\langle\varphi|$ is then ascribed, which, however, does not belong to the space $\mathcal{H}$ of the $|\varphi\rangle$'s, but to a dual space $\mathcal{H}^*$. According to Dirac one uses the notation *bra- and ket-vectors*,

$$\begin{array}{c} \langle\varphi| \quad |\psi\rangle \ , \\ \nwarrow \quad \nearrow \\ \text{bra} - \text{c} - \text{ket} \end{array}$$

since their *product* shall represent the *bra-c-ket* of the scalar product.

Mathematically correctly one introduces the dual space $\mathcal{H}^*$ via linear functionals,

$$F_\varphi(|\psi\rangle) \ ; \quad |\psi\rangle \in \mathcal{H} \ ,$$

of the elements of the space $\mathcal{H}$:

$$\mathcal{H}^* = \left\{F_\varphi \ ; \quad F_\varphi : \mathcal{H} \longrightarrow \mathbb{C} \ ; \quad F_\varphi \text{ linear} \right\} \ . \tag{3.35}$$

Linearity means:

$$\begin{aligned} F_\varphi(c_1|\psi_1\rangle + c_2|\psi_2\rangle) &= c_1\, F_\varphi(|\psi_1\rangle) + c_2\, F_\varphi(|\psi_2\rangle) \\ c_{1,2} \in \mathbb{C} \quad ; \quad |\psi_{1,2}\rangle &\in \mathcal{H} \ . \end{aligned} \tag{3.36}$$

One can easily see that with respect to the connections,

$$F_{\varphi_1+\varphi_2}(|\psi\rangle) = F_{\varphi_1}(|\psi\rangle) + F_{\varphi_2}(|\psi\rangle)\,, \tag{3.37}$$

$$F_{c\,\varphi}(|\psi\rangle) = c^*\,F_{\varphi}(|\psi\rangle)\,; \qquad c \in \mathbb{C}\,, \tag{3.38}$$

$\mathcal{H}^*$ itself is a linear vector space. We recognize now by (3.36) the linearity (3.16), (3.17) of the scalar product with respect to the second factor and by (3.37), (3.38) the *anti-linearity* with respect to the first factor. If we therefore agree upon the notation

$$\begin{aligned} F_\varphi &\equiv \langle\varphi| \qquad (\textit{bra-vector})\,, \\ F_\varphi(|\psi\rangle) &\equiv \langle\varphi|\psi\rangle\,, \end{aligned} \tag{3.39}$$

then the scalar product (3.15) can be formally interpreted as product of one vector of $\mathcal{H}$ and one of $\mathcal{H}^*$.

The bra-vector $\langle\varphi|$ is considered as uniquely defined by the specification of the scalar products $\langle\varphi|\alpha_n\rangle$ of $\langle\varphi|$ with the CON-basis $\{|\alpha_n\rangle\}$ in $\mathcal{H}$. In particular we have:

$$\langle\varphi_1| = \langle\varphi_2| \Longleftrightarrow \langle\varphi_1|\alpha_n\rangle = \langle\varphi_2|\alpha_n\rangle \quad \forall n\,, \tag{3.40}$$

$$\langle\varphi| = \langle 0| \Longleftrightarrow \langle\varphi|\alpha_n\rangle = 0 \quad \forall n\,. \tag{3.41}$$

It follows therewith via

$$|\varphi\rangle = \sum_j |\alpha_j\rangle\langle\alpha_j|\varphi\rangle = \sum_j |\alpha_j\rangle\langle\varphi|\alpha_j\rangle^* \tag{3.42}$$

an explicit relationship between $|\varphi\rangle$ and $\langle\varphi|$. To each $|\varphi\rangle \in \mathcal{H}$ there belongs just one $\langle\varphi| \in \mathcal{H}^*$. In detail, the following assignments are decisive:

$$\begin{gathered} \mathcal{H} \Longleftrightarrow \mathcal{H}^*\,, \\ \underset{\text{(ket-vector)}}{|\varphi\rangle} \Longleftrightarrow \underset{\text{(bra-vector)}}{\langle\varphi|}\,, \\ |\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle \Longleftrightarrow \langle\psi| = c_1^*\langle\psi_1| + c_2^*\langle\psi_2|\,. \end{gathered}$$

We know a prominent example of use from solid state physics. The assignment crystal lattice $\Longleftrightarrow$ reciprocal lattice corresponds to that of dual spaces. Each vector of the reciprocal lattice is uniquely given by the determination of the scalar products of the vector with three linearly independent vectors of the real lattice (see Sect. 1.4.3).

The introduction of the dual space, however, turns out to be not at all necessary for the understanding of elementary Quantum Mechanics. In principle, it is sufficient, simply to interpret $\langle\varphi|\psi\rangle$ as a symbol for the scalar product of the vectors $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$.

3.2.4 Improper (Dirac-)Vectors

For the description of many important quantum features, the restriction to states, which are represented by vectors of the so far introduced Hilbert space, is certainly not sufficient. One has simply to think, e.g., of a position measurement, to which a *continuous* distribution of possible measured values are available. Accordingly, the position states $|\mathbf{r}\rangle$ can not be countable. The axiom of separability is not satisfiable. On the other hand, it is clear that such important observables, as e.g. the position and momentum, can not simply be excluded from a quantum-theoretical treatment. We have to look for a practicable but also unambiguous extension of the Hilbert space. In particular, the scalar product (3.15) and the eminently important expansion law (3.27) are untenable in their present forms. In the case that the physical quantity α has a continuous set of values, the indexing (α_j) makes of course no longer sense. The scalar product $\langle\alpha_j|\varphi\rangle$ will have to be changed into a (in general complex-valued) function $\varphi(\alpha)$ and the sum $\sum_j$ into a corresponding integral.

One therefore introduces, besides the so far discussed *proper* Hilbert vectors, also the so-called *improper* vectors, which are also denoted as *Dirac vectors*. The Hilbert space shall be extended to incorporate also these Dirac vectors. The underlying mathematical idea is, to let the improper states arise from the proper ones by certain limiting processes. This can be schematically illustrated as follows: We first start at a countable orthonormalized set of (proper) vectors $|\alpha_j\rangle$. The index j is always a non-negative integer. We can of course formally also write $|\alpha_{p,\,\Delta p}\rangle$, where p shall be a natural number and $\Delta p = 1$. We build the scalar product with an arbitrary but fixed Hilbert vector $|\psi\rangle$:

$$\langle\alpha_j|\psi\rangle \Longleftrightarrow \langle\alpha_{p,\,\Delta p}|\psi\rangle \ .$$

The absolute values are then real numbers, which one can schematically plot in dependence on j and p, respectively. It results in a *vertical-bar diagram* as represented in Fig. 3.9. We now extend our considerations by assuming that p can take arbitrary real values and Δp can be made arbitrarily small. We thus imagine a *filter* (see Sect. 3.1.2), which is able to continuously change its spectrum in dependence of a certain parameter. The limiting process $\Delta p \to 0$,

$$\psi(p) = \lim_{\Delta p \to 0} \frac{\langle\alpha_{p,\,\Delta p}|\psi\rangle}{\sqrt{\Delta p}} \ ,$$

then defines a continuous function of the variable p, which can be interpreted as scalar product

$$\psi(p) = \langle\overline{\alpha}_p|\psi\rangle$$

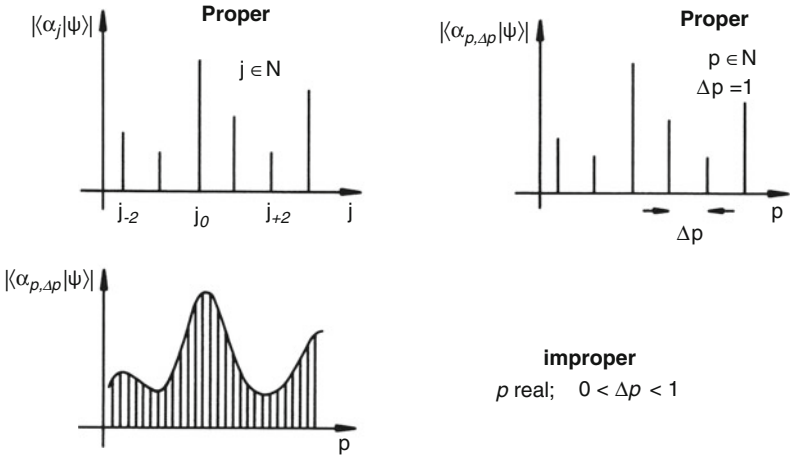

Fig. 3.9 Schematic spectral representation of a proper state for the explanation of the limiting process to an improper Dirac state

between $|\psi\rangle$ and the formal Dirac vector

$$|\overline{\alpha}_p\rangle = \lim_{\Delta p \to 0} \frac{|\alpha_{p,\,\Delta p}\rangle}{\sqrt{\Delta p}} \,. \tag{3.43}$$

Now we can rewrite the expansion law (3.27) by use of such Dirac vectors:

$$\begin{aligned} |\psi\rangle &= \lim_{\Delta p \to 0} \sum_p |\alpha_{p,\,\Delta p}\rangle \langle \alpha_{p,\,\Delta p}|\psi\rangle \\ &= \lim_{\Delta p \to 0} \sum_p \frac{|\alpha_{p,\,\Delta p}\rangle}{\Delta p} \frac{\langle \alpha_{p,\Delta p}|\psi\rangle}{\Delta p} \Delta p \\ &= \lim_{\Delta p \to 0} \sum_p |\overline{\alpha}_p\rangle \langle \overline{\alpha}_p|\psi\rangle \, \Delta p \,. \end{aligned}$$

We thus have, in comparison to (3.27), as supposed, to replace the sum by a Riemann-integral :

$$|\psi\rangle = \int dp \, |\overline{\alpha}_p\rangle \langle \overline{\alpha}_p|\psi\rangle \,. \tag{3.44}$$

Multiplying this expression from the left side by the bra-vector $\langle \overline{\alpha}_{p'}|$ we get a relation,

$$\langle \overline{\alpha}_{p'}|\psi\rangle = \int dp \, \langle \overline{\alpha}_{p'}|\overline{\alpha}_p\rangle \langle \overline{\alpha}_p|\psi\rangle \,,$$

which for arbitrary $|\psi\rangle$ can be fulfilled only by

$$\langle\overline{\alpha}_{p'}|\overline{\alpha}_p\rangle = \delta(p'-p)\ . \tag{3.45}$$

This important relation states that

improper (Dirac) vectors are normalized to δ-functions.

In Sect. 1.1 of Vol. 3 we got to know the properties of Dirac's δ-function. The reader should assure himself of being still familiar with them. In the orthonormalization-condition (3.45) the Kronecker delta (3.25), valid for proper state vectors, is replaced by the δ-function, i.e., by a distribution. That formally means that Dirac vectors possess an infinitely large norm (*length*), but, otherwise also, that even arbitrarily closely neighboring vectors are orthogonal to each other. Dirac vectors thus can not be genuine Hilbert vectors.

One can apply the expansion law (3.44) of course also for the representation of the vector $|\alpha_{p,\,\Delta p}\rangle$:

$$\begin{aligned}|\alpha_{p,\,\Delta p}\rangle &= \int dp'\,|\overline{\alpha}_{p'}\rangle\langle\overline{\alpha}_{p'}|\alpha_{p,\,\Delta p}\rangle \\ &= \int\limits_{p-\frac{1}{2}\Delta p}^{p+\frac{1}{2}\Delta p} dp'\,|\overline{\alpha}_{p'}\rangle\langle\overline{\alpha}_{p'}|\alpha_{p,\,\Delta p}\rangle\ .\end{aligned}$$

Because of the orthogonality of the scalar product in the integrand we can choose the integration limit as given in the second line. For sufficiently small Δp one can still replace, because of (3.43), $\langle\overline{\alpha}_{p'}|\alpha_{p,\,\Delta p}\rangle$ by $1/\sqrt{\Delta p}$:

$$|\alpha_{p,\Delta p}\rangle \to \mathrm{ED}(\overline{\alpha}_p) = \underbrace{\frac{1}{\sqrt{\Delta p}}\int_{p-\frac{1}{2}\Delta p}^{p+\Delta p} dp'|\overline{\alpha}_{p'}\rangle}_{\text{'eigen-differential of } |\overline{\alpha}_p\rangle\text{'}} \tag{3.46}$$

The reverse obviously reads:

$$|\overline{\alpha}_p\rangle = \lim_{\Delta p\to 0}\frac{1}{\sqrt{\Delta p}}\,\mathrm{ED}(\overline{\alpha}_p)$$

This expression has to be compared with (3.43).

Although the Dirac vectors $|\overline{\alpha}_p\rangle$ are not proper elements of the Hilbert space, the eigen-differentials do fulfill all the axioms of the Hilbert space. In particular, they are normalizable:

$$\langle \mathrm{ED}\,(\overline{\alpha}_p)|\mathrm{ED}\,(\overline{\alpha}_p)\rangle = \frac{1}{\Delta p}\iint\limits_{p-\frac{1}{2}\Delta p}^{p+\frac{1}{2}\Delta p} dp'\,dp''\,\langle\overline{\alpha}_{p'}|\overline{\alpha}_{p''}\rangle$$

$$= \frac{1}{\Delta p}\iint\limits_{p-\frac{1}{2}\Delta p}^{p+\frac{1}{2}\Delta p} dp'\,dp''\,\delta(p'-p'') = 1\ .$$

When we have got a Dirac vector $|\overline{\alpha}_p\rangle$ by procedures, which are still to be learned, then we find, by insertion into (3.46) and an integration over an interval of the width Δp, with the eigen-differential a *correct* Hilbert vector. In this sense, we agree upon the following definition:

'Extended' Hilbert space = set of the proper and the improper state vectors

When there is no possibility of confusion, we will use the same symbols for both the proper and the improper vectors. We therefore omit in the following the bars on the Dirac vectors (3.43). In particular, we mark the *extended* Hilbert space, too, by the symbol $\mathcal{H}$.

In order to be able to formulate the expansion law in its most general statement,

$$|\varphi\rangle = \sum\!\!\!\!\!\!\int_j |\alpha_j\rangle\langle\alpha_j|\varphi\rangle\ , \tag{3.47}$$

we introduce a new sign:

$$\sum\!\!\!\!\!\!\int_j \Longleftrightarrow \begin{cases} \sum_j & : \text{proper states} \\ \int dj & : \text{improper states} \\ \sum_j \ldots + \int dj \ldots & : \text{proper as well as improper states} \end{cases} \tag{3.48}$$

That avoids a troublesome case-by-case analysis. Analogously one can use

$$\delta(i,j) \Longleftrightarrow \begin{cases} \delta_{ij} & : \text{discrete} \\ \delta(i-j) & : \text{continuous} \end{cases} \tag{3.49}$$

to combine the orthonormalization conditions (3.25) and (3.45):

$$\langle\alpha_i|\alpha_j\rangle = \delta(i,j)\ . \tag{3.50}$$

3.2.5 *Linear Operators*

The Quantum Mechanics deals with the results of physical measurements, which in turn are to be considered as *operations* (*manipulations*) on the given states of the system. On the therewith arising central role of the operators, we have already reflected in Sect. 3.1.3. We have to now place this such an important concept of the *operator* in the theory developed so far. How do operators act on the states of the Hilbert space?

Definition 3.2.1 (Operator A**)** *Mapping relation, which assigns to each element* $|\alpha\rangle$ *from the partial set* $D_A \subseteq \mathcal{H}$ *uniquely an element* $|\beta\rangle \in W_A \subseteq \mathcal{H}$*:*

$$|\beta\rangle = A|\alpha\rangle = |A\,\alpha\rangle \ . \tag{3.51}$$

One denotes D_A as the *domain of definition of* A; the set of all $|\beta\rangle$ is called the *co-domain* W_A *of* A. In what follows we want to mark operators by capital letters, leaving out, however, the previously used ($\widehat{\ }$) above the capital letters, at least as long as there is no possibility of confusion.

We see that for the fixing of an operator two ingredients are necessary, since the domain of definition as well as the mapping relation must be known. Consequently, two operators A_1 and A_2 are considered as to be identical, if they have the same domain of definition, and if it is for all $|\alpha\rangle \in D_{A_1} = D_{A_2}$:

$$A_1|\alpha\rangle = A_2|\alpha\rangle \ .$$

This is then written shortly as an operator identity:

$$A_1 = A_2 \ .$$

Sum and product, we have already pointed up in Sect. 3.1.2:

$$(A_1 + A_2)|\alpha\rangle = A_1|\alpha\rangle + A_2|\alpha\rangle \ ; \qquad |\alpha\rangle \in D_{A_1} \wedge D_{A_2} \ , \tag{3.52}$$

$$(A_1\,A_2)|\alpha\rangle = A_1(A_2|\varphi\rangle) \ . \tag{3.53}$$

The domain of definition of A_1 in (3.53) must contain the co-domain of A_2. Only in exceptional cases ($\rightarrow$ *commutable operators*), the order of the operators is arbitrary. Operators are normally non-commutable. We have already analyzed this issue in Sect. 2.1.3.

The zero operator $\widehat{0}$ maps each vector to the zero vector:

$$\widehat{0}|\alpha\rangle = |0\rangle \qquad \forall |\alpha\rangle \in \mathcal{H} \ . \tag{3.54}$$

The identity (unit) operator $\mathbb{1}$ transfers each element into itself:

$$\mathbb{1}\,|\alpha\rangle = |\alpha\rangle \qquad \forall |\alpha\rangle \in \mathcal{H}\ . \tag{3.55}$$

To each operator there belongs an adjoint operator A^+, which is defined as follows:

Definition 3.2.2 (To A Adjoint Operator A^+)

1. D_{A^+}: Set of all $|\gamma\rangle \in \mathcal{H}$, for which a $|\overline{\gamma}\rangle \in \mathcal{H}$ exists with:

$$\langle\gamma|A|\alpha\rangle = \langle\overline{\gamma}|\alpha\rangle \qquad \forall |\alpha\rangle \in D_A\ .$$

2. Mapping condition:

$$A^+|\gamma\rangle = |\overline{\gamma}\rangle\ .$$

Let us draw from this definition some **conclusions**:

a) Let be $|\alpha\rangle \in D_A$ and $|\gamma\rangle \in D_{A^+}$, then it is:

$$\langle\gamma|A|\alpha\rangle = \langle\alpha|A^+|\gamma\rangle^*\ , \tag{3.56}$$

because:

$$\langle\gamma|A|\alpha\rangle = \langle\overline{\gamma}|\alpha\rangle = \langle\alpha|\overline{\gamma}\rangle^* = \langle\alpha|A^+|\gamma\rangle^*\ .$$

b) By the assignment

$$|\overline{\alpha}\rangle = A|\alpha\rangle = |A\,\alpha\rangle \Longleftrightarrow \langle\overline{\alpha}| = \langle\alpha|A^+ = \langle A\,\alpha| \tag{3.57}$$

A^+ acts in the dual space $\mathcal{H}^*$ just as A does in $\mathcal{H}$!

c) For *suitable* domains of definition, which from now on we will no longer indicate explicitly, if they are obvious, the following operator identity is valid:

$$(A^+)^+ = A\ . \tag{3.58}$$

Proof

$$\langle\gamma|A|\alpha\rangle = \langle\alpha|A^+|\gamma\rangle^* = (\langle\gamma|(A^+)^+|\alpha\rangle^*)^* = \langle\gamma|(A^+)^+|\alpha\rangle\ .$$

d) The adjoint operator of a product $A\,B$ of two operators A and B is calculated according to the formula:

$$(A\,B)^+ = B^+\,A^+\ . \tag{3.59}$$

One has to pay attention to the sequence of the operators on the right-hand side!

Proof

$$\langle\gamma|(A\,B)|\alpha\rangle \overset{(3.56)}{=} \langle\alpha|(A\,B)^+|\gamma\rangle^* \ ,$$

$$\langle\gamma|(A\,B)|\alpha\rangle \overset{(3.57)}{=} \langle A^+\gamma|B|\alpha\rangle = \langle B^+A^+\gamma|\alpha\rangle =$$

$$= \langle\alpha|B^+A^+\gamma\rangle^* = \langle\alpha|B^+A^+|\gamma\rangle^* \ .$$

By comparison one recognizes the assertion!

e) One verifies, similarly easily, two further identities:

$$(A+B)^+ = A^+ + B^+ \ , \tag{3.60}$$

$$(c\,A)^+ = c^*A^+; \quad c \in \mathbb{C} \ . \tag{3.61}$$

From the whole group of thinkable operators, only a certain subclass is relevant for Quantum Mechanics, namely the linear operators:

Definition 3.2.3 (Linear Operator A)

1. D_A linear subspace of $\mathcal{H}$.
2. For arbitrary $|\alpha_1\rangle,\ |\alpha_2\rangle \in D_A$ and $c_1, c_2 \in \mathbb{C}$ it holds:

$$A(c_1|\alpha_1\rangle + c_2|\alpha_2\rangle) = c_1\,A|\alpha_1\rangle + c_2\,A|\alpha_2\rangle \ .$$

We will explain in the next section why among the linear operators a further special subclass stands out. These are the Hermitian operators, which we will later identify with the quantum-mechanical observables (Sect. 3.1.3).

Definition 3.2.4 (Hermitian Operator A)

1. $D_A = D_{A^+} = \mathcal{H}$.
2. $A|\alpha\rangle = A^+|\alpha\rangle \qquad \forall|\alpha\rangle \in \mathcal{H}$,
   short: $A = A^+$.

In Sect. 3.2.6 we will deal with the properties of Hermitian operators, which are decisively important for Quantum Mechanics. Before that, let us still add two further definitions:

Definition 3.2.5 (Bounded Operator) There exists a $c > 0$, such that

$$\| A\,\alpha \| \leq c \ \| \alpha \| \qquad \forall|\alpha\rangle \in D_A \ .$$

Definition 3.2.6 (Continuous Operator A) For each sequence $\{|\alpha_n\rangle\} \longrightarrow |\alpha\rangle$ it holds:

$$\{A|\alpha_n\rangle\} \longrightarrow A|\alpha\rangle \ .$$

3.2.6 Eigen-Value Problem

A linear operator A assigns to a vector $|\alpha\rangle \in D_A$ another vector $|\beta\rangle \in \mathcal{H}$. A typical object of Quantum Mechanics presents, in this sense, a special case. An exceptional position, in particular with respect to the subsequent physical interpretation, is taken by those elements $|a\rangle$ of the domain of definition, which, after the application of the operator A, change into vectors *parallel* to them. The task to find these special vectors is called an *eigen-value problem* (Fig. 3.10). They are solutions of the *eigen-value equation*:

$$A|a\rangle = a|a\rangle \ . \tag{3.62}$$

a is the (in general complex) *eigen-value* and $|a\rangle$ the corresponding *eigen-vector* of the operator A. The whole ensemble of all possible eigen-values defines the *spectrum* of A, which can be discrete (finite or countably infinite) as well as continuous. If $|a\rangle$ is a proper Hilbert vector, the spectrum will be certainly discrete with, at most, countably infinite eigen-states and eigen-values (axiom of separability). If there are for one and the same eigen-value a more than one linearly independent eigen-states, then one says that a is *degenerate*. One denotes the maximal number of linearly independent eigen-states with the same eigen-value as the *degree of degeneracy*. Any linear combination of these eigen-states is then of course also an eigen-state with the same eigen-value. Therefore, these linearly independent states span a subspace of $\mathcal{H}$, the so-called *eigen-space to a*, whose dimension of course agrees with the degree of degeneracy. One can make them, with one of the usual orthogonalization methods (Exercise 3.2.4), a CON-basis of the eigen-space.

The eigen-value equations of Hermitian operators are of outstanding importance, since we will identify these operators in the next section, by postulate, with the observables of the system, where their eigen-values represent the possible measured values. The central mathematical exercise therefore consists in solving (3.62), i.e., in determining the eigen-values and eigen-states of specific linear Hermitian operators, predetermined by the physical situation at hand. The results are of course specific for

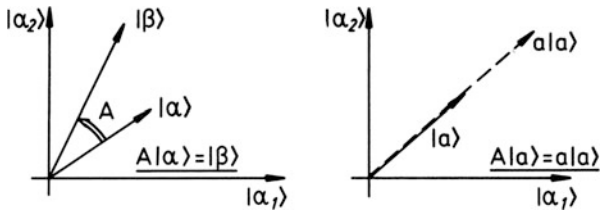

Fig. 3.10 Graphical representation of the action of a linear operator on a state vector, to the *left*: general, to the *right*: the special case of an eigen-vector

the respective operator.There are, however, some very important properties, which are valid **for all Hermitian operators**:

1) Expectation values are always real

Let be $|\alpha\rangle,\ |\beta\rangle \in D_A = \mathcal{H}$. Because of $A = A^+$ it follows from (3.56):

$$\langle\alpha|A|\beta\rangle = \langle\beta|A|\alpha\rangle^* \ . \tag{3.63}$$

But then $\langle\alpha|A|\alpha\rangle$ must be real!

2) Eigen-values are real

For the eigen-value a of the observable A it holds according to (3.62):

$$a = \frac{\langle a|A|a\rangle}{\langle a|a\rangle} \ . \tag{3.64}$$

Numerator and denominator are real, thus also a.

3) Eigen-states are orthogonal

a) without degeneracy

In the expression

$$A|a_i\rangle = a_i|a_i\rangle$$

the state vector $|a_i\rangle$. It is with a discrete index i a proper Hilbert vector, and with a continuous index i, it is an improper Dirac vector. If now $i \neq j$, then:

$$\begin{aligned}\langle a_i|A|a_j\rangle &= a_j\langle a_i|a_j\rangle = (\langle a_j|A|a_i\rangle)^* = \\ &= a_i^*\ \langle a_j|a_i\rangle^* \overset{2)}{=} a_i\langle a_i|a_j\rangle \ .\end{aligned}$$

The assertion is now fulfilled because $a_i \neq a_j$:

$$(a_i - a_j)\langle a_i|a_j\rangle = 0 \Longrightarrow \langle a_i|a_j\rangle = 0 \ .$$

b) with degeneracy

For eigen-states from different eigen-spaces the line of argument is the same as in a). Within the same eigen-space, however, the very last step is no longer valid conclusively, because $a_i = a_j$. But we can always orthonormalize the linearly independent basis states of the eigen-space to a_i. If we take these as the eigen-states, in the spirit of 3), then the assertion follows, in this case also.

4) Eigen states build a CON-basis

We have seen that the proper and the improper eigen-states of a Hermitian operator can be orthonormalized:

$$\langle a_i | a_j \rangle = \delta(i,j) \; . \tag{3.65}$$

They therewith fulfill a necessary condition for being recognized as basis of the Hilbert space $\mathcal{H}$. This condition becomes sufficient, however, only if we can prove its completeness. To show this for arbitrary Hermitian operators is in general a non-trivial problem, which we want to assume here always as somehow solved. Under this presumption we can then write for an arbitrary state $|\psi\rangle \in \mathcal{H}$:

$$|\psi\rangle = \sum\!\!\!\!\!\!\int_j |a_j\rangle \langle a_j | \psi \rangle \; . \tag{3.66}$$

We now let the operator A act on this state and exploit its eigen-value equation:

$$A|\psi\rangle = \sum\!\!\!\!\!\!\int_j a_j |a_j\rangle \langle a_j | \psi \rangle \; . \tag{3.67}$$

Since that is valid for **all** $|\psi\rangle \in \mathcal{H}$, there follows the important operator identity:

Spectral representation:

$$A = \sum\!\!\!\!\!\!\int_j a_j |a_j\rangle \langle a_j| \; . \tag{3.68}$$

In particular; we can express the completeness of the eigen-states of the Hermitian operator A as assumed in (3.66), because of $|\psi\rangle = \mathbb{1}|\psi\rangle$, by a special representation of the unit operator $\mathbb{1}$:

Completeness relation:

$$\mathbb{1} = \sum\!\!\!\!\!\!\int_j |a_j\rangle \langle a_j| \; . \tag{3.69}$$

The Eqs. (3.68) and (3.69) turn out to be extremely useful for the explicit execution of many quantum-mechanical calculations. One can, for instance, insert the $\mathbb{1}$-operator into operator equations and vector equations, respectively, at arbitrary positions without violating the validity of the equation. If one writes *the identity* $\mathbb{1}$ in the form of the right-hand side of Eq. (3.69), then it is possible that by this *trick*, which is usually called *'insertion of intermediate states'*, a completely new way of solution opens up. Two examples, important for later considerations, are mentioned here. The first will be helpful for us in Sect. 3.3 in connection with the physical interpretation of the quantum-mechanical postulates. It concerns the expectation

value of the Hermitian operator A in the state $|\psi\rangle$:

$$\begin{aligned}\langle\psi|A|\psi\rangle &= \langle\psi|\mathbb{1}\,A\,\mathbb{1}|\psi\rangle = \\ &= \sum_i \sum_j \langle\psi|a_i\rangle\langle a_i|A|a_j\rangle\langle a_j|\psi\rangle = \\ &= \sum_i \sum_j a_j\langle\psi|a_i\rangle\langle a_i|a_j\rangle\langle a_j|\psi\rangle = \\ &= \sum_i a_i\langle\psi|a_i\rangle\langle a_i|\psi\rangle \ .\end{aligned}$$

We have used here the eigen-value equation of the operator A and (3.65). We see that the expectation value of A can be expressed by the eigen-values a_i, which, however, get weight factors, determined by the *components* of the state vector $|\psi\rangle$ with respect to the eigen-states $|a_i\rangle$:

$$\langle\psi|A|\psi\rangle = \sum_i a_i|\langle a_i|\psi\rangle|^2 \ . \tag{3.70}$$

At a later stage, we will have to analyze this expression physically more precisely.

The second example leads to a practical method of solution for eigen-value problems. We assume a discrete basis system $|\varphi_n\rangle$ and try to find the eigen-values and eigen-states of the linear Hermitian operator A. We extend the eigen-value equation

$$A|a\rangle = a|a\rangle$$

by inserting the identity (3.69):

$$\begin{aligned}\mathbb{1}\,A\,\mathbb{1}|a\rangle &= a\mathbb{1}\,|a\rangle \\ \Longrightarrow \sum_{n,n'} |\varphi_n\rangle\langle\varphi_n|A|\varphi_{n'}\rangle\langle\varphi_{n'}|a\rangle &= a\sum_n |\varphi_n\rangle\langle\varphi_n|a\rangle \ .\end{aligned}$$

The $|\varphi_n\rangle$ are linearly independent (CON-system). Therefore, it must even hold:

$$\sum_{n'} \left(\langle\varphi_n|A|\varphi_{n'}\rangle - a\,\delta_{n\,n'}\right)\langle\varphi_{n'}|a\rangle = 0 \qquad \forall n \ . \tag{3.71}$$

This is obviously a homogeneous, finite or countably infinite, linear system of equations. According to ((1.224), Vol. 1) non-trivial solution can be expected only when the secular determinant vanishes:

$$\det\left(\langle\varphi_n|A|\varphi_{n'}\rangle - a\,\delta_{n\,n'}\right) \stackrel{!}{=} 0 \ . \tag{3.72}$$

In the case of calculable terms $\langle\varphi_n|A|\varphi_{n'}\rangle$ (*matrix elements*), the eigen-values a_i can be derived from this condition. Then we can calculate with (3.71) for each a_i the components $\langle\varphi_{n'}|a_i\rangle$ and therewith via (3.66) the eigen-state $|a_i\rangle$ which belongs to a_i.

The case of a continuous spectrum is not so clearly laid out. Instead of (3.71) an integral equation is now to besolved:

$$\int dn' \, \langle\varphi_n|A|\varphi_{n'}\rangle\langle\varphi_{n'}|a\rangle = a\langle\varphi_n|a\rangle \; . \tag{3.73}$$

We want to close this section with the proof of an important theorem:

Theorem 3.2.1 *The linear, Hermitian operators A and B are commutable,*

$$[A, B]_- = A\,B - B\,A = 0 \; , \tag{3.74}$$

if and only if they possess a common CON-system $|\varphi_n\rangle$ *as eigen-states.*

Proof

1. We assume that A and B possess the same eigen-states $|\varphi_n\rangle$:

$$\begin{aligned} A|\varphi_n\rangle &= a_n|\varphi_n\rangle \; ; \\ B|\varphi_n\rangle &= b_n|\varphi_n\rangle \; . \end{aligned}$$

Let $|\psi\rangle$ be an arbitrary vector in $\mathcal{H}$. Then we have:

$$\begin{aligned} |\psi\rangle &= \sum\!\!\!\!\!\!\int_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle \\ \Longrightarrow A\,B|\psi\rangle &= \sum\!\!\!\!\!\!\int_n A\,b_n|\varphi_n\rangle\langle\varphi_n|\psi\rangle = \sum\!\!\!\!\!\!\int_n b_n\,A|\varphi_n\rangle\langle\varphi_n|\psi\rangle \\ &= \sum\!\!\!\!\!\!\int_n b_n\,a_n|\varphi_n\rangle\langle\varphi_n|\psi\rangle \; . \end{aligned}$$

Analogously one finds:

$$B\,A|\psi\rangle = \sum\!\!\!\!\!\!\int_n a_n\,b_n|\varphi_n\rangle\langle\varphi_n|\psi\rangle \; .$$

Because of identical spectral representations we can conclude:

$$A\,B = B\,A \; .$$

2. Let $A\,B = B\,A$ and furthermore $A|\varphi_n\rangle = a_n|\varphi_n\rangle$. But then it follows also:

$$A\,B|\varphi_n\rangle = B\,A|\varphi_n\rangle = a_n\,B|\varphi_n\rangle \ .$$

If we exclude degeneracy, then this equation means that $B|\varphi_n\rangle$ must be an eigen-state of A with the eigen-value a_n. This has the consequence:

$$B|\varphi_n\rangle \sim |\varphi_n\rangle \Longleftrightarrow B|\varphi_n\rangle = b_n|\varphi_n\rangle$$

Commutable operators therefore have the same set of eigen-states! Note that our conclusion holds only if there is no degeneracy.

3.2.7 Special Operators

We introduce in this section some special operators, which are important for subsequent considerations, and list their properties in note form:

1) Dyadic product

The spectral representation (3.68) has already shown that one can build up operators by states. The simplest case of this kind is the dyadic product of two states $|\alpha\rangle,\ |\beta\rangle \in \mathcal{H}$:

$$D_{\alpha\,\beta} \equiv |\alpha\rangle\langle\beta| \ . \tag{3.75}$$

This, of course, must not be confused with the scalar product $\langle\alpha|\beta\rangle$, which is a number, not an operator. The application of $D_{\alpha\,\beta}$ to any state vector $|\psi\rangle \in \mathcal{H}$ yields a state, parallel to $|\alpha\rangle$ and with a length modified by a factor $|\langle\beta|\psi\rangle|$.

The order of the states in $D_{\alpha\,\beta}$ is not commutable. It rather holds (Exercise 3.2.8):

$$(|\alpha\rangle\langle\beta|)^{+} = |\beta\rangle\langle\alpha| \ . \tag{3.76}$$

Let $|a_n\rangle$ be the eigen-states of a Hermitean operator, which build a CON-system. Then we can use the completeness relation (3.69) in order to represent an arbitrary operator X by dyadic products:

$$X = X\,\mathbb{1} = \sum_j X|a_j\rangle\langle a_j| = \sum_j |X\,a_j\rangle\langle a_j| \ . \tag{3.77}$$

The state $|X\,a_j\rangle$ is of course in general not parallel to $|a_j\rangle$.

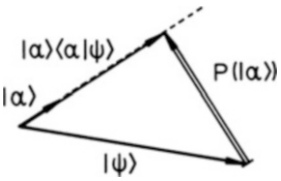

Fig. 3.11 Mode of action of the projection operator

2) Projection operator

The *diagonal* dyadic products are of special importance. They can be interpreted as projectors if $|\alpha\rangle$ is normalized (Fig. 3.11):

$$P(|\alpha\rangle) \equiv |\alpha\rangle\langle\alpha| \; ; \qquad \| \, \alpha \, \| = 1 \; . \tag{3.78}$$

Illustratively, $P(|\alpha\rangle)$ projects an arbitrary state vector $|\psi\rangle$ onto the *direction* of $|\alpha\rangle$. If $|\alpha\rangle$ is an eigen-state of an Hermitian operator, then $P(|\alpha\rangle)$ corresponds just to the effect of a *filter* which we qualitatively introduced in Sect. 3.1.2. The projection operator has a few striking, but nevertheless easily provable properties. Its domain of definition is the whole Hilbert space $\mathcal{H}$. It is a linear and Hermitian operator. The latter follows immediately from (3.76). Furthermore, it is idempotent, i.e., :

$$P^2(|\alpha\rangle) = |\alpha\rangle\langle\alpha|\alpha\rangle\langle\alpha| = |\alpha\rangle\langle\alpha| = P(|\alpha\rangle) \; . \tag{3.79}$$

The *connection in series* of two projection operators onto orthogonal states $|\alpha_i\rangle$, $|\alpha_j\rangle$ ($\langle\alpha_i|\alpha_j\rangle = 0$) has the effect of the zero-operator (3.54):

$$P(|\alpha_i\rangle)\, P(|\alpha_j\rangle) = \widehat{0} \; . \tag{3.80}$$

The idempotency (3.79) needs of course the normalizability of the state $|\alpha\rangle$, therefore holds only for the proper state vectors of the Hilbert space. If the definition (3.78) is extended to Dirac vectors (3.43), then one merges the two properties (3.79) and (3.80) conveniently as follows:

$$P(|\alpha_i\rangle)\, P(|\alpha_j\rangle) = \delta(i,j) \; . \tag{3.81}$$

$\delta(i,j)$ is defined in (3.49).

Occasionally, also projections onto multi-dimensional subspaces of $\mathcal{H}$, instead of onto a single vector, can be interesting. The suitable extension of the definition (3.78) is obvious:

$$\begin{aligned} &M \text{ unitary subspace of } \mathcal{H} \; , \\ &\{|\varphi_\nu\rangle\} : \text{ CON-basis of } M \; , \\ &P_M = \sum_\nu |\varphi_\nu\rangle\langle\varphi_\nu| \; ; \quad D_{P_M} = \mathcal{H} \; . \end{aligned} \tag{3.82}$$

On the vectors of M, P_M acts like the unit-operator $\mathbb{1}$. The projection operator P_M fulfills the eigen-value equation:

$$P_M|p\rangle = \sum_{\nu}^{f} |\varphi_\nu\rangle\langle\varphi_\nu|p\rangle \stackrel{!}{=} p|p\rangle \ . \tag{3.83}$$

Immediately we recognize one special set of eigen-states. These are just the orthonormalized basis states $|\varphi_\nu\rangle$ of the subspace M itself:

$$|p\rangle = |\varphi_\mu\rangle : P_M|\varphi_\mu\rangle = \sum_{\nu}^{f} |\varphi_\nu\rangle\langle\varphi_\nu|\varphi_\mu\rangle = \sum_{\nu}^{f} |\varphi_\nu\rangle\, \delta(\nu,\mu) = |\varphi_\mu\rangle \ .$$

They all belong to the eigen-value 1, which is obviously degenerate accordingly to the dimension of M. The corresponding eigen-space is identical to M.

There are further eigen-states with the eigen-value 0. These are the linearly independent states $|\psi\rangle \in \mathcal{H}$, which are orthogonal to M, i.e.:

$$\langle\varphi_\nu|\psi\rangle = 0 \qquad \forall|\varphi_\nu\rangle \in M \ .$$

We prove as Exercise 3.2.17 further properties of the projection operator:

a) P_M depends only on M and does **not** depend on the special basis $\{|\varphi_\nu\rangle\}$!
b) P_M is Hermitian:

$$P_M^+ = P_M \ . \tag{3.84}$$

c) P_M is idempotent:

$$P_M^2 = P_M \ . \tag{3.85}$$

The Hilbert space $\mathcal{H}$ is projected by P_M onto M. P_M *thus inquires*, whether or not a physical quantity, to which the space M is mathematically ascribed, is covered by the state of the system $|\psi\rangle$.

3) Inverse (reciprocal) operator

Let A be a linear operator with a one-to-one mapping prescription

$$|\beta\rangle = A|\alpha\rangle \ ,$$

where domain of definition D_A and co-domain W_A coincide. Then the to A inverse operator A^{-1} is defined by

$$A^{-1}|\beta\rangle = |\alpha\rangle$$

with

$$D_{A^{-1}} = W_A \; ; \quad W_{A^{-1}} = D_A \; . \tag{3.86}$$

Because of $D_A = W_A$ we have the operator identity:

$$A^{-1} A = A A^{-1} = \mathbb{1} \; . \tag{3.87}$$

We find the adjoint operator of A^{-1} by the following consideration:

$$\begin{aligned} \mathbb{1} = \mathbb{1}^+ = (A^{-1} A)^+ &\overset{(3.59)}{=} A^+ (A^{-1})^+ \\ \Longrightarrow (A^+)^{-1} &= (A^{-1})^+ \; . \end{aligned} \tag{3.88}$$

A^{-1} is therefore Hermitian if A is Hermitian. One can easily convince oneself (Exercise 3.2.21) that the eigen-states of A^{-1} are the same as those of A, where the eigen-values are just the reciprocal to the eigen-values of A.

4) Unitary operator

The physical interpretation in Sect. 3.3 will make clear that the experimentally verifiable results of Quantum Mechanics will correspond to

$$\begin{array}{ll} \text{eigen-values } a_i & (A|a_i\rangle = a_i|a_i\rangle) \; , \\ \text{scalar products} & \langle\varphi|\psi\rangle \; , \\ \text{expectation values} & \langle\psi|A|\psi\rangle \; . \end{array}$$

Actually, the state vectors themselves are not the decisive terms. They can be changed (transformed) *almost arbitrarily*, if it is only guaranteed that the above measurands thereby remain unaffected.

Definition 3.2.7 (Unitary Operator U)

$$U^+ U = U U^+ = \mathbb{1} \Longleftrightarrow U^+ = U^{-1} \; . \tag{3.89}$$

Definition 3.2.8 (Unitary Transformation)

$$\begin{array}{ll} \text{for states:} & |\overline{\psi}\rangle = U|\psi\rangle \; , \\ \text{for operators:} & \overline{A} = U A U^+ \; . \end{array} \tag{3.90}$$

We now show the invariance of the above-listed measurands with respect to a unitary transformation:

a)

$$\langle\overline{\psi}|\overline{\varphi}\rangle = \langle\psi|U^+ U|\varphi\rangle = \langle\psi|\varphi\rangle \; . \tag{3.91}$$

b)

$$\langle\overline{\psi}|\overline{A}|\overline{\psi}\rangle = \langle\psi|U^+\,U\,A\,U^+U|\psi\rangle = \langle\psi|A|\psi\rangle\ . \tag{3.92}$$

c)

$$\begin{aligned} &A|a_i\rangle = a_i|a_i\rangle\ ; \quad \overline{A}|\overline{a}_i\rangle = \overline{a}_i|\overline{a}_i\rangle\ , \\ &\overline{A}|\overline{a}_i\rangle = U\,A\,U^+\,U|a_i\rangle = U\,A|a_i\rangle = a_i U|a_i\rangle = a_i|\overline{a}_i\rangle \\ &\Longrightarrow \overline{a}_i = a_i\ . \end{aligned} \tag{3.93}$$

A unitary transformation *does not change the physics!*

Eventually, the

infinitesimal unitary transformation

$$U_\varepsilon = \mathbb{1} + i\,\varepsilon\,F\ ; \quad F = F^+ \qquad (\varepsilon \text{ real, infinitesimally small}) \tag{3.94}$$

is of interest. Equation (3.89) is valid for this transformation, if one neglects quadratic terms of ε. Such a transformation changes the operator A as follows:

$$\overline{A} = (\mathbb{1} + i\,\varepsilon\,F)\,A(\mathbb{1} - i\,\varepsilon\,F) = A + i\,\varepsilon\,[F, A]_- + \mathcal{O}(\varepsilon^2)\ . \tag{3.95}$$

5) Functions of operators

We already got to know the sum and the product of two operators in (3.52) and (3.53). Based on this, somewhat more complicated functions of operators can also be understood.

a) Powers

It follows directly from the definition of the operator product (3.53):

$$A^n|\psi\rangle = A^{n-1}(A|\psi\rangle) = \ldots = A(A(\ldots(A|\psi\rangle)\ldots))\ , \tag{3.96}$$

$$A^o = \mathbb{1}\ . \tag{3.97}$$

b) Polynomials

If one combines (3.96) with the definition (3.52) of the sum of operators, then the mode of action of expressions of the type

$$P_n(A) = c_0\mathbb{1} + c_1\,A + \ldots + c_n\,A^n\ , \quad c_i \in \mathbb{C} \tag{3.98}$$

is fixed.

c) Power series

The logical generalization of b) are infinite sums of operator powers if only convergence is guaranteed. So it holds, for instance, for the exponential function of an operator A:

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n \ . \tag{3.99}$$

Now it is obvious how one has to understand polynomials and power series of more than one operator. Thereby, however, the possible non-commutability of the operators must be strictly kept in mind. So

$$e^A \, e^B = e^{A+B} \text{ is valid only if } [A, B]_- = 0 \ . \tag{3.100}$$

d) Operator functions

In the sense of the above discussion, we consider a general function of an operator A,

$$f(A) \ ,$$

exactly then as defined, if it is possible, at least in principle, to represent the function by sums, products, powers, polynomials, or power series. That holds then correspondingly for functions $f(A, B, C, \ldots)$ of more than one operator. For the so defined operator functions it must follow from

$$A|a\rangle = a|a\rangle$$

the eigen-value equation

$$f(A)|a\rangle = f(a)|a\rangle \ . \tag{3.101}$$

6) Derivatives of operators

We have to distinguish two different differentiation processes:

a) Differentiation with respect to a real parameter

Let the operator $A = A(\eta)$ depend on a real parameter η, as for instance the time t. Then we define:

$$\frac{dA}{d\eta} = \lim_{\varepsilon \to 0} \frac{A(\eta + \varepsilon) - A(\eta)}{\varepsilon} \ . \tag{3.102}$$

Some of the relevant rules of calculation will be proved as Exercise 3.2.25!

b) Differentiation with respect to an operator

We assume an operator function $f(A)$ as explained in 5d). Then the obvious definition,

$$\frac{d}{dA} f(A) = \lim_{\varepsilon \to 0} \frac{f(A + \varepsilon \mathbb{1}) - f(A)}{\varepsilon} , \tag{3.103}$$

leads to the *familiar* calculation rules of differentiation, where, however, as the case may be, the sequence of the operators has to be obeyed (Exercise 3.2.24):

$$\frac{d}{dA} \left(f(A) + g(A) \right) = \frac{d}{dA} f(A) + \frac{d}{dA} g(A) , \tag{3.104}$$

$$\frac{d}{dA} \left(f(A)\, g(A) \right) = \frac{df}{dA} g(A) + f(A) \frac{dg}{dA} , \tag{3.105}$$

$$\frac{d}{dA} A^n = n A^{n-1} \quad ; \quad \frac{d}{dA} e^{cA} = c\, e^{cA} , \quad c \in \mathbb{C} . \tag{3.106}$$

If the considered functions depend on more than one operator then we should be capable of performing partial differentiations also:

$$\frac{\partial}{\partial B} f(A, B, C, \ldots) = \lim_{\varepsilon \to 0} \frac{f(A, B + \varepsilon \mathbb{1}, C, \ldots) - f(A, B, C, \ldots)}{\varepsilon} . \tag{3.107}$$

3.2.8 Linear Operators as Matrices

So far we have regarded the Hilbert space as a set of abstract state vectors. But the representation (3.66) of a general state $|\psi\rangle$ by the eigen-states $|a_i\rangle$ of a linear Hermitian operator A already indicates that this state $|\psi\rangle$ is completely determined by its components with respect to a pre-given CON-basis. The practical method of solution of eigen-value problems is based on the fact that, as formulated in (3.71) and (3.72), respectively, the operator A appears in the form of its *matrix elements*. We now want to recapitulate this idea once more, in order to further deepen it.

Let the Hilbert space $\mathcal{H}$ be spanned by any

$$\text{countable CON-system} : \quad \{|\varphi_n\rangle\} \quad n = 1, 2, \ldots \quad .$$

Let $|\psi\rangle$ be an arbitrary state in $\mathcal{H}$, which can be expressed according to (3.66) as:

$$|\psi\rangle = \sum_n |\varphi_n\rangle \langle \varphi_n | \psi \rangle . \tag{3.108}$$

Since the components of $|\psi\rangle$ with respect to the basis $|\varphi_n\rangle$ uniquely fix the state $|\psi\rangle$, we can ascribe to it a column vector,

$$|\psi\rangle \longleftrightarrow \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_m \\ \vdots \end{pmatrix} , \tag{3.109}$$

whose elements just represent the *projections* of $|\psi\rangle$ onto the basis states $|\varphi_n\rangle$:

$$\psi_n = \langle\varphi_n|\psi\rangle \; ; \qquad n = 1, 2, 3, \ldots \tag{3.110}$$

We prove as Exercise 3.2.6 that these column vectors fulfill the axioms of the Hilbert space, i.e., that they can themselves be interpreted as elements of a Hilbert space.

Analogously, we can now write an operator A, because of

$$A = \mathbb{1}A\mathbb{1} = \sum_{n,m} |\varphi_n\rangle\langle\varphi_n|A|\varphi_m\rangle\langle\varphi_m| \; , \tag{3.111}$$

in form of a matrix:

$$A = (A_{nm}) = \begin{pmatrix} A_{11} & A_{12} & \ldots & A_{1m} & \ldots \\ A_{21} & A_{22} & \ldots & A_{2m} & \ldots \\ \vdots & \vdots & & \vdots & \\ A_{n1} & A_{n2} & \ldots & A_{nm} & \ldots \\ \vdots & \vdots & & \vdots & \end{pmatrix} . \tag{3.112}$$

The matrix elements are again uniquely fixed by the given basis:

$$A_{nm} = \langle\varphi_n|A|\varphi_m\rangle \; . \tag{3.113}$$

If the Hilbert space is n-dimensional, then A is a quadratic $n \times n$-matrix. In the case of a countably infinite basis, the matrix is formally built up by infinite rows and infinite columns. If, however, the basis consists of improper Hilbert vectors, the sums in (3.111) have to be replaced by integrals; n and m become continuous index variables. A matrix definition is then actually no longer reasonable. Nevertheless, even in such a case one denotes expressions of the form (3.113) as *matrix elements*.

If the state $|\psi\rangle$ is mapped by the operator A onto the state $|\chi\rangle$ then:

$$|\chi\rangle = A|\psi\rangle = \sum_m A|\varphi_m\rangle\langle\varphi_m|\psi\rangle \; .$$

If we define, in analogy to (3.110), the components χ_n of the state $|\chi\rangle$ with respect to the basis $\{|\varphi_n\rangle\}$, then we can write the last equation also as follows:

$$\chi_n = \sum_m A_{nm}\,\psi_m \ .$$

On the right-hand side we recognize the multiplication of a matrix by a column vector:

$$\begin{pmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_n \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & \dots \\ A_{21} & A_{22} & \dots & \dots \\ \vdots & \vdots & \vdots & \\ \cdots & \cdots & A_{nm} & \dots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_m \\ \vdots \end{pmatrix} . \tag{3.114}$$

For the special case of an eigen-value equation, (3.71) is to be translated correspondingly into a matrix equation ($a_n = \langle\varphi_n|a\rangle$):

$$\begin{pmatrix} (A_{11}-a) & A_{12} & \cdots & \cdots & \cdots \\ A_{21} & (A_{22}-a) & \cdots & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots & \\ A_{n1} & A_{n2} & & (A_{nn}-a) & \cdots \\ \vdots & \vdots & \vdots & \ddots & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \vdots \end{pmatrix} . \tag{3.115}$$

While we can perceive the ket-state $|\psi\rangle$ as column vector (3.109), we have to write the corresponding bra-state $\langle\psi|$ as row vector with complex conjugate components:

$$\langle\psi| = \sum_n \langle\psi|\varphi_n\rangle\langle\varphi_n| = \sum_n \langle\varphi_n|\psi\rangle^*\langle\varphi_n| \ , \tag{3.116}$$

$$\langle\psi| \longleftrightarrow \left(\psi_1^*\ \psi_2^* \dots \psi_m^* \dots\right) . \tag{3.117}$$

For the scalar product of two Hilbert vectors we have, according to our former considerations:

$$\langle\chi|\psi\rangle \ = \ \sum_n \langle\chi|\varphi_n\rangle\langle\varphi_n|\psi\rangle = \sum_n \chi_n^*\,\psi_n \ , \tag{3.118}$$

$$\langle\chi|\psi\rangle \longleftrightarrow \left(\chi_1^*\ \chi_2^* \dots \chi_n^* \dots\right) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \\ \vdots \end{pmatrix} . \tag{3.119}$$

We can, eventually, very easily find out, how the matrix A^+, which is the operator adjoint to A adjoint operator, has to look like. It follows immediately from (3.56):

$$(A^+)_{nm} = A^*_{mn} \; . \tag{3.120}$$

Hence we obtain the matrix A^+ from A by interchanging rows and columns and changing the elements to their complex conjugate values. For a Hermitian matrix it holds in particular $A_{nm} = A^*_{mn}$. Reflection at the main diagonal converts the matrix elements into their complex conjugate values. The diagonal elements of a Hermitian matrix are real.

The product of two operators A and B corresponds to the well-known multiplication of matrices, because we have:

$$(A\,B)_{ij} = \langle\varphi_i|A\,B|\varphi_j\rangle = \sum_n \langle\varphi_i|A|\varphi_n\rangle\langle\varphi_n|B|\varphi_j\rangle = \sum_n A_{in}\,B_{nj} \; . \tag{3.121}$$

In the second step we have inserted a complete set of eigen-states (3.69) between the operators A and B.

The matrices of unitary operators represent a special case. For these it holds because of (3.89) $U^+ = U^{-1}$:

$$\left(U^{-1}\right)_{nm} = U^*_{mn} \; . \tag{3.122}$$

One easily realizes that rows and columns of a unitary matrix are orthonormalized:

$$\begin{aligned} U^+\,U = \mathbb{1} &\underset{(3.121)}{\longrightarrow} \sum_m (U^+)_{im}\,U_{mj} = \delta_{ij} \\ &\underset{(3.120)}{\longrightarrow} \sum_m U^*_{mi}\,U_{mj} = \delta_{ij} \; . \end{aligned} \tag{3.123}$$

If one chooses as the basis of $\mathcal{H}$ just the complete set $|a_n\rangle$ of eigen-states of the Hermitian operator A, then the matrix A has a diagonal form, where on the main diagonal just the eigen-values a_n of A appear:

$$A|a_n\rangle \;\; = \;\; a_n|a_n\rangle \longrightarrow \langle a_n|A|a_m\rangle = A_{nm} = a_n\,\delta_{nm} \; ,$$

$$A \longleftrightarrow \begin{pmatrix} a_1 & & & & \\ & a_2 & & 0 & \\ & & \ddots & & \\ & & & a_n & \\ & 0 & & & \ddots \end{pmatrix} \; . \tag{3.124}$$

It is important in this connection that there always exists a unitary transformation which brings a matrix A into the diagonal form (3.124). That can be seen as follows:

$$a_i\,\delta_{ij} = \langle a_i|A|a_j\rangle = \sum_{n,m} \langle a_i|\varphi_n\rangle\langle\varphi_n|A|\varphi_m\rangle\langle\varphi_m|a_j\rangle \ .$$

$\langle\varphi_n|A|\varphi_m\rangle = A_{nm}$ is the (n,m)-matrix element of A in the *φ-basis*. We define

$$U_{in} = \langle a_i|\varphi_n\rangle \tag{3.125}$$

as the $(i,\ n)$-element of the matrix U. According to (3.120), the scalar product

$$\langle\varphi_m|a_j\rangle = \langle a_j|\varphi_m\rangle^* = U^*_{jm} = (U^+)_{mj}$$

is then the (m,j)-element of the adjoint matrix U^+. That means for the above equation:

$$a_i\,\delta_{ij} = \sum_{n,m} U_{in}\,A_{nm}\,(U^+)_{mj}$$

$$(\overline{A} = U\,A\,U^+) \ . \tag{3.126}$$

We see that the unitary matrix U, which diagonalizes A, is built up by the eigenvectors of A. The complex conjugate components of the i-th eigen-state $|a_i\rangle$ in the *φ-basis* (3.125) form the i-th row of U. One easily convinces oneself that the condition (3.89), $U^+U = \mathbb{1}$, is fulfilled.

At the end of this section we introduce a term which is frequently used in connection with matrices:

Definition 3.2.9 *'trace of a matrix'* $\equiv$ *sum of its diagonal elements*

This definition would be hardly meaningful without the statement of the following theorem:

Theorem 3.2.2 *The trace of a matrix is independent of its representation, i.e., independent of the used CON-basis!*

Proof Let $\{|\varphi_n\rangle\}$ and $\{|\psi_\nu\rangle\}$ be two different CON-basis systems of $\mathcal{H}$:

$$\begin{aligned}
\mathrm{Sp}\,A &= \sum_n \langle\varphi_n|A|\varphi_n\rangle = \\
&= \sum_n \sum_{\nu\mu} \langle\varphi_n|\psi_\nu\rangle\langle\psi_\nu|A|\psi_\mu\rangle\langle\psi_\mu|\varphi_n\rangle = \\
&= \sum_{\nu,\mu} \langle\psi_\mu| \left(\sum_n |\varphi_n\rangle\langle\varphi_n| \right) |\psi_\nu\rangle\langle\psi_\nu|A|\psi_\mu\rangle =
\end{aligned}$$

$$= \sum_{\nu,\mu} \langle \psi_\mu | \mathbb{1} | \psi_\nu \rangle \langle \psi_\nu | A | \psi_\mu \rangle =$$

$$= \sum_{\nu,\mu} \delta_{\nu\mu} \langle \psi_\nu | A | \psi_\mu \rangle =$$

$$= \sum_{\nu} \langle \psi_\nu | A | \psi_\nu \rangle \ .$$

That is the assertion of the theorem!

3.2.9 Exercises

Exercise 3.2.1 Let $\mathcal{H}$ be a Hilbert space and $|\alpha\rangle$, $|\beta\rangle$ arbitrary states of $\mathcal{H}$. Prove the so-called parallelogram equation:

$$\| \alpha + \beta \|^2 + \| \alpha - \beta \|^2 = 2 \| \alpha \|^2 + 2 \| \beta \|^2 \ .$$

Exercise 3.2.2 Prove with the presumptions of Exercise 3.2.1 the Schwarz's inequality

$$|\langle \alpha | \beta \rangle| \leq \| \alpha \| \| \beta \| \ .$$

It may be convenient, first to decompose the vector $|\beta\rangle$ into the components parallel and perpendicular to $|\alpha\rangle$, and then to calculate $\| \beta \|^2$.

Exercise 3.2.3 Verify by the use of the Schwarz's inequality the triangle inequality:

$$| \| \alpha \| - \| \beta \| | \leq \| \alpha + \beta \| \leq \| \alpha \| + \| \beta \| \ .$$

Exercise 3.2.4 Let $|\psi_i\rangle$ be a system of linearly independent Hilbert vectors, which, however, are not all pairwise orthogonal. Show that, recursively, a system of orthonormal vectors is produced by:

$$|d_j\rangle = \frac{|\psi_j\rangle - \sum_{i=1}^{j-1} \langle d_i | \psi_j \rangle |d_i\rangle}{\left\| \left\{ |\psi_j\rangle - \sum_{i=1}^{j-1} \langle d_i | \psi_j \rangle |d_i\rangle \right\} \right\|}$$

Exercise 3.2.5

1. Let $|v_1\rangle$ and $|v_2\rangle$ be unnormalized but orthogonal, discrete vectors of a Hilbert space. Show that the states

$$|\varphi_1\rangle = a|v_1\rangle + i\,b|v_2\rangle \,,$$
$$|\varphi_2\rangle = a|v_1\rangle - i\,b|v_2\rangle$$

   are orthonormalized for suitably chosen real constants a and b.
2. Calculate the norm and the scalar product of the vectors:

$$|\psi_1\rangle = \sqrt{\frac{2}{\pi}} \int_a^{a+\pi} dp|v_p\rangle \cos p \,,$$
$$|\psi_2\rangle = \sqrt{\frac{2}{\pi}} \int_a^{a+\pi} dp|v_p\rangle \sin p \,,$$

   where $|v_p\rangle$ is an orthonormalized improper (Dirac) vector.

Exercise 3.2.6 Let $\mathcal{H}$ be the ensemble of all column vectors

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = (a_n) \,,$$

whose components are complex numbers with

$$\sum_{n=1}^{\infty} |a_n|^2 < \infty \,.$$

Addition and multiplication by a complex number are performed component-by-component:

$$\mathbf{a} + \mathbf{b} = (a_n + b_n) \,,$$
$$c\,\mathbf{a} = (c\,a_n) \,.$$

Let the scalar product be defined as follows:

$$\mathbf{a} \cdot \mathbf{b} = \sum_{n=1}^{\infty} a_n^* \, b_n \,.$$

Show that $\mathcal{H}$ is a Hilbert space.

Exercise 3.2.7 Let $\mathcal{H}$ be the Hilbert space of the square-integrable functions $f(x)$ in the interval $a \leq x \leq b$ (a, b reell) with the properties:

1. scalar product

$$\langle f_1 | f_2 \rangle = \int_a^b dx\, f_1^*(x) f_2(x)$$

2.

$$\langle f | f \rangle < \infty$$

3.

$$f(a) = f(b) = 0$$

Let A be a linear operator ($D_A = \mathcal{H}$) with the mapping prescription:

$$A|f\rangle \longrightarrow f'(x)$$

Show that A is antihermitian in $\mathcal{H}$ ($A^\dagger = -A$).

Exercise 3.2.8 Determine the adjoint operators of

1. $A + B$ (A, B : operators),
2. cA (A : operator , $c \in \mathbb{C}$),
3. $|\varphi\rangle\langle\psi|$,
4. $\mathbb{1}$.

Exercise 3.2.9

1. Under which condition is the product of two Hermitian operators again a Hermitian operator?
2. Let A and B be Hermitian operators.
   - 2a) What is the adjoint operator of the commutator$[A, B]_-$?
   - 2b) Find a suitable numerical factor by which $[A, B]_-$ becomes a Hermitian operator!

Exercise 3.2.10 Testify whether or not the following operators are Hermitian:

1.

$$x$$

2.

$$\frac{d}{dx}$$

3.

$$\frac{\hbar}{i}\frac{d}{dx}$$

4.

$$xp_y\,; \quad xp_x$$

5.

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \quad (V(x) \text{ real})$$

Exercise 3.2.11 $|\alpha\rangle$ is an eigen-state of the linear Hermitian operator A. Calculate the expectation value in the state $|\alpha\rangle$ of the commutator of A with an arbitrary operator B:

$$\langle\alpha|[A, B]_-|\alpha\rangle\ .$$

Exercise 3.2.12 Let A, B, C be linear operators with

$$[A, B]_- = 0\,; \qquad [B, C]_- = 0\ .$$

Does it then necessarily follow that also $[A, C]_- = 0$?

Exercise 3.2.13 Let A, B, C be linear operators. For these operators, prove the following useful relations:

1. $[A,\, B\,C]_- = B[A,\, C]_- + [A,\, B]_-\, C$,
2. $[A\,B,\, C]_- = A[B,\, C]_- + [A,\, C]_-\, B$,
3. Jacobi identity:

$$[A,\, [B,\, C]_-]_- + [B,\, [C,\, A]_-]_- + [C,\, [A,\, B]_-]_- = 0\ .$$

Exercise 3.2.14 For two operators A and B we have:

$$[A,\, B]_- = i\,\mathbb{1}\ .$$

Verify that it follows for $n = 1, 2, 3, \ldots$:

1. $[A,\, B^n]_- = i\,n\,B^{n-1} = i\,(d/dB)\,B^n$,
2. $[A^n,\, B]_- = i\,n\,A^{n-1} = i\,(d/dA)\,A^n$.

Exercise 3.2.15 Let A and $B_1, \ldots, B_n$ be not necessarily commutable operators.

1. Prove the following relation:

$$\left[A, \prod_{i=1}^{n} B_i\right]_- = \sum_{m=1}^{n} B_1 \cdot B_2 \cdot \cdots \cdot B_{m-1} \cdot [A, B_m]_- \cdot B_{m+1} \cdot \cdots \cdot B_n \ .$$

2. Calculate

$$[A, B^n]_- \ !$$

   What results for the special case $[A, B]_- = 0$?
3. Calculate

$$[A, B^n]_-$$

   under the assumption that $[A, B]_- \neq 0$, but

$$[[A, B]_- , B]_- = 0 \ .$$

Exercise 3.2.16 Let A and B be linear operators with $A \neq A(\lambda)$ and $B \neq B(\lambda)$, $\lambda \in \mathbb{R}$.

1. Write

$$e^{\lambda A} B e^{-\lambda A} = \sum_{n=0}^{\infty} \alpha_n \lambda^n \quad (\alpha_n \text{ operators!})$$

   and determine the coefficients α_n.
2. Show that if

$$[A, [A, B]_-]_- = 0$$

   one can use:

$$e^{\lambda A} B e^{-\lambda A} = B + \lambda \, [A, B]_- \ .$$

3. Use the partial results in 1. and 2., in order to derive the differential equation

$$\frac{d}{d\lambda} \left(e^{\lambda A} e^{\lambda B}\right) = (A + B + \lambda \, [A, B]_-) \left(e^{\lambda A} e^{\lambda B}\right)$$

   for $[A, [A, B]_-]_- = [B, [A, B]_-]_- = 0$.

4. Prove with 3.:

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]_-} ,$$

if $[A,[A,B]_-]_- = [B,[A,B]_-]_- = 0$.

Exercise 3.2.17 Let P_L and P_M be projection operators onto the subspaces $L, M \in \mathcal{H}$. Verify the following properties:

1. P_M depends only on M, however, not on the special basis of M,
2. $P_M^+ = P_M$: Hermitian,
3. $P_M^2 = P_M$: idempotent.
4. Under which conditions are

$$P_L P_M , \quad P_L + P_M , \quad P_L - P_M$$

also projection operators? Onto which subspaces do these operator combinations project?

Exercise 3.2.18 Given is a two-dimensional Hilbert space $\mathcal{H}$ with a CON-basis $\{|\varphi_1\rangle, |\varphi_2\rangle\}$. One has found for the operator A:

$$A|\varphi_1\rangle = -|\varphi_2\rangle ; \quad A|\varphi_2\rangle = -|\varphi_1\rangle .$$

1. Write A as linear combination of dyadic products $|\varphi_i\rangle\langle\varphi_j|$.
2. Is A Hermtian?
3. Calculate $A\,A^+$, A^+A, A^2!
4. Determine the eigen-values and eigen-states of A!

Exercise 3.2.19 In a three-dimensional Hilbert space $\mathcal{H}$ two linear operators are defined by their actions on the vectors of an orthonormalized basis: $\{|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle\}$

$$\begin{aligned} A|\alpha_1\rangle &= 3|\alpha_1\rangle - i\sqrt{2}|\alpha_2\rangle + |\alpha_3\rangle \\ A|\alpha_2\rangle &= i\sqrt{2}|\alpha_1\rangle + 2|\alpha_2\rangle - i\sqrt{2}|\alpha_3\rangle \\ A|\alpha_3\rangle &= |\alpha_1\rangle + i\sqrt{2}|\alpha_2\rangle + 3|\alpha_3\rangle \end{aligned}$$

$$\begin{aligned} B|\alpha_1\rangle &= |\alpha_1\rangle + i\sqrt{2}|\alpha_2\rangle + |\alpha_3\rangle \\ B|\alpha_2\rangle &= -i\sqrt{2}|\alpha_1\rangle + i\sqrt{2}|\alpha_3\rangle \\ B|\alpha_3\rangle &= |\alpha_1\rangle - i\sqrt{2}|\alpha_2\rangle + |\alpha_3\rangle \end{aligned}$$

1. Check whether A and B are Hermitian!
2. Determine the eigen-values and the eigen-states of the operators!
3. Are A and B commutable?

Exercise 3.2.20 A Hermitian operator A with a discrete spectrum is called *positive definite* in the Hilbert space $\mathcal{H}$, if it holds:

$$\langle\psi|A|\psi\rangle > 0 \quad \forall\ |\psi\rangle \in \mathcal{H} \quad |\psi\rangle \neq |0\rangle\ .$$

1. Show that A is positive definite if and only if all eigen-values a_i are positive.
2. Let the three-dimensional Hilbert space $\mathcal{H}$ be spanned by orthonormalized states $|\varphi_1\rangle$, $|\varphi_2\rangle$ and $|\varphi_3\rangle$, and let the action of A on these states be given by:

$$\begin{aligned} A\,|\varphi_1\rangle &= |\varphi_1\rangle - \sqrt{2}|\varphi_3\rangle \\ A\,|\varphi_2\rangle &= 3|\varphi_2\rangle \\ A\,|\varphi_3\rangle &= -\sqrt{2}|\varphi_1\rangle + 5|\varphi_3\rangle \end{aligned}$$

   Show that A is Hermitian and positive definite.

Exercise 3.2.21 The linear operator A satisfies the eigen-value equation,

$$A|a\rangle = a|a\rangle\ ,$$

and the inverse operator A^{-1} exists. Show that it possesses the same eigen-state, and calculate the corresponding eigen-value.

Exercise 3.2.22 Does an inverse operator exist for the projection operator $P\,(|\alpha\rangle) = |\alpha\rangle\langle\alpha|$?

Exercise 3.2.23

1. Show that the eigenvalues of an unitary operator U are complex numbers of the absolute value 1.
2. Is a Hermitian operator after a unitary transformation still Hermitian?
3. Do two commutable operators A and B remain commutable after a unitary transformation?

Exercise 3.2.24 Let $f(A)$ and $g(A)$ be functions of the operator A. Prove the rules of differentiation:

1.

$$\frac{d}{dA}\,(f(A) + g(A)) = \frac{df}{dA} + \frac{dg}{dA}\ ,$$

2.

$$\frac{d}{dA}\,(f(A)\,g(A)) = \frac{df}{dA}\,g(A) + f(A)\,\frac{dg}{dA}\ ,$$

3.

$$\frac{d}{dA}A^n = nA^{n-1}\ ; \quad n = 1, 2, 3, \ldots$$

Exercise 3.2.25 Let the operators $A = A(\eta)$ and $B = B(\eta)$ depend on a real parameter η. Prove the following rules of differentiation:

1.

$$\frac{d}{d\eta}(A\,B) = \frac{dA}{d\eta}B + A\,\frac{dB}{d\eta}\ ,$$

2.

$$\frac{d}{d\eta}A^n = \sum_{\mu=1}^{n} A^{\mu-1}\,\frac{dA}{d\eta}\,A^{n-\mu}\ ; \quad n = 1, 2, \ldots\ ,$$

3.

$$\frac{d}{d\eta}A^{-1} = -A^{-1}\,\frac{dA}{d\eta}\,A^{-1}\ .$$

Exercise 3.2.26 Let the two observables A and B comply with the commutator relation

$$[A, B]_- = C\ .$$

Assume that the operator C commutes with A as well as with B. Show that it then holds for the operator functions $f(B)$ and $g(A)$:

$$[A, f(B)]_- = C\frac{d}{dB}f(B)$$
$$[g(A), B]_- = C\frac{d}{dA}g(A)\ .$$

Exercise 3.2.27 Let $|\rho\rangle = \begin{pmatrix}1\\1\\0\end{pmatrix}$ and $|\psi\rangle = \begin{pmatrix}1\\0\\1\end{pmatrix}$ be two vectors of the three-dimensional Hilbert space $\mathcal{H}$, which is spanned by the CON-basis

$$|e_1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}\ ; \quad |e_2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}\ ; \quad |e_3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}\ .$$

1. Find the matrix representation of the dyadic product

$$D = |\rho\rangle\langle\psi| \, .$$

2. Calculate the adjoint operator D^+. Is D Hermitian?
3. Determine the eigen-values of D!
4. Demonstrate the idempotency of D. Is D therewith a projection operator?

Exercise 3.2.28 Given is the Hermitian matrix

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \, .$$

1. Calculate the eigen-values E_1 and E_2!
2. Determine the corresponding eigen-states!

Exercise 3.2.29 Given is the matrix

$$A = \begin{pmatrix} 3 & 2i \\ -2i & 0 \end{pmatrix} \, .$$

Determine

1. the eigen-values a_1, a_2,
2. the eigen-vectors $|a_1\rangle$, $|a_2\rangle$,
3. the unitary transformation which diagonalizes A.

Exercise 3.2.30 Find the unitary transformation which transfers the matrices

$$A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

simultaneously into diagonal form.

Exercise 3.2.31 Let the Hermitian operator A have, in a given CON-basis of a two-dimensional Hilbert space, the representation

$$A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

1. How does the matrix representation of the operator

$$T(\alpha) = e^{i\alpha A} \, ; \quad \alpha \in \mathbb{R}$$

look like?

2. Verify for the derivative of the operator the expression:

$$\left(\frac{dT}{d\alpha}\right)_{ij} = \frac{dT_{ij}(\alpha)}{d\alpha} .$$

Exercise 3.2.32 Let

$$F = F(A, B)$$

be an operator function. Show that the transformed operator

$$\overline{F} = U F U^{+}$$

can be found by inserting the transformed operators $\overline{A} = U A U^{+}, \overline{B} = U B U^{+}$ into the argument of F:

$$\overline{F} = F(\overline{A}, \overline{B}) .$$

Exercise 3.2.33

1. Prove the *cyclic invariance* of the trace

$$\mathrm{Tr}(A B) = \mathrm{Tr}(B A) ,$$

   where A, B are two not necessarily commutable operators.
2. Show:

$$\mathrm{Tr}\overline{A} = \mathrm{Tr} A \qquad (\overline{A} = U A U^{+}) .$$

Exercise 3.2.34 Let $|\alpha\rangle$, $|\beta\rangle$ be two orthogonal states. Calculate the trace of the dyadic product:

$$D = |\alpha\rangle\langle\beta| .$$

Exercise 3.2.35 Given are the following matrix representations of the operators L_x, L_y, L_z:

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} ; \quad L_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} ; \quad L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} .$$

1. Show that all the three operators possess the same eigen-values!
2. Find the unitary matrix U, which diagonalizes L_y.
3. Calculate therewith also $\overline{L}_x = U L_x U^{+}, \overline{L}_z = U L_z U^{+}$.

Exercise 3.2.36 The states $|\alpha_1\rangle$, $|\alpha_2\rangle$ build an orthonormalized basis of a two-dimensional Hilbert space. Another orthonormalized basis $|\beta_1\rangle$, $|\beta_2\rangle$ is given by

$$|\beta_1\rangle = \tfrac{1}{\sqrt{2}}\left(|\alpha_1\rangle + i|\alpha_2\rangle\right)$$
$$|\beta_2\rangle = \tfrac{1}{\sqrt{2}}\left(|\alpha_1\rangle - i|\alpha_2\rangle\right)$$

1. The transition from the *'α-representation'* to the *'β-representation'* is mediated by a unitary operator U. Express U by the states $|\alpha_i\rangle$ and $|\beta_k\rangle$!
2. Find the matrix belonging to U in the *'α-representation'*!
3. Let the state $|\psi\rangle$ be given in the *'α-representation'* by

$$|\psi_\alpha\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}.$$

   How does it look like in the *'β-representation'*?
4. The operator A reads in the *'α-representation'*:

$$A_\alpha = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}.$$

   How does it read in the *'β-representation'*?

Exercise 3.2.37 Let $\{|\alpha_n\rangle\}$ and $\{|\beta_n\rangle\}$ be two complete orthonormal systems of the infinite-dimensional Hilbert space $\mathcal{H}$. A linear operator is defined in $\mathcal{H}$ by

$$L = \sum_{n=1}^{\infty} |\beta_{n+1}\rangle \langle\alpha_n| .$$

1. Is L unitary in $\mathcal{H}$?
2. Let $\mathcal{H}'$ be the subspace which is spanned only by the vectors

$$\{|\beta_n\rangle \;;\quad n = 2, 3, \ldots\} .$$

   Show that L is unitary in $\mathcal{H}'$!

3.3 Physical Interpretation

What does it actually mean *to understand Quantum Mechanics*? As a start, the mathematical formalism has of course to be mastered. Without that, it does not work; any basis for further discussions would be lacking! But in addition there

are some other conceptual novelties of Quantum Mechanics by which we have to extend our *classical* world of imagination. In general, that may be the more difficult part for a real understanding of Quantum Mechanics. However, with respect to the conceptual difficulties, it is not at all the theory, which is to be complained about. The theory has proven itself up to now to be *absolutely correct*. It is rather exclusively our restricted *classical* power of imagination. We therefore want to bring, in this sense, our so far preparatory qualitative considerations of Sect. 3.1 into contact with the abstract mathematical concepts of Sect. 3.2.

3.3.1 Postulates of Quantum Mechanics

We had already formulated that the *prediction and interpretation of results of physical measurements on atomic (microscopic) systems* is the essential challenge of Quantum Mechanics. In particular, we have to therefore make an effort to clarify the meaning of the measurement process in Quantum Mechanics. At first we have to distinguish two classes of physical quantities. The one consists of the physically relevant quantities, which are directly experimentally observable. The other class contains the indirect quantities, which are not directly amenable to the experiment, but which are indispensable, in order to be able to derive theoretical predictions for the experiment. In this sense, the state vector $|\psi\rangle$ or the (linear, Hermitian) operator A have actually no real meaning, but are, however, indispensable for the representation of objective data in the form of expectation values $\langle\psi|A|\psi\rangle$, eigenvalues $a_i = \langle a_i|A|a_i\rangle$, scalar products $\langle\varphi|\psi\rangle$ and probabilities, which are all counted as relevant quantities.

With the aid of the following postulates we create the basic connection between the experimental observation and the Quantum Theory. Some of them appear perhaps rather *self-evident* due to our pre-considerations, but ultimately they must all draw their justification from experimental experience, the *'supreme judge of every theory'*

Postulate 1

$$\begin{array}{l}\textit{measuring equipment for a certain}\\ \textit{physical quantity (observable)}\end{array} \quad \Longleftrightarrow \quad \begin{array}{l}\textit{linear, Hermitian}\\ \textit{operator.}\end{array}$$

This postulate implicitly requires also that such a measuring equipment is always, at least in principle, realizable for the interesting physical quantities. That is already hidden in the term *observable*.

Postulate 2

$$\begin{array}{l}\textit{pure state of the}\\ \textit{quantum system}\end{array} \quad \Longleftrightarrow \quad \textit{Hilbert vector } |\psi\rangle .$$

What is to be understood by a *pure* state, has been commented upon in Sect. 3.1.1. We will come back once more to this important concept in the course of this section.

Postulate 3

$$\textit{measurement} \cong \textit{interaction between system and apparatus} \iff \begin{array}{l}\textit{application of the operator } A \\ \textit{on the state } |\psi\rangle : \\ A|\psi\rangle = \sum_i a_i |a_i\rangle\langle a_i|\psi\rangle \\ \xrightarrow[\text{filter}]{} |a_j\rangle\langle a_j|\psi\rangle \ .\end{array}$$

First, the apparatus takes care for a spectral decomposition of the state $|\psi\rangle$ into components *parallel* to the eigen-states $|a_i\rangle$ of A. The actual measurement is done by a filter $P(a_i)$ (see Sect. 3.1.2), which *filters out* **all except one** component. One speaks of a *'reduction of state'* from the original system state $|\psi\rangle$.

Postulate 4

$$\textit{results of measurement} \iff \textit{eigen-values } a_i \textit{ of the operator } A \ .$$

Which eigen-value is really measured, is in general uncertain, delimited only by probability statements. For that we need

Postulate 5

$$\textit{measuring probability for } a_i \iff w(a_i|\psi) = |\langle a_i|\psi\rangle|^2 \ .$$

Classical Mechanics is deterministic in such a sense that all observables, in particular position and momentum, are determinable with arbitrary accuracy, by the solution of respective equations of motion. This determinism does not exist in Quantum Mechanics. Its statements are essentially weaker, since it can answer only questions of the following kind:

a) Which results are possible at all?

The actually measured value belongs to a set of numbers, which can be found as the eigen-values of a corresponding observable. These can build a discrete manifold, but can also continuously fill whole intervals of values. The answering of question a) therefore aims at a property of the measuring apparatus, independently of the system to be investigated!

b) What is the probability of actually observing a particular value when a measurement is made?

According to postulate 5 this question is answered by the state of the system $|\psi\rangle$! Obviously, this probability equals one, i.e., only then is a *'certainty'*, when $|\psi\rangle$ is identical to the eigen-state $|a_i\rangle$ of A. It is typical for Quantum Mechanics—and in this sense the theory is not deterministic—that, in the general case, it can not exactly predict, which of the *possible* results really appears in a single measurement. One

can offer only probability distributions for many measurements on the same system or for one simultaneous measurement on a great number ($N \to \infty$) of identical single systems (see double-slit experiment in Sect. 2.1.3).

We want to intensify these considerations further in the next sections.

3.3.2 *Measuring Process*

Three self-contained components are involved in the measuring process:

1) system, 2) measuring equipment, 3) observer

A measurement can be on only if there are interactions among these three components. Classical Mechanics basically presumes that these interactions can, in principle, be made arbitrarily small, so that neither the properties of the system 1) nor the function of 2) are influenced in a noteworthy manner. This assumption is no longer tenable for Quantum Mechanics. The mutual influence of 2) and 3) can surely further be neglected, however, not that of 1) and 2). The switching on of the (macroscopic) measuring apparatus leads unavoidably to an uncontrolled disturbance of the (atomic, microscopic) system. A measurement will in general change its state, so that a subsequent, second measurement will already find the system in another state. Different measuring equipments, corresponding to different observables, will influence the state of the system in a different manner, so that it is not necessarily guaranteed that one gets the same results, when one measures the different observables in a different order. In such a case one says that the two quantities can not simultaneously be precisely measured. The corresponding operators are not commutable. They are considered as non-compatible.

Let us inspect once more, but in a bit more detail, a measuring equipment for the observable A, which we have introduced in Sect. 3.1.2 abstractly as a filter $P(a_i)$ ($\cong$ separator $T(A)+$ system of blinds). Let A have a discrete spectrum. Before the measurement let the system be in a state $|\psi\rangle$ which we assume to be known. The filter $P(a_i)$ transfers, via postulate 3 (Fig. 3.3), the system into an eigen-state $|a_i\rangle$ of the observable A, so that the corresponding eigen-value a_i is measured (postulate 4). Into which state $|a_i\rangle$ the system actually changes, is, however, undetermined. According to postulate 5, we know only the probability by which a certain value a_i is indeed measured. One can write this probability as expectation value of the projection operator:

$$P(a_i) = |a_i\rangle\langle a_i| : \qquad w(a_i|\psi) = |\langle a_i|\psi\rangle|^2 = \langle\psi|P(a_i)|\psi\rangle \ . \tag{3.127}$$

In this sense, the projector, too, is an observable, which answers with 'yes' or 'no' to the question, whether or not the system is in the state $|a_i\rangle$. Accordingly, its eigenvalues are 1 and 0 (3.83). The expectation value is then a number in between 0 and 1.

It follows with the completeness relation (3.69) that in any case the system after the measurements is in one of the eigen-states:

$$\sum_i w(a_i|\psi) = \sum_i \langle\psi|a_i\rangle\langle a_i|\psi\rangle = \langle\psi|\mathbb{1}|\psi\rangle = \langle\psi|\psi\rangle = 1 \ .$$

Thus with certainty, one of the eigen-values out of the spectrum of A is measured. An immediate second measurement with the same apparatus, the same filter, will yield exactly the same value, since then the system is already in an eigen-state of A. The probability to get another eigen-value by the second measurement is therefore zero. That agrees with our qualitative considerations in Sect. 3.1.2 (see (3.3)):

$$w(a_j|a_i) = |\langle a_j|a_i\rangle|^2 = \delta_{ij} \ . \tag{3.128}$$

The eigen-states of A thus have to be orthogonal. That is one of the reasons why we have to represent observables by Hermitian operators (postulate 1).

Practically the same considerations are valid also for observables with continuous spectra. But thereby one has to regard, though, that each real measuring system can fix the measuring value only with a finite width. The initial state $|\psi\rangle$ is manipulated by the measurement in the following manner:

$$|\psi\rangle \overset{\text{measurement}}{\Longrightarrow} \int_{j-\frac{1}{2}\Delta j}^{j+\frac{1}{2}\Delta j} dj' \, |\overline{a}_{j'}\rangle\langle\overline{a}_{j'}|\psi\rangle \ . \tag{3.129}$$

The eigen-states $|\overline{a}_j\rangle$ are now Dirac vectors ((3.43), (3.44)). The measured value will lie within an interval of the width Δj, actually being measured with the probability

$$w_{\Delta j}(a_j|\psi) = \int_{j-\frac{1}{2}\Delta j}^{j+\frac{1}{2}\Delta j} dj' \, |\langle\overline{a}_{j'}|\psi\rangle|^2 \ . \tag{3.130}$$

The square of the absolute value is therefore now a probability density, as we have it already discussed in Chap. 2 in connection with $\rho(\mathbf{r})$ (2.26) for the special case of a measurement of the position. The scalar product $\langle\overline{\mathbf{r}}|\psi\rangle$ between the (improper) eigen-state of the position operator $|\overline{\mathbf{r}}\rangle$ and the state $|\psi\rangle$, we will later indeed identify as the wave function (*position representation*) (3.238) which is ascribed to the state of the system $|\psi\rangle$. The position-eigen states, too, build a complete system, so that each $|\psi\rangle$ can be expanded in them:

$$|\psi\rangle = \int d^3r' \, |\overline{\mathbf{r}'}\rangle\langle\overline{\mathbf{r}'}|\psi\rangle \ . \tag{3.131}$$

The integral encompasses the whole space. $|\psi\rangle$ may describe, for instance, the state of an electron. If we now perform a measurement of the position by use of a detector, which *covers* just the small volume $v(\mathbf{r})$ at $\mathbf{r}$, the electron will go due to the measurement into the state $|\widehat{\psi}(\mathbf{r})\rangle$:

$$|\psi\rangle \overset{\text{measurement}}{\Longrightarrow} |\widehat{\psi}(\mathbf{r})\rangle = \int\limits_{v(\mathbf{r})} d^3r' |\overline{\mathbf{r}'}\rangle\langle\overline{\mathbf{r}'}|\psi\rangle \ . \tag{3.132}$$

The probability, to find indeed the electron in the volume $v(\mathbf{r})$, is given by

$$w(\mathbf{r}|\psi) = \int\limits_{v(\mathbf{r})} d^3r' |\langle\overline{\mathbf{r}'}|\psi\rangle|^2 \ . \tag{3.133}$$

That couples seamlessly to the considerations of Chap. 2. We thus recognize that Schrödinger's wave mechanics represents a special realization of the abstract quantum-mechanical apparatus.

In the case of a degenerate eigen-value a we write instead of (3.127) and (3.130) for the measuring probability:

$$w(M(a)|\psi) = \langle\psi|P_{M(a)}|\psi\rangle \ . \tag{3.134}$$

$P_{M(a)}$ is the projection operator onto the whole eigen-space $M(a)$ of the degenerate eigen-value a:

$$P_{M(a)} = \sum\!\!\!\!\!\!\int\limits_{M(a)} |a_j\rangle\langle a_j| \ . \tag{3.135}$$

In this expression, (3.127) and (3.130) are contained as special cases.

For single measurements the so far introduced probabilities are actually *empty, meaningless*, i.e., not controllable expressions. Only by a great number ($N \to \infty$) of measurements on the same system under always the same conditions, or simultaneously on many non-interacting, completely equivalent systems, the probability function w for the distribution (*scattering*) of the single results can be made directly observable. In such a case it is reasonable, as already seen in Sect. 2.2.6, to introduce average values and expectation values, respectively, for the measurement of the observable A on a system (or an ensemble of systems) in the state $|\psi\rangle$. These we get, rather plausibly, by the prescription to multiply each thinkable measuring value by the probability of its appearance, and then to add up:

$$\begin{aligned} \sum\!\!\!\!\!\!\int\limits_i a_i w(a_i|\psi) &= \sum\!\!\!\!\!\!\int\limits_i a_i |\langle a_i|\psi\rangle|^2 = \\ &= \sum\!\!\!\!\!\!\int\limits_i \langle\psi|A|a_i\rangle\langle a_i|\psi\rangle = \langle\psi|A|\psi\rangle \end{aligned} \tag{3.136}$$

expectation value of A in the state $|\psi\rangle$.

For a discrete spectrum this relation can also be written as follows:

$$\langle\psi|A|\psi\rangle = \sum_i \langle a_i|\psi\rangle\langle\psi|A|a_i\rangle = \mathrm{Tr}\left(P(\psi)\,A\right) . \tag{3.137}$$

In the section after the next one section we will be able to read off from this expression that the projector $P(|\psi\rangle)$ corresponds to the so-called density matrix of the pure state $|\psi\rangle$. The concept of the density matrix is not yet known here, but will be introduced in that section.

Analogously to (2.84), we can define a *mean square deviation* as a measure of the *spreading* of the results of measurement around the expectation value:

$$\Delta A_\psi = \left(\langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2\right)^{1/2} . \tag{3.138}$$

ΔA_ψ is zero if and only if $|\psi\rangle$ is an eigen-state of A. One direction of the proof is trivial. When $|\psi\rangle$ is an eigen-state ($A|\psi\rangle = a|\psi\rangle$), then the right-hand side of (3.138) of course vanishes. However, the reversal is also true. It follows with $\Delta A_\psi = 0$:

$$\begin{aligned}
0 &= \langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2 = \langle\psi|(A - \langle\psi|A|\psi\rangle)^2|\psi\rangle = \\
&= \langle\psi|\left(\sum_j |a_j\rangle\langle a_j|a_j - \langle\psi|A|\psi\rangle\right)^2|\psi\rangle = \\
&= \langle\psi|\sum_j |a_j\rangle\langle a_j|(a_j - \langle\psi|A|\psi\rangle)^2|\psi\rangle = \\
&= \sum_j \langle\psi|a_j\rangle\langle a_j|\psi\rangle(a_j - \langle\psi|A|\psi\rangle)^2 .
\end{aligned}$$

In the third line we have used the orthogonality of the eigen-states $|a_j\rangle$. The summands are all non-negative. Each summand itself must thus already be zero:

$$\langle\psi|a_j\rangle\langle a_j|\psi\rangle(a_j - \langle\psi|A|\psi\rangle)^2 = 0 .$$

The eigen-states $|a_j\rangle$ build a CON-system. Therefore there must exist at least one j for which $\langle a_j|\psi\rangle \neq 0$. But then the bracket must vanish: $a_j = \langle\psi|A|\psi\rangle$. Furthermore, since $\langle\psi|A|\psi\rangle$ is a number independent of j, the bracket must be unequal zero for all states $|a_k\rangle$, which are not degenerate with $|a_j\rangle$, and therewith $\langle a_k|\psi\rangle = 0$. If $\langle a_j|\psi\rangle \neq 0$ for exactly one j, then $|\psi\rangle$ is an eigen-state of A, parallel to $|a_j\rangle$ and perpendicular to all the others $|a_k\rangle$. On the other hand, if there is more than one j, for which $\langle a_j|\psi\rangle \neq 0$, then the eigen-value $a_j = \langle\psi|A|\psi\rangle \equiv a$ is correspondingly highly degenerate and it must be possible to write $|\psi\rangle$ as a linear combination of these linearly independent $|a_j\rangle$. $|\psi\rangle$ is therewith an element of the eigen-space to the eigen-value a and thus an eigen-state of the operator A.

3.3.3 Compatible, Non-compatible Observables

Typical differences with Classical Physics emerge for the description of combined measurements of two operators A and B. From a classical point of view, the order how we perform two partial measurements,—whether first A and then B ore vice versa—, is completely inconsequential, since neither of the measurements changes the state of the system. For both the measurements, always the same initial situation is present, independently of their sequence. That no longer holds, though, for Quantum Mechanics. We got to know of the characteristic non-commutability of operators already in other contexts (see Sects. 2.3.2, 3.1.1). Now, however, we are able to relate this non-commutability to the quantum-mechanical measuring process.

Let $|\psi\rangle$ be the initial state of the system, on to which we apply at first A and then B. We assume that the first measurement yields the eigen-value a_i, the second the eigen-value b_j:

$$|\psi\rangle \xrightarrow{A} |\psi_1\rangle = |a_i\rangle\langle a_i|\psi\rangle \xrightarrow{B} |\psi_2\rangle = |b_j\rangle\langle b_j|\psi_1\rangle \ . \tag{3.139}$$

As in Sect. 3.1.2 we will denote observables as *compatible*, if they do not *interfere with each other* each other in the measuring process the measurement, so that the particular sequence of their actions does not matter. That means in particular that, in the arrangement given in (3.139), a repeated measurement of A at the end yields *with certainty* again the value a_i. The final state $|\psi_2\rangle$ in (3.139) is therefore simultaneously eigen-state of A **and** B. That means according to (3.74):

$$A,\ B\ \textit{compatible} \Longleftrightarrow [A,B]_- = 0 \ . \tag{3.140}$$

But we have to, on the other hand, also conclude that the state $|\psi_1\rangle$, which results from a measurement of A, is still undetermined (degenerate) with respect to the eigen-values of B. Hence it can not yet be about a *completely prepared* pure state. At least a part of the lack of knowledge is lifted by the subsequent application of B and $|\psi_2\rangle$ is already characterized by two numerical values:

$$|\psi_2\rangle \sim |a_i\, b_j\rangle \ , \quad \text{if } [A,B]_- = 0 \ .$$

If there is a further observable C, which commutes with both A and B, then $|\psi_2\rangle$ is not completely determined yet. C has to still be measured. The procedure must be continued until a *complete set* of commutable observables leads to a *unique preparation* of the state.

Definition 3.3.1 *The observables A, B, $C, \ldots, M$ build a **complete (maximal)** set of commuting observables, if there exists **only one** common system of eigen-states.*

Definition 3.3.2 *A **pure state** is **'prepared'** by measuring a complete set of commutable observables A, B, C, . . . , M:*

$$|\psi\rangle = |a\, b\, c, \ldots, m\rangle \ .$$

We have already talked about this last definition, qualitatively, in Sect. 3.1.2.

Non-compatible observables A and B do not have a common set of eigen-states, and therefore do not commute. An application of A on $|\psi_2\rangle$ in (3.139) no longer yields with certainty the measuring value a_i. The effect of preparation due to A is set aside again by B. The add-on *'no longer with certainty'* is important. The measurement of A for **arbitrary** states leads of course always to the **full** spectrum. That includes also a_i, being measured, however, no longer with the probability 1. After the B-measurement the number a_i is for the state $|\psi_2\rangle$ no more a reasonable identification mark.

Subsequent to the definition (3.138) we had shown that the mean square deviation ΔA_ψ equals zero just when $|\psi\rangle$ is an eigen-state of the observable A. The statement that A and B **do not have** a common CON-set of eigen-states, is therefore equivalent to the fact that the *deviations* ΔA_ψ and ΔB_ψ in general can not vanish *at the same time*. A and B can not be sharply measured simultaneously for the same state $|\psi\rangle$. As a rule, the product $\Delta A_\psi\, \Delta B_\psi$ will be truly greater than zero. We therefore want to now calculate an upper bound for this product.

If A and B are Hermitian operators, then the extensions

$$a = A - \langle\psi|A|\psi\rangle\, \mathbb{1} \ ; \quad b = B - \langle\psi|B|\psi\rangle\, \mathbb{1}$$

are also Hermitian operators, so that the mean square deviations ΔA_ψ, ΔB_ψ,

$$\begin{aligned} \Delta A_\psi^2 &= \langle\psi|(A - \langle\psi|A|\psi\rangle\, \mathbb{1})^2|\psi\rangle = \| \ a\, \psi \ \|^2 \ , \\ \Delta B_\psi^2 &= \langle\psi|(B - \langle\psi|B|\psi\rangle\, \mathbb{1})^2|\psi\rangle = \| \ b\, \psi \ \|^2 \ , \end{aligned} \tag{3.141}$$

can be understood as the *lengths* of the vectors $a|\psi\rangle$ and $b|\psi\rangle$. Schwarz's inequality (3.20) then yields the estimation:

$$\Delta A_\psi^2\, \Delta B_\psi^2 \geq |\langle a\, \psi|b\, \psi\rangle|^2 = \langle\psi|a\, b|\psi\rangle\langle\psi|b\, a|\psi\rangle \ .$$

The product of two Hermitian operators is also Hermitian only when the two operators commute. In the decompositions

$$\begin{aligned} a\, b &= \frac{1}{2}(a\, b + b\, a) + \frac{1}{2}[a, b]_- \ , \\ b\, a &= \frac{1}{2}(a\, b + b\, a) - \frac{1}{2}[a, b]_- \end{aligned}$$

each of the first summands is Hermitian, while the second summands are anti-Hermitian. An operator X is called *anti-Hermitian* if $X^+ = -X$. The operator iX is then Hermitian. The inequality

$$\Delta A_\psi^2 \, \Delta B_\psi^2 \geq \frac{1}{4} \langle \psi | (a\,b + b\,a) | \psi \rangle^2 + \frac{1}{4} \langle \psi | i[a,b]_- | \psi \rangle^2$$

contains on the right-hand side the expectation values of Hermitian operators, which must be real according to (3.63). That justifies eventually the estimation

$$\Delta A_\psi \, \Delta B_\psi \geq \frac{1}{2} |\langle \psi | [A,B]_- | \psi \rangle| \, , \tag{3.142}$$

where we still have made use of $[a,b]_- = [A,B]_-$. This is a remarkable result! The quantities on the left-hand side concern, as *scatterings* of the measured values of A and B for a system in the state $|\psi\rangle$, the *uncertainty* of the quantum-mechanical measurement. This is obviously correlated with the *non-commutability* of the operators. One denotes (3.142) as

generalized Heisenberg uncertainty principle (relation).

It interrelates two typical quantum-mechanical phenomena. For the position q and the momentum p (one-dimensional!) of a particle it follows from $[q,p]_- = i\hbar$ (2.102) the actual Heisenberg uncertainty relation (1.5):

$$\Delta p \, \Delta q \geq \frac{\hbar}{2} \, . \tag{3.143}$$

The lower bound is in this special case even independent of the state of the system $|\psi\rangle$. Apart from that, it can of course give special states $|\psi\rangle$, for which the right-hand side of (3.142) vanishes. The *non-compatibility* of the operators A and B does not of course exclude, nevertheless, that there can exist the one or the other common eigen-state.

3.3.4 Density Matrix (Statistical Operator)

In our considerations so far, we have always assumed that the underlying quantum systems are in pure states. By postulate 2, a Hilbert vector $|\psi\rangle$ is ascribed to such a pure state. Furthermore, we have assumed, when investigating the measuring process, that the state before the measurement is *completely prepared*. That means that a complete set of commuting observables has been measured. Only then we *know* the state. But now it is not difficult to imagine that in most practical cases such a complete preparation is not available. Think of a macroscopic solid, which consists of some 10^{23} atomic nuclei and electrons. How can one get complete information for this system? One does not actually need to have in mind necessarily

only macroscopic systems. Incomplete preliminary investigations can prevent, even for in principle simple systems, the definition of a pure state. Scattering experiments with unpolarized electrons can serve as prominent examples.

On the other hand, the complete preparation of a pure state does not always appear to be absolutely necessary for the analysis of empirical findings. Thermodynamics, for instance, comes, within certain limits, absolutely to satisfying results, although it uses only macroscopic variables such as pressure, volume, energy, magnetization, etc..

If for a quantum-mechanical description only an incomplete set of specifications about the system is available, then the so far developed methods are to be complemented by statistical procedures. A corresponding concept of the density matrix, which will now be introduced, and for which other equivalent nomenclature is applied as, e.g., density operator or statistical operator. It is the most general form of a quantum-mechanical description of physical systems. The density matrix is of central importance in the framework of Quantum Statistics, which is the topic of Vol. 8 of this ground course in Theoretical Physics.

If the set of observables, which has been measured at a certain point of time, is not complete, i.e., therefore does not exist sufficient information about the system, then one says that the system is only *weakly prepared*, or that it is in a

mixed state

In such a case it is not describable by a Hilbert vector. However, the following statement might be possible:

The system is with the probability p_m in the pure state $|\psi_m\rangle; m = 1, 2, \ldots$

$$0 \leq p_m \leq 1 \; ; \qquad \sum_m p_m = 1 \; . \tag{3.144}$$

$|\psi_m\rangle$ is an eigen-state of all the observables, which have actually been measured, and simultaneously of those, whose measurements are lacking for a complete preparation. $|\psi_m\rangle$ is thus one of the *thinkable* states, which the system, about which only incomplete information is available, might occupy. It is an essential task for Quantum Statistics (Vol. 8) to develop concrete expressions for the related probabilities p_m. Since they are eigen-states of certain observables, we can presume the $|\psi_m\rangle$ to be orthonormalized:

$$\langle \psi_m | \psi_n \rangle = \delta_{mn} \; . \tag{3.145}$$

Strictly speaking, we need for the following only the normalization, not necessarily the orthogonality (see Exercise 3.3.12). For simplicity we restrict our considerations here to the case where m is a discrete index. The transfer to the continuous case turns out to be unproblematic.

If the system were in the pure state $|\psi_m\rangle$, then the expectation value $\langle \psi_m | A | \psi_m \rangle$ would actually be the measured value for the observable A. But because of our incomplete information about the system, we are now forced to perform an additional statistical averaging, since we know only the probability p_m with which the system actually occupies this state:

expectation value of A in the mixed state

$$\langle A\rangle = \sum_m p_m \langle\psi_m|A|\psi_m\rangle \ . \tag{3.146}$$

One should bear in mind the two different types of averaging in this expression. The statistical averaging over the weights p_m is due to our incomplete information and could, fully or at least partially, be removed by corresponding additional measurements. In contrast, the quantum-mechanical averaging is of intrinsic nature. It is, as we have discussed in the preceding sections, a consequence of the outcome of the quantum-mechanical measuring process. The quantum-mechanical averaging ($\{|b_i\rangle\}$: CON-system)

$$\langle\psi_m|A|\psi_m\rangle = \sum_{i,j} \langle\psi_m|b_i\rangle\, A_{ij} \langle b_j|\psi_m\rangle \ ,$$

$$A_{ij} = \langle b_i|A|b_j\rangle \tag{3.147}$$

is performed by use of probability amplitudes $\langle b_j|\psi_m\rangle$, therefore concerns states and leads to the well-known effects of interference. The statistical averaging, on the other hand, aims directly at the expectation values and not at the states, so that the different pure states $|\psi_m\rangle$ of the mixture do not interfere with each other. The mixed state thus results from an incoherent superposition of pure states.

The consistent handling of the two different averaging processes is accomplished by use the of the

density matrix (statistical operator)

$$\rho = \sum_m p_m |\psi_m\rangle\langle\psi_m| \ , \tag{3.148}$$

which is of outstanding importance for the whole of Quantum Statistics. As in (3.146), the sum in (3.148) runs over all *thinkable* pure states. Let us compile the most important properties of the density matrix (actually better: density operator) in the form of the following listing:

1) Expectation values

Let $\{|\varphi_n\rangle\}$ be an arbitrary CON-system. Then it holds for the expectation value of an observable A, starting at (3.146):

$$\begin{aligned}\langle A\rangle &= \sum_m \sum_{i,j} p_m \langle\psi_m|\varphi_i\rangle\langle\varphi_i|A|\varphi_j\rangle\langle\varphi_j|\psi_m\rangle = \\ &= \sum_{i,j} \langle\varphi_i|A|\varphi_j\rangle \sum_m p_m \langle\varphi_j|\psi_m\rangle\langle\psi_m|\varphi_i\rangle = \\ &= \sum_{i,j} A_{ij}\,\rho_{ji} = \sum_i (A\,\rho)_{ii} \ .\end{aligned}$$

Not surprisingly, the original goal, namely the calculation of the expectation values of observables can be performed by the use of ρ:

$$\langle A \rangle = \mathrm{Tr}(\rho A) = \mathrm{Tr}(A \rho) \; . \tag{3.149}$$

We remember that the trace is independent of the applied CON-basis. This can lead to a great computational advantage. For an explicit evaluation, one should apply the basis *as convenient as possible*.

2) $\rho = \rho^+$: Hermitian

ρ itself can therewith be interpreted as an observable. The proof of the hermiticity follows directly from the definition (3.148). The weights p_m are real and the projection operator $|\psi_m\rangle\langle\psi_m|$ is Hermitian.

3) ρ: positive-definite

It holds for an arbitrary state $|\varphi\rangle$:

$$\langle\varphi|\rho|\varphi\rangle = \sum_m p_m |\langle\varphi|\psi_m\rangle|^2 \geq 0 \; . \tag{3.150}$$

The expectation value of ρ in the normalized state $|\varphi\rangle$ expresses the probability to find the system in this state $|\varphi\rangle$. When we represent the density matrix in the CON-basis $\{|a_i\rangle\}$ of the observable A, then, in the diagonal at the i-th position, one has just the probability for the measurement yielding the value a_i in the mixed state.

In connection with (3.127), we had identified the projector $P(\psi) = |\psi\rangle\langle\psi|$ as an observable, which answer with 'yes' (1) or 'no' (0) whether or not the system is in the state $|\psi\rangle$. The expectation value $\langle\varphi|P(\psi)|\varphi\rangle$ in a pure state $|\varphi\rangle$ corresponds then, according to (3.127), to the probability with which $|\varphi\rangle$ is contained in $|\psi\rangle$. The result for the expectation value in a mixed state reads analogously:

$$\begin{aligned}
\langle P(\psi)\rangle &= \mathrm{Tr}(|\psi\rangle\langle\psi|\rho) = \\
&= \mathrm{Tr}\left(\sum_m p_m |\psi\rangle\langle\psi|\psi_m\rangle\langle\psi_m|\right) = \\
&= \sum_{m,n} p_m \langle\varphi_n|\psi\rangle\langle\psi|\psi_m\rangle\langle\psi_m|\varphi_n\rangle = \\
&= \sum_{m,n} p_m \langle\psi|\psi_m\rangle\langle\psi_m|\varphi_n\rangle\langle\varphi_n|\psi\rangle = \\
&= \sum_n \langle\psi|\rho|\varphi_n\rangle\langle\varphi_n|\psi\rangle \; .
\end{aligned}$$

Thus it also holds:

$$\langle P(\psi)\rangle = \langle\psi|\rho|\psi\rangle \; . \tag{3.151}$$

4) Trace

Let $\{|\varphi_n\rangle\}$ be an arbitrary CON-system:

$$\mathrm{Tr}\,\rho = \sum_n \langle\varphi_n|\rho|\varphi_n\rangle = \sum_{n,m} \langle\varphi_n|\psi_m\rangle\langle\psi_m|\varphi_n\rangle p_m =$$

$$= \sum_m p_m \langle\psi_m| \underbrace{\left(\sum_n |\varphi_n\rangle\langle\varphi_n|\right)}_{\mathbb{1}} |\psi_m\rangle = \sum_m p_m \langle\psi_m|\psi_m\rangle \ .$$

Therefore we get

$$\mathrm{Tr}\,\rho = 1 \ , \tag{3.152}$$

a relation which is compatible with the probability-interpretation (3.150). It follows, incidentally, for $A = \mathbb{1}$ also directly from (3.149).

5) Pure state

Pure states also can be treated, as special cases, by the density-matrix formalism. The highest degree of information corresponds to them, which is realized by $p_1 = 1$; $p_m = 0 \ \forall m \neq 1$. The general definition (3.148) then reads:

$$\rho_\psi = |\psi\rangle\langle\psi| = P(\psi) \ . \tag{3.153}$$

When we insert this result into (3.149), then we obtain for the expectation value of an observable A in the pure state $|\psi\rangle$ the already previously derived expression (3.137).

6) Square of the density matrix

Via ρ^2 pure and mixed states can be distinguished. That can be seen as follows:

$$\rho^2 = \sum_{n,m} p_n p_m |\psi_n\rangle\langle\psi_n|\psi_m\rangle\langle\psi_m| \overset{(3.145)}{=} \sum_n p_n^2 |\psi_n\rangle\langle\psi_n| \ .$$

Because of

$$\mathrm{Tr}\,\rho^2 = \sum_n p_n^2 \,\mathrm{Tr}\left(\rho_{\psi_n}\right) \overset{(3.152)}{=} \sum_n p_n^2$$

the following useful criterion arises:

$$\mathrm{Tr}\,\rho^2 = \sum_n p_n^2 \qquad \begin{cases} = 1 & \longleftrightarrow \text{ pure state} \ , \\ < 1 & \longleftrightarrow \text{ mixed state} \ . \end{cases} \tag{3.154}$$

Since all experimentally verifiable statements about a given physical system can be calculated with the density matrix, one agrees that:

Two mixed states are identical, if they are described by the same density matrix!

The precise structure of the density matrix is determined by the actually present pre-information about the system to be described. To find the density matrix is a typical problem of the Quantum Statistics (Vol. 8).

3.3.5 *Uncertainty Relation*

At the end of this Sect. 3.3 we want to come back once more to the

generalized Heisenberg uncertainty relation

which we could formulate already in (3.142) for pure states. Because of its fundamental meaning we want to demonstrate now that it is valid in completely analogous form also for systems in mixed states.

Theorem 3.3.1 *Let A, B be two non-commutable Hermitian operators,*

$$[A,B]_- = \frac{\hbar}{i}\,C\,,$$

with the indeterminacies:

$$\Delta A = \sqrt{\langle (A - \langle A\rangle \mathbb{1})^2\rangle}\,,$$
$$\Delta B = \sqrt{\langle (B - \langle B\rangle \mathbb{1})^2\rangle}\,.$$

For these, one has the estimation:

$$\Delta A\,\Delta B \geq \frac{\hbar}{2}|\langle C\rangle| = \frac{1}{2}|\langle [A,B]_-\rangle|\,. \tag{3.155}$$

Proof We define as for (3.141):

$$a = A - \langle A\rangle \mathbb{1} \Longrightarrow \Delta A^2 = \langle a^2\rangle = \mathrm{Tr}(\rho\, a^2)\,,$$
$$b = B - \langle B\rangle \mathbb{1} \Longrightarrow \Delta B^2 = \langle b^2\rangle = \mathrm{Tr}(\rho\, b^2)\,.$$

Let the system be in a mixed state, to which the density matrix ρ is ascribed. Together with A and B, a and b also are of course Hermitian operators with

$$[a,b]_- = [A,B]_- = \frac{\hbar}{i}\,C\,.$$

With a real parameter λ, we introduce the non-Hermitian operator

$$d = a + i\,\lambda\, b\,.$$

Then we have:

$$\mathrm{Tr}(d^+\,\rho\,d) = \sum_n \langle\varphi_n|d^+\,\rho\,d|\varphi_n\rangle = \sum_n \langle d\varphi_n|\rho|d\,\varphi_n\rangle \geq 0\ .$$

Let $\{|\varphi_n\}$ be thereby any CON-system. The given estimation then results from the positive-definiteness of the density matrix (3.150). It further follows with (3.149):

$$\begin{aligned} 0 \leq \mathrm{Tr}(d^+\rho\,d) &= \mathrm{Tr}(\rho\,d\,d^+) = \\ &= \mathrm{Tr}[\rho(a + i\,\lambda\,b)\,(a - i\,\lambda\,b)] = \\ &= \mathrm{Tr}[\rho(a^2 + \lambda^2 b^2 - i\,\lambda[a,b]_-] = \\ &= \langle a^2\rangle + \lambda^2\langle b^2\rangle - i\,\lambda\langle[a,b]_-\rangle\ . \end{aligned}$$

This holds for arbitrary λ, i.e. also for that λ_0, which makes $\mathrm{Tr}(d^+\rho\,d)$ minimal:

$$\begin{aligned} \frac{d}{d\lambda}\ \mathrm{Tr}(d^+\,\rho\,d)\big|_{\lambda=\lambda_0} &\stackrel{!}{=} 0 = 2\,\lambda_0\langle b^2\rangle - \hbar\langle C\rangle \\ &\longrightarrow \lambda_0 = \frac{\hbar\langle C\rangle}{2\langle b^2\rangle}\ . \end{aligned}$$

This λ_0 we insert into the above estimation:

$$0 \leq \langle a^2\rangle - \frac{\hbar^2\langle C\rangle^2}{4\langle b^2\rangle}\ .$$

This leads immediately to the assertion! One easily convinces oneself that (3.142) is contained as special case in (3.155).

3.3.6 *Exercises*

Exercise 3.3.1 Let the linear Hermitian operator A have countably-infinite eigenvalues a_i with orthonormalized eigen-states $|a_i\rangle$. What are the probabilities for the values a_2 and a_3 to be measured for the system in the state

$$|\psi\rangle = |a_1\rangle + \frac{i}{2}|a_2\rangle\ ?$$

Exercise 3.3.2 Under which preconditions for the pure state $|\psi\rangle$ is the equality sign valid in the generalized uncertainty relation (3.142)?

Exercise 3.3.3 From the generalized Heisenberg uncertainty relation (3.155) derive for systems in arbitrary, not necessarily pure states the condition for *minimal uncertainty*. Compare the result with that of Exercise 3.3.2.

Exercise 3.3.4

1. Can

$$\widehat{\rho} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

be a density matrix?
2. The system is in a mixed state described by the density matrix

$$\rho = \begin{pmatrix} \frac{1}{2} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{2} \end{pmatrix} .$$

Evaluate explicitly for the observables

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} ; \qquad B = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

the generalized Heisenberg uncertainty relation (3.155)!

Exercise 3.3.5 To the observable *electron spin* (Sects. 5.2 and 5.3, Vol. 7) the operator

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} ; \qquad \boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$$

is ascribed, where the $\sigma_{x,y,z}$ are Pauli's spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} ; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The eigen-states of the observable σ_z have been used as CON-basis for the representation of the operators $\sigma_{x,y,z}$, what can be realized by a Stern-Gerlach apparatus, oriented in z-direction (see Sect. 1.3.2).

1. Calculate the eigen-states $|\pm\rangle$ and the eigen-values $\lambda_\pm$ of the operator σ_z.
2. Show that σ_x and σ_y have the same eigen-values as σ_z. Is that also true for the eigen-states?
3. Calculate the uncertainty relation for the operator-pairs (σ_x, σ_y), (σ_x, σ_z) and (σ_y, σ_z)!

Exercise 3.3.6 With the eigen-states of σ_z as CON-basis, the observables A, B, C have the following matrix representations:

$$A = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix} ; \quad B = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} ; \quad C = \begin{pmatrix} 0 & 2i \\ -2i & 0 \end{pmatrix} .$$

The following expectation values were measured on a spin state:

$$\langle A\rangle = 2\,; \quad \langle B\rangle = \frac{1}{2}\,; \quad \langle C\rangle = 0\,.$$

1. Determine the density matrix ρ of the spin state!
2. Is it a pure or a mixed spin state?
3. What is the probability of finding the spin value $+1$ (or $+\hbar/2$) with a measurement in z-direction?
4. Calculate $\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle$!

Exercise 3.3.7

1. An (idealized) Stern-Gerlach apparatus is oriented in the direction

$$\mathbf{e} = (\sin\vartheta\cos\varphi,\ \sin\vartheta\sin\varphi,\ \cos\vartheta)$$

   and prepares the pure spin states $|\mathbf{e}_\pm\rangle$. Calculate these states!
2. How do the density matrices $\rho_{e_\pm}$ for the pure states from 1) read:

   a) in the basis $|\mathbf{e}_\pm\rangle$,
   b) in the basis $|\pm\rangle$ (Exercise 3.3.5, part 1))?

3. The electron-spin polarization $\mathbf{P}$ is defined by

$$\mathbf{P} = \langle\boldsymbol{\sigma}\rangle = \mathrm{Tr}(\rho\,\boldsymbol{\sigma})$$

   ($\boldsymbol{\sigma}$ as in Exercise 3.3.5). Let the pure state $|\mathbf{e}_+\rangle$ be prepared. Which polarizations are measured in $x-$, $y-$, z-direction?

Exercise 3.3.8 We use the same notations as in the three preceding exercises. Let now $p_\pm$ be the weights of the states $|\mathbf{e}_\pm\rangle$ in a mixed spin state.

1. Express the density matrix ρ and the electron-spin polarization $\mathbf{P}$ by $p_\pm$ and show therewith that

$$\rho = \frac{1}{2}\,(\mathbb{1} + \mathbf{P}\cdot\boldsymbol{\sigma})\,.$$

2. Determine the eigen-values of ρ.
3. Show that

$$P_z = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}\,,$$

   where $N_{\uparrow,\downarrow}$ means the number of the electrons, which have their spin parallel (anti-parallel) to the z-direction.

Exercise 3.3.9 Let

$$\rho = \frac{1}{2}\left(\mathbb{1} + \mathbf{P}\cdot\boldsymbol{\sigma}\right)$$

be the density matrix for electrons in a mixed spin state. Show that the vector of the spin polarization $\mathbf{P}$ can then be written as:

$$\mathbf{P} = \langle\boldsymbol{\sigma}\rangle \ .$$

(Definition of $\boldsymbol{\sigma}$ in Exercise 3.3.5.)

Exercise 3.3.10 $|+\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|-\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ are the eigen-states of the z-component of the electron spin. Let N_0 identical electrons be in the pure spin state

$$|\psi_0\rangle = \frac{1}{5}\begin{pmatrix}3\\4\end{pmatrix} \ .$$

They pass through two Stern-Gerlach apparatus. The first is oriented in ($\vartheta = \pi/2$, $\varphi = 0$)-direction letting through only electrons with spin $+\hbar/2$ (filter!). The second has the direction ($\vartheta = \pi$, $\varphi = \pi$) and lets pass only electrons with spin $-\hbar/2$. Which fractional amount of particles passes through the whole set-up?

Exercise 3.3.11 Inspect whether the density matrix

$$\rho = \frac{1}{3}\begin{pmatrix}1 & 0 & -1\\ 0 & 1 & 0\\ -1 & 0 & 1\end{pmatrix}$$

describes a pure state and calculate the expectation value of the observable

$$A = \begin{pmatrix}0 & 0 & i\\ 0 & 0 & 0\\ -i & 0 & 0\end{pmatrix}$$

in this state.

Exercise 3.3.12 Prove that the characteristic properties of the statistical operator (density matrix)

$$\rho = \sum_m p_m |\psi_m\rangle\langle\psi_m|$$

remain unchanged even then when the states $|\psi_m\rangle$ are normalized, but not orthogonal.

3.4 Dynamics of Quantum Systems

Up to now we have considered the quantities, which are important for Quantum Mechanics, namely

states, observables, scalar products, expectation values, ... ,

at a given same fixed point of time. The experiment, however, requires also relationships between these quantities at different points of time. We therefore need statements about the dynamical evolution of quantum systems.

We begin with the remark that the time t is a parameter, a so-called c-number, which we determine as in the classical, non-relativistic Mechanics (Vol. 1), namely by looking at the movement of the hand of a macroscopic clock. The time is thus not to be understood as the eigen-value of any physical operator. All attempts to introduce an observable *time* run into insurmountable, basic difficulties, which, however, we cannot inspect here in detail.

The central challenge of this section is the following: Let the state of the system be known, by a measurement at the time t_0. Which statements are then possible for $t > t_0$ if the system is not *disturbed* in the meantime by any other measurement, i.e if it is left alone! In order to answer this question, we need equations of motion of states and observables, which are then to be integrated. The next subsections deal with such equations of motion.

3.4.1 Time Evolution of the States (Schrödinger Picture)

Let the

pure states $|\psi(t_0)\rangle$

be prepared at the time $t = t_0$. How does this state evolve by the time $t > t_0$, if no further measurement is done in the interval $[t_0, t]$? By the ansatz

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle \tag{3.156}$$

we shift the answer of this question to the

time evolution operator $U(t, t_0)$**.**

We list some basic requirements which must be fulfilled by $U(t, t_0)$:

1. For the probability statements it is necessary that the norm of the state is constant in time:

$$\langle\psi(t)|\psi(t)\rangle \stackrel{!}{=} \langle\psi(t_0)|\psi(t_0)\rangle \ .$$

But that is possible only if

$$U \text{is unitary} \Longleftrightarrow U^{+}(t,t_0) = U^{-1}(t,t_0)\ . \tag{3.157}$$

2.

$$U(t_0,t_0) = \mathbb{1}\ . \tag{3.158}$$

3.

$$U(t,t_0) = U(t,t')\,U(t',t_0)\ . \tag{3.159}$$

These last two conditions can be combined:

$$U(t,t_0) = U^{-1}(t_0,t)\ . \tag{3.160}$$

4. In closed (conservative) systems only time**differences** matter; the zero of time is by no means significant:

$$U(t,t_0) = U(t-t_0)\ . \tag{3.161}$$

This relation is of course no longer valid when the system underlies the influence of time-dependent external forces, so that the properties of the system become explicitly time-dependent.

Let us now consider an
infinitesimal time-translation

$$U(t+dt,t) = \mathbb{1} + \left(\frac{\partial}{\partial t'}\,U(t',t)\right)_{t'=t} dt + \mathcal{O}(dt^2)\ , \tag{3.162}$$

for which a Taylor expansion can be terminated after the linear term. We have introduced in Sect. 3.2.7 the derivative of operators with respect to a real parameter. For the second summand we write:

$$\left(\frac{\partial}{\partial t'}\,U(t',t)\right)_{t'=t} = -\frac{i}{\hbar}\,H(t)\ . \tag{3.163}$$

The extracted factor $-1/\hbar$ is only a convention and has no deeper physical meaning. The imaginary unit i takes care for the fact that according to (3.94) the *generator of the time-translation* H is a Hermitian operator. Only then, U is unitary. Strictly speaking, we have not yet gained very much by the ansatz (3.163), since the unknown operator U has been replaced by the at first equally unknown operator H. The physical meaning of H is provided ultimately only after the principle of

correspondence is discussed in Sect. 3.5. We therefore have to at this stage accept the identification

$$H: \quad \text{Hamilton operator} ,$$

more or less axiomatically. According to all experiences so far any other identification quickly leads to contradictions (see Sect. 3.5). We met the Hamilton operator (Hamiltonian) for the first time in (2.16). The rule of correspondence in Sect. 2.3.2 shows how to come to this operator starting with the classical Hamilton function.

Equation (3.162),

$$U(t + dt,\, t) = \mathbb{1} - \frac{i}{\hbar} H(t)\, dt , \tag{3.164}$$

leads us now to the required equation of motion for the state vectors:

$$i\hbar|\dot{\psi}(t)\rangle = i\hbar \frac{|\psi(t + dt)\rangle - |\psi(t)\rangle}{dt} = i\hbar \frac{[U(t + dt,\, t) - \mathbb{1}]}{dt} |\psi(t)\rangle .$$

That results in the fundamental

time-dependent Schrödinger equation

$$i\hbar|\dot{\psi}(t)\rangle = H|\psi(t)\rangle . \tag{3.165}$$

If we describe the state especially by a space-dependent wave function, this equation turns into the equation of motion (2.18), which we previously *'derived'* using another method. We could also have taken this analogy to identify H as the Hamilton operator. The explicit transition from the abstract Hilbert-space vector $|\psi(t)\rangle$ to the wave function $\psi(\mathbf{r}, t)$ will be performed in Sect. 3.5.2.

In the same manner, as above one derives the Schrödinger equation for the bra-vector:

$$-i\hbar\langle\dot{\psi}(t)| = \langle\psi(t)|H . \tag{3.166}$$

The hermiticity of the Hamilton operator H comes here, of course, into play.

Equations (3.165) and (3.166) are the equations of motion for pure states. Mixed states are ascribed to density matrices (3.148). When we differentiate them with respect to time then it follows with (3.165) and (3.166):

$$\dot{\rho} = \sum_m p_m(|\dot{\psi}_m\rangle\langle\psi_m| + |\psi_m\rangle\langle\dot{\psi}_m|) =$$

$$= -\frac{i}{\hbar} \sum_m p_m(H|\psi_m\rangle\langle\psi_m| - |\psi_m\rangle\langle\psi_m|H) .$$

The weights p_m are time-independent since the *state of information* can not change before the next measurement. The equations of motion, however, shall be valid here for time intervals in which no measurement is performed. The

equation of motion of the density matrix

$$\dot{\rho} = \frac{i}{\hbar} [\rho, H]_- \tag{3.167}$$

is sometimes denoted as *von Neumann's differential equation*. It is the quantum-mechanical analog to the classical *Liouville equation*, which we will get to know in the framework of the Classical Statistical Mechanics in Vol. 8.

This kind of describing the dynamics of quantum systems is not the only possible one, as we will demonstrate later in this section. Typical for this so-called

Schrödinger picture (state picture)

is that the temporal evolution of the system is carried by time-dependent states, whereas the operators (observables) are time-independent, so long as they do not *explicitly* depend on time, as for instance by switching on and switching off processes or by the presence of time-dependent external fields:

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} \, . \tag{3.168}$$

The unitarity of the time evolution operator U takes care for the fact that the *lengths* of the state vectors in the Hilbert space and the *angles* between them remain temporally invariant. The time-dependence consists, according to that, apparently of a *rigid rotation* of the vectors in the Hilbert space.

3.4.2 Time Evolution Operator

The Schrödinger Eq. (3.165) and the definition Eq. (3.156) for $U(t, t_0)$ can be combined as the equation of motion for the time evolution operator:

$$i\hbar \frac{d}{dt} U(t, t_0) = H(t) \, U(t, t_0) \, . \tag{3.169}$$

This can be formally integrated with the boundary condition (3.158):

$$U(t, t_0) = \mathbb{1} + \frac{1}{i\hbar} \int_{t_0}^{t} dt_1 \, H(t_1) \, U(t_1, t_0) \, . \tag{3.170}$$

We can perform an iteration, by which it follows, for instance, in the second step:

$$U(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} dt_1\, H(t_1) + \frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)\, H(t_2)\, U(t_2,t_0)\ .$$

That can obviously be continued leading eventually to the **von Neumann's series**:

$$U(t,t_0) = \mathbb{1} + \sum_{n=1}^{\infty} U^{(n)}(t,t_0)\ , \tag{3.171}$$

$$U^{(n)}(t,t_0) = \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)\, H(t_2) \cdots H(t_n)$$

$$(t \geq t_1 \geq t_2 \geq \ldots \geq t_n \geq t_0)\ . \tag{3.172}$$

In the last expression one has to strictly obey the time ordering, since the Hamilton operators at different points of time, in case of explicit time-dependence, do not necessarily commute. The operator with the earliest time stands farthest to the right.

For a further transformation, we introduce **Dyson's time ordering operator**:

$$T\left(A(t_1)\,B(t_2)\right) = \begin{cases} A(t_1)\,B(t_2) & \text{for } t_1 > t_2\ , \\ B(t_2)\,A(t_1) & \text{for } t_2 > t_1\ . \end{cases} \tag{3.173}$$

The generalization to more than two operators is obvious. By the way, simultaneity does not mean an uncertainty in (3.172), since then the Hamiltonians commute anyway.

Let us consider the $n = 2$-term in (3.172). The lower triangle in Fig. 3.12 represents the region of integration. As indicated, we can settle the integration *stripe by stripe* in two different manners. This means:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)\, H(t_2) = \int_{t_0}^{t} dt_2 \int_{t_2}^{t} dt_1\, H(t_1)\, H(t_2)\ .$$

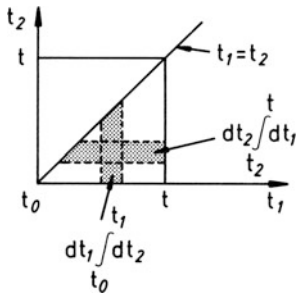

Fig. 3.12 Illustration of the equivalence of two variants of integration for the $n = 2$-term of von Neumann's series

On the right-hand side we interchange the times t_1 and t_2:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)\, H(t_2) = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, H(t_2)\, H(t_1) \ .$$

The last two equations can be combined as follows:

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)\, H(t_2) = \frac{1}{2} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdot$$
$$\cdot \left(H(t_1)\, H(t_2)\, \Theta(t_1 - t_2) + H(t_2)\, H(t_1)\, \Theta(t_2 - t_1) \right) \ .$$

Θ is thereby the *step function*:

$$\Theta(t) = \begin{cases} 1 \ , & \text{if } \ t > 0 \ , \\ 0 & \text{otherwise} \ . \end{cases} \tag{3.174}$$

It thus results with (3.173):

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H(t_1)\, H(t_2) = \frac{1}{2} \iint_{t_0}^{t} dt_1\, dt_2\, T\left(H(t_1)\, H(t_2) \right) \ .$$

That can be generalized to n terms so that (3.172) takes the following form:

$$U^{(n)}(t, t_0) = \frac{1}{n!} \left(-\frac{i}{\hbar} \right)^n \int_{t_0}^{t} \ldots \int_{t_0}^{t} dt_1, \ldots, dt_n\, T\left(H(t_1)\, H(t_2) \ldots H(t_n) \right) \ . \tag{3.175}$$

If one inserts this result into (3.171), one finds a very compact representation of the time evolution operator in the Schrödinger picture:

$$U(t, t_0) = T \exp\left(-\frac{i}{\hbar} \int_{t_0}^{t} dt'\, H(t') \right) \ . \tag{3.176}$$

However, this compact and elegant representation must not mislead one, because for concrete evaluations, one has to revert to the original formulation (3.171), unless one of the two following special cases is realized:

1. If we can assume

$$[H(t),\, H(t')]_- = 0 \qquad \forall t, t' \ ,$$

then the time ordering operator has only the effect of the identity,

$$T \longrightarrow \mathbb{1} \ ,$$

can therefore be left out in (3.176).

2. In the case of a closed, conservative system the Hamilton operator in (3.176) looses its explicit time-dependence:

$$\frac{\partial H}{\partial t} = 0 \ .$$

Then the time evolution operator U reduces to a comparatively simple form:

$$U(t, t_0) = U(t - t_0) = \exp\left[-\frac{i}{\hbar} H(t - t_0)\right] \ . \tag{3.177}$$

From this we can conclude that the eigen-states of the Hamiltonian,

$$H|E_n\rangle = E_n|E_n\rangle \ , \tag{3.178}$$

exhibit only a trivial time-dependence:

$$|E_n(t)\rangle = U(t, 0)|E_n\rangle = e^{-\frac{i}{\hbar}E_n t}\,|E_n\rangle \ . \tag{3.179}$$

The probability that the state $|E_n(t')\rangle$, which has been prepared at the time t', continues to exist at the time $t > t'$, is constant and is equal to 1:

$$|\langle E_n(t)|E_n(t')\rangle|^2 = |e^{\frac{i}{\hbar}E_n(t-t')}\langle E_n|E_n\rangle|^2 = 1 \ . \tag{3.180}$$

Such states are called *stationary states* or *states of infinite lifetime*.

For an arbitrary state of a closed system, on the other hand, it holds:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}\,|\psi(0)\rangle = e^{-\frac{i}{\hbar}Ht}\sum_n |E_n\rangle\langle E_n|\psi(0)\rangle =$$

$$= \sum_n e^{-\frac{i}{\hbar}E_n t}|E_n\rangle\langle E_n|\psi(0)\rangle \ . \tag{3.181}$$

Such a state is not necessarily stationary:

$$|\langle\psi(t)|\psi(t')\rangle|^2 =$$

$$= \left|\sum_{n,m} e^{\frac{i}{\hbar}(E_n t - E_m t')}\,\langle E_n|E_m\rangle\langle\psi(0)|E_n\rangle\langle E_m|\psi(0)\rangle\right|^2 =$$

$$= \left|\sum_n e^{\frac{i}{\hbar}E_n(t-t')}|\langle E_n|\psi(0)\rangle|^2\right|^2 \leq \sum_n |\langle E_n|\psi(0)\rangle|^2 = \langle\psi(0)|\psi(0)\rangle \ .$$

So we have:

$$|\langle\psi(t)|\psi(t')\rangle|^2 \leq 1 \,. \tag{3.182}$$

Possibly, this state has only a finite lifetime. The exponential function $\exp\left(\frac{i}{\hbar}E_n(t-t')\right)$, with increasing time difference $(t-t')$, distributes itself gradually over the unit circle of the plane of complex number and, by destructive interference, ensures that the above square of the absolute value vanishes ($\rightarrow$ quasi-particle concept of the many-body theory; Vol. 9).

3.4.3 *Time Evolution of the Observables (Heisenberg Picture)*

The Schrödinger picture is not at all *compulsory*, i.e., it is not the only possible formulation of the dynamics of quantum systems. The special representation (*'picture'*) can be changed *almost arbitrarily* so long as physically relevant quantities and relations, i.e., the measurable quantities such as

expectation values, eigen-values, scalar products, ...,

remain thereby unaffected. We know from Sect. 3.2.7 that this requirement is fulfilled by unitary transformations ((3.90)–(3.92)). Which picture one actually chooses, depends on, where the actual physical problem can be laid out most clearly.

In the Schrödinger picture the full time-dependence is carried by the states. However, the expectation values, for instance, are built up by state vectors **and** operators. One can therefore easily imagine that for such measurable values, only the *relative position* of operators and states in the Hilbert space $\mathcal{H}$ is of importance. It is therefore imaginable that, instead of the states, the observables take over the full time-dependence. This is exactly the case in the so-called Heisenberg picture, which arises out of the Schrödinger picture by a suitable unitary transformation.

Let us assume that it holds for the states in the Heisenberg picture:

$$|\psi_H(t)\rangle \equiv |\psi_H\rangle \stackrel{!}{=} |\psi(t_0)\rangle \,. \tag{3.183}$$

At an arbitrary but fixed point of time t_0 (e.g. $t_0 = 0$) the time-independent *Heisenberg state* shall coincide with the corresponding Schrödinger state. From now on, all quantities of the Heisenberg picture get an index H in order to distinguish them from those of the Schrödinger picture, which shall remain without index.

The equations of motion for pure and mixed states in the Heisenberg picture are of course trivial:

$$|\dot{\psi}_H\rangle = 0 \,, \tag{3.184}$$

$$\dot{\rho}_H = \sum_m p_m \left\{|\dot{\psi}_{m\,H}\rangle\langle\psi_{m\,H}| + |\psi_{m\,H}\rangle\langle\dot{\psi}_{m\,H}|\right\} = 0 \,. \tag{3.185}$$

Now we get with the time evolution operator of the Schrödinger picture ((3.156), (3.160)):

$$|\psi_H\rangle = U^+(t,t_0)|\psi(t)\rangle = U(t_0,t)|\psi(t)\rangle \ . \tag{3.186}$$

The reverse transformation is obvious:

$$|\psi(t)\rangle = U(t,t_0)|\psi_H\rangle \ .$$

The corresponding unitary transformation for the operators then must read:

$$A_H(t) = U^+(t,t_0)\, A\, U(t,t_0) \ . \tag{3.187}$$

Here also, the reversal is clear:

$$A = U(t,t_0)\, A_H(t)\, U^+(t,t_0) \ . \tag{3.188}$$

The physics does not change by the transformation. Let us check that:

1. Expectation values remain unchanged:

$$\begin{aligned}\langle\psi_H|A_H(t)|\psi_H\rangle &= \langle\psi(t)|U(t,t_0)\, U^+(t,t_0)\, A\, U(t,t_0)\, U^+(t,t_0)|\psi(t)\rangle = \\ &= \langle\psi(t)|A|\psi(t)\rangle \ .\end{aligned}$$

2. Scalar products are also invariant:

$$\langle\psi_H|\varphi_H\rangle = \langle\psi(t)|U(t,t_0)\, U^+(t,t_0)|\varphi(t)\rangle = \langle\psi(t)|\varphi(t)\rangle \ .$$

3. Commutation relations are of outstanding importance in Quantum Mechanics. It is therefore decisive to know that commutators are form-invariant under unitary transformations:

$$\begin{aligned}[A,B]_- &= C \\ &= AB - BA = UA_HU^+UB_HU^+ - UB_HU^+UA_HU^+ \\ &= U[A_H\ , B_H]_-\, U^+ \ .\end{aligned}$$

Thus:

$$[A_H,\, B_H]_- = U^+\, C\, U = C_H \ . \tag{3.189}$$

The equation of motion of the operators is important. It follows simply from the definition for the operator A:

$$\begin{aligned}\frac{d}{dt}A_H(t) &= \frac{\partial U^+}{\partial t}\,A\,U + U^+\,\frac{\partial A}{\partial t}\,U + U^+\,A\,\frac{\partial U}{\partial t} \\ &\overset{(3.169)}{=} -\frac{1}{i\hbar}(H\,U)^+\,A\,U + U^+\,\frac{\partial A}{\partial t}\,U + U^+\,A\,\frac{1}{i\hbar}\,(H\,U) = \\ &= \frac{1}{i\hbar}\,U^+\,[A,H]_-\,U + U^+\,\frac{\partial A}{\partial t}\,U\;.\end{aligned}$$

We define:

$$\frac{\partial A_H}{\partial t} = U^+(t,t_0)\frac{\partial A}{\partial t}U(t,t_0)\;. \tag{3.190}$$

That corresponds, in a certain sense, to a commutability of time-differentiation and unitary transformation. The expression vanishes when the Schrödinger operator is not explicitly time-dependent. So it follows with (3.189):

$$i\hbar\,\frac{d}{dt}\,A_H(t) = [A_H,H_H]_- + i\hbar\,\frac{\partial A_H}{\partial t}\;. \tag{3.191}$$

The closed system represents again an important special case:

$$\begin{aligned}\frac{\partial H}{\partial t} = 0 \overset{(3.177)}{\longrightarrow} U(t,t_0) &= \exp\left[-\frac{i}{\hbar}H(t-t_0)\right] \\ \longrightarrow [H,U]_- = 0 \Longleftrightarrow H_H(t) \equiv H_H &= H\;.\end{aligned} \tag{3.192}$$

The Hamilton operator is then time-independent, while it holds for other observables of the closed system according to (3.187):

$$A_H(t) = e^{\frac{i}{\hbar}H(t-t_0)}\,A\,e^{-\frac{i}{\hbar}H(t-t_0)}\;. \tag{3.193}$$

Heisenberg's equation of motion (3.191) for operators replaces the Schrödinger Eq. (3.165) of the state vectors in the Schrödinger picture. In a certain sense, the operators *rotate* in the Heisenberg picture *contrariwise* to the states in the Schrödinger picture.

There are special operators,which are time-independent even in the Heisenberg representation. They are called:

$$\begin{gathered}\textit{integrals (constants) of motion (conserved quantities)} \\ \Longleftrightarrow \;\textit{observable}\;\; C_H\;\;\textit{with} \\ \text{a)}\;\frac{\partial C}{\partial t} = 0\;; \qquad \text{b)}\;[H_H,\,C_H]_- = 0\;.\end{gathered} \tag{3.194}$$

For instance, in a closed system the Hamilton operator itself is an integral of motion (3.192).

At first glance, the Heisenberg picture appears more abstract, less illustrative than the Schrödinger picture. The *rotation* of vectors is of course easier to visualize than that of operators. Nevertheless, from a quantum-mechanical point of view it is actually *conceptually more consistent*. In particular, it is easier to bring the Heisenberg picture, by use of the principle of correspondence (Sect. 3.5), into contact with Classical Physics. The statement

$$|\dot{\psi}_H\rangle = 0$$

is better understood if one replaces the word *state* by *state of information*. The state $|\psi\rangle$ contains exactly that information, which has been found at the point of time of its preparation by the measurement of a complete set of observables. But this state of information is now indeed constant until the next measurement. Otherwise, it can certainly make a difference, at which time an observable is analyzed.

To the quantum-mechanical state $|\psi_H\rangle$ there is ascribed in Classical Mechanics the *timeless* trajectory of the system in the phase space, i.e. the entirety of points in the phase space, which are available for the system as solutions of the Hamilton equations of motion with corresponding initial conditions. Think of the phase-space ellipse of the harmonic oscillator. The quantum-mechanical observable $A_H(t)$ corresponds to the classical phase-space function $A(\mathbf{q}(t), \mathbf{p}(t), t)$ (*dynamical variable*), which assumes on the *timeless* path different values at different times (see Sect. 3.5.1).

3.4.4 Interaction Representation (Dirac Picture)

There is another representation of the dynamics of quantum systems, which takes an intermediate position between the Schrödinger and the Heisenberg picture because it distributes the time-dependences over states as well as operators. It is called the *interaction representation* or the *Dirac picture*. Starting point is the typical situation, for which the Hamilton operator can be decomposed as follows:

$$H = H_0 + H_1^t \,. \tag{3.195}$$

H_0 is the time-independent Hamilton operator of a system which is more easily treatable than the full one. The *'perturbation term'* H_1^t, however, carries possibly an explicit time-dependence. In many cases one understands by H_0 the *free*, not interacting system, while H_1^t comprises the interactions. The idea of the Dirac picture consists now therein, to transfer the dynamical time-dependence, which is

due to the *free* motion (H_0), to the observables, while the influence of the interaction H_1^t is taken by the states. That succeeds with the following ansatz:

$$|\psi_{\mathrm{D}}(t_0)\rangle = |\psi_H\rangle = |\psi(t_0)\rangle \,, \tag{3.196}$$

$$|\psi_{\mathrm{D}}(t)\rangle = U_{\mathrm{D}}(t,t')|\psi_{\mathrm{D}}(t')\rangle \,, \tag{3.197}$$

$$|\psi_{\mathrm{D}}(t)\rangle = U_0(t_0,t)|\psi(t)\rangle \,. \tag{3.198}$$

All *Dirac quantities* are badged in the following by the index 'D'. t_0 is the given point of time at which Heisenberg and Schrödinger states coincide (3.183). $U_{\mathrm{D}}(t,t')$ is the time evolution operator in the Dirac picture. U_0 means the time evolution operator of the *free* system. Because of $\partial H_0/\partial t = 0$ we have for this according to (3.177):

$$U_0(t,t') = U_0(t-t') = \exp\left[-\frac{i}{\hbar}H_0(t-t')\right] . \tag{3.199}$$

When one compares (3.198) with (3.186), one recognizes that in cases without interaction, i.e., when H_0 is already the *full* Hamilton operator of the system, the Dirac picture is identical to the Heisenberg picture.

The Eqs. (3.196)–(3.198) permit the following rearrangement:

$$\begin{aligned}|\psi_{\mathrm{D}}(t)\rangle &= U_0(t_0,t)|\psi(t)\rangle = U_0^+(t,t_0)\,U(t,t')|\psi(t')\rangle = \\ &= U_0^+(t,t_0)\,U(t,t')\,U_0^{-1}(t_0,t')|\psi_{\mathrm{D}}(t')\rangle \,.\end{aligned}$$

We remember that quantities without index are meant to be in the Schrödinger picture. The comparison of this expression with (3.197) yields the connection between Dirac's and Schrödinger's time evolution operators:

$$U_{\mathrm{D}}(t,t') = U_0^+(t,t_0)\,U(t,t')\,U_0(t',t_0) \,. \tag{3.200}$$

If there is no interaction ($H_1^t \equiv 0$) then it is $U \equiv U_0$ and therewith $U_{\mathrm{D}} \equiv \mathbb{1}$. That means, according to (3.197), that the state in the Dirac picture becomes time-independent as the Heisenberg state. The time-dependence of the states is obviously determined by the interaction.

For the transformation of an arbitrary observable A we have to require:

$$\begin{aligned}\langle\psi_{\mathrm{D}}(t)|A_{\mathrm{D}}(t)|\psi_{\mathrm{D}}(t)\rangle &\overset{!}{=} \langle\psi(t)|A|\psi(t)\rangle \\ &\overset{(3.198)}{=} \langle\psi_{\mathrm{D}}(t)|U_0(t_0,t)\,A\,U_0^{-1}(t_0,t)|\psi_{\mathrm{D}}(t)\rangle \,.\end{aligned}$$

This means:

$$A_{\mathrm{D}}(t) = e^{\frac{i}{\hbar}H_0(t-t_0)}\,A\,e^{-\frac{i}{\hbar}H_0(t-t_0)} \,. \tag{3.201}$$

The dynamics of the observables is therefore, as projected, fixed by H_0. That one realizes in particular by the equation of motion of a Dirac-observable, which is derived directly from (3.201):

$$i\hbar \frac{d}{dt} A_{\mathrm{D}}(t) = [A_{\mathrm{D}}(t), H_0]_- + i\hbar \frac{\partial A_{\mathrm{D}}}{\partial t} . \tag{3.202}$$

In analogy to (3.190) we have defined here:

$$\frac{\partial A_{\mathrm{D}}}{\partial t} = e^{\frac{i}{\hbar} H_0 (t - t_0)} \frac{\partial A}{\partial t} e^{-\frac{i}{\hbar} H_0 (t - t_0)} . \tag{3.203}$$

The equation of motion (3.202) agrees *almost* with that of the Heisenberg picture, except for the fact that now in the commutator there does not appear the *full* Hamiltonian H, but only the *free* part H_0.

If one evaluates (3.201) especially for the Hamilton operator, then one finds for the *free* system:

$$H_{0\mathrm{D}}(t) \equiv H_0 . \tag{3.204}$$

But since H_0 and H_1^t in general do not commute, the *Dirac-interaction* $H_{1\mathrm{D}}^t(t)$ can not in any case be equated with the *Schrödinger-interaction*:

$$H_{1\mathrm{D}}^t(t) = e^{\frac{i}{\hbar} H_0 (t - t_0)} H_1^t e^{-\frac{i}{\hbar} H_0 (t - t_0)} . \tag{3.205}$$

One should pay attention to the two different time-dependences. The explicit time-dependence of the interaction, which also exists in the Schrödinger picture, is therefore labeled consciously as upper index in (3.195).

Let us eventually investigate the time-dependence of the states in the Dirac picture. For this purpose we differentiate (3.198) with respect to time:

$$\begin{aligned} |\dot{\psi}_{\mathrm{D}}(t)\rangle &= \dot{U}_0(t_0, t)|\psi(t)\rangle + U_0(t_0, t)|\dot{\psi}(t)\rangle = \\ &= \frac{i}{\hbar} \left[U_0^+(t, t_0)\, H_0 - U_0^+(t, t_0)\, H \right] |\psi(t)\rangle = \\ &= \frac{i}{\hbar} U_0^+(t, t_0)(-H_1^t)\, U_0(t, t_0)|\psi_{\mathrm{D}}(t)\rangle . \end{aligned}$$

This results in an equation of motion, which is formally very similar to the Schrödinger Eq. (3.165):

$$i\hbar |\dot{\psi}_{\mathrm{D}}(t)\rangle = H_{1\mathrm{D}}^t(t)|\psi_{\mathrm{D}}(t)\rangle . \tag{3.206}$$

On the right-hand side, the full Hamilton operator is *merely* replaced by the interaction term. The temporal evolution of the states is thus determined by the

interaction term. This of course does not only hold for pure but also for mixed states, as one recognizes by the equation of motion,

$$\dot{\rho}_{\mathrm{D}}(t) = \frac{i}{\hbar}\left[\rho_{\mathrm{D}}(t),\, H^t_{1\mathrm{D}}(t)\right]_- \,, \tag{3.207}$$

of the density matrix

$$\rho_{\mathrm{D}}(t) = \sum_m p_m |\psi_{m\mathrm{D}}(t)\rangle\langle\psi_{m\mathrm{D}}(t)| \,. \tag{3.208}$$

Equation (3.207) is immediately derived, with (3.206), from the definition Eq. (3.208).

The

time evolution operator of the Dirac picture

is of practical interest for later applications. It is formally derived exactly as in the Schrödinger picture. With (3.197) and (3.206) we find for it an equation of motion,

$$i\hbar\,\frac{d}{dt}\,U_{\mathrm{D}}(t,t_0) = H^t_{1\mathrm{D}}(t)\,U_{\mathrm{D}}(t,t_0) \,, \tag{3.209}$$

which can be integrated in the same way of calculation as for (3.169). Completely analogously to (3.176) one finds:

$$U_{\mathrm{D}}(t,t_0) = T\,\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,H^{t'}_{1\mathrm{D}}(t')\right) . \tag{3.210}$$

One should bear in mind that U_{D}, in contrast to U in (3.176), can not be further simplified, even if there is no explicit time-dependence of the Hamilton operator, because in that case $H^{t'}_{1\mathrm{D}}(t')$ is only to be replaced by $H_{1\mathrm{D}}(t')$. In any case, one of the two time-dependences will still remain.

3.4.5 Quantum-Theoretical Equations of Motion

Let us gather once more the equations of motion derived so far, for a system which is characterized by the Hamilton operator

$$H = H_0 + H^t_1 \,.$$

1) Schrödinger picture

$$\text{pure state:} \qquad i\hbar|\dot{\psi}(t)\rangle = H|\psi(t)\rangle \ ,$$

$$\text{density matrix:} \ \dot{\rho}(t) = \tfrac{i}{\hbar}\,[\rho, H]_-(t) \ ,$$

$$\text{observable:} \qquad \tfrac{d}{dt}A = \tfrac{\partial}{\partial t}A \ .$$

2) Heisenberg picture

$$\text{pure state:} \qquad |\dot{\psi}_H\rangle = 0 \ ,$$

$$\text{density matrix:} \ \dot{\rho}_{\rm H} = 0 \ ,$$

$$\text{observable:} \qquad i\hbar\tfrac{d}{dt}A_{\rm H} = [A_{\rm H}, H_{\rm H}]_-(t) + i\hbar\tfrac{\partial}{\partial t}A_{\rm H} \ ,$$

$$\textit{connections:} \qquad |\psi_H\rangle = U^+(t,t_0)|\psi(t)\rangle \ ,$$

$$A_{\rm H}(t) = U^+(t,t_0)\,A\,U(t,t_0) \ ,$$

$$U(t,t_0) = T\,\exp\left[-\tfrac{i}{\hbar}\int\limits_{t_0}^{t} dt'\,H(t')\right] \ .$$

3) Dirac picture

$$\text{pure state:} \qquad i\hbar|\dot{\psi}_{\rm D}(t)\rangle = H^t_{\rm 1D}(t)|\psi_{\rm D}(t)\rangle \ ,$$

$$\text{density matrix:} \ \dot{\rho}_{\rm D}(t) = \tfrac{i}{\hbar}\,[\rho_{\rm D},\, H^t_{\rm 1D}]_-(t) \ ,$$

$$\text{observable:} \qquad i\hbar\tfrac{d}{dt}A_{\rm D} = [A_{\rm D}, H_0]_-(t) + i\hbar\tfrac{\partial}{\partial t}A_{\rm D} \ ,$$

$$\textit{connections:} \qquad |\psi_{\rm D}(t)\rangle = U_0(t_0,t)|\psi(t)\rangle \ ,$$

$$A_{\rm D}(t) = U_0^+(t,t_0)\,A\,U_0(t,t_0) \ ,$$

$$U_0(t,t_0) = \exp\left[-\tfrac{i}{\hbar}H_0(t-t_0)\right] \ .$$

In spite of the rather different structures, it can be shown that the physically relevant expectation values of the observables, which follow from these relations, are form-invariant. We prove as Exercise 3.4.8 that it holds in all the three pictures for pure as well as mixed states:

$$i\hbar\,\frac{d}{dt}\langle A\rangle = \langle [A,H]_-\rangle + i\hbar\left\langle\frac{\partial A}{\partial t}\right\rangle \ . \tag{3.211}$$

This relation is called the *Ehrenfest's theorem*, which states that classical equations of motion appear in Quantum Mechanics for the expectation values. We will learn to understand this statement in the next section in connection with the principle of correspondence. Here we make do with an illustrative example.

Let the Hamilton operator

$$H = \frac{p^2}{2\,m} + V(q) \tag{3.212}$$

describe the one-dimensional motion of a particle in a potential V. We have proven as Exercise 3.2.14 that for two operators A and B with

$$[A,\, B]_- = i\mathbb{1} \tag{3.213}$$

it follows

$$[A,\, B^n]_- = i\,n\,B^{n-1}$$

and therewith, if we understand, as previously agreed upon, $f(B)$ as a polynomial or a power series in B (Exercise 3.2.26):

$$[A, f(B)]_- = i\,\frac{d}{dB} f(B)\ . \tag{3.214}$$

We have introduced the differentiation with respect to an operator in Sect. 3.2.7. We exploit (3.214) for our example (3.212). With $[q, p]_- = i\,\hbar$ one gets

$$[p, H]_- = \frac{\hbar}{i}\,\frac{d}{dq}\,V(q)\ , \tag{3.215}$$

and

$$[q, H]_- = \frac{i\,\hbar}{m}\,p\ . \tag{3.216}$$

Position q and momentum p are not explicitly time-dependent, so that we can conclude with the Ehrenfest's theorem (3.211):

$$\frac{d}{dt}\langle q\rangle = \frac{1}{i\,\hbar}\langle [q, H]_-\rangle = \frac{1}{m}\langle p\rangle\ , \tag{3.217}$$

$$\frac{d}{dt}\langle p\rangle = \frac{1}{i\,\hbar}\langle [p, H]_-\rangle = -\left\langle \frac{d}{dq}\,V(q)\right\rangle \tag{3.218}$$

If we define as the operator of the force,

$$F(q) = -\frac{d}{dq}\, V(q), \tag{3.219}$$

then the combination of (3.217) and (3.218) leads to:

$$m\,\frac{d^2}{dt^2}\langle q\rangle = \langle F(q)\rangle\ . \tag{3.220}$$

This relation indeed reminds strongly of the law of inertia of Classical Mechanics. However, the analogy has a *minor flaw* since in general one has to assume

$$\langle F(q)\rangle \neq F(\langle q\rangle)\ .$$

If there were on the right-hand side of (3.220) $F(\langle q\rangle)$, then the statement of the Ehrenefest's theorem (3.211) would be that the expectation values $\langle q\rangle$ and $\langle p\rangle$ strictly obey the classical equations of motion.

3.4.6 Energy-Time Uncertainty Relation

At the beginning of this section we have already commented on the special role of the *time* in Quantum Mechanics. It is a parameter, which cannot be ascribed as eigen-value to any observable. The energy-time uncertainty relation

$$\Delta E\,\Delta t \geq \frac{\hbar}{2} \tag{3.221}$$

is therefore of special kind and needs a precise interpretation. While the position-momentum uncertainty (1.5) is determined by the structure of Quantum Mechanics—position and momentum are operators!—(3.221) represents only an estimation of the time intervals and energy distributions, which are connected to transient oscillations and decay processes, processes of disintegration (decays) and similar things. In addition, the energy is in principle exactly measurable at any point of time. Before the application of the relation (3.221) one has therefore to be clear on what is actually meant by ΔE and Δt.

As an illustrative example we discuss at first a wave packet of the width Δq (Sect. 2.2.3), which is built up by free matter waves. A possible interpretation of Δt could be to regard it as the time, which the maximum of the packet q_0 needs to travel distance of the width of the uncertainty Δq (Fig. 3.13). That would otherwise correspond to the time, during which the particle can be found with finite probability at a certain position q_0. If now p_0/m is the group velocity of the packet, it thus holds:

$$\Delta t = \frac{m}{p_0}\,\Delta q\ .$$

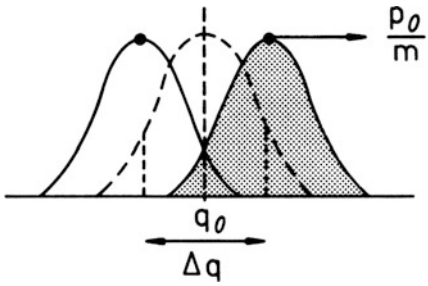

Fig. 3.13 Illustration of the energy-time uncertainty relation by inspecting the shift of a wave packet

Because of the indeterminacy Δq of the position, in a certain sense also the time, at which the particle can be found at a given position, is predictable only up to an accuracy of Δt. We can interpret the energy-indeterminacy ΔE as the difference of the energies at two points of time which are separated by Δt:

$$\Delta E = \Delta \left(\frac{p^2}{2\,m} \right)_0 = \frac{p_0}{m} \, \Delta p \; .$$

The indeterminacy of the momentum Δp thus causes ΔE. Combining the last two relations we get with the already known position-momentum uncertainty relation (3.143) the corresponding one for time and energy (3.221):

$$\Delta E \, \Delta t = \Delta p \, \Delta q \geq \frac{\hbar}{2} \; .$$

In a forthcoming chapter about *time-dependent perturbation theory* (Sect. 7.3, Vol. 7) we will be able to give reasons for (3.221), inspecting the special case of the connection between the lifetimes of excited atomic states and the energetic widths of the particles (photons) emitted by deexcitation.

The justification of the energy-time uncertainty relation (3.221) succeeds a bit more precisely and more generally with the aid of the Ehrenfest's theorem (3.211) and the generalized uncertainty relation (3.155). Let us assume that the Hamilton operator H and the observable A are not explicitly time-dependent. Then the following estimation is valid:

$$\Delta A \, \Delta H \geq \frac{1}{2} |\langle [A, H]_- \rangle| = \frac{\hbar}{2} \left| \frac{d}{dt} \langle A \rangle \right| \; .$$

This relation suggests the introduction of a characteristic time Δt_A as the time interval, in which the expectation value $\langle A \rangle$ of the observable A shifts just by the mean square deviation ΔA (see the above example (Fig. 3.13)):

$$\Delta t_A = \frac{\Delta A}{|\frac{d}{dt} \langle A \rangle|} \; . \tag{3.222}$$

Such times, which are at least necessary for significant changes of the statistical distribution of measuring values, can be defined for all observables. We therefore omit from now on the index A and deduce from the last two expressions:

$$\Delta H \, \Delta t \geq \frac{\hbar}{2} \, . \tag{3.223}$$

If we now further take into consideration the fact that the Hamilton operator stands for the observable *energy*, as we have concluded in Sect. 2.3.3 from an analogy to the classical Hamilton function, then we can write $\Delta H = \Delta E$, having therewith reproduced (3.221) with (3.223).

If the system occupies a stationary state, i.e., an eigen-state of H, then we have $\langle\psi|[A,H]_-|\psi\rangle = 0 = (d/dt)\langle A\rangle$ and therewith $\Delta t = \infty$. That must not necessarily be seen as contradiction to (3.221) since then we have also $\Delta E = 0$.

3.4.7 Exercises

Exercise 3.4.1 The Hamilton operator of a physical system is not explicitly time-dependent:

$$\frac{\partial H}{\partial t} \equiv 0 \, .$$

Show that then Schrödinger's time evolution operator reads

$$U(t,t_0) = U(t-t_0) = \exp\left[-\frac{i}{\hbar}H(t-t_0)\right] \, .$$

For the proof, evaluate explicitly the von Neumann's series (3.171)!

Exercise 3.4.2 To the observable *'spin*-1/2*'* (Sects. 5.2, 5.3, Vol. 7) the operator

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \; ; \qquad \boldsymbol{\sigma} = (\sigma_x, \, \sigma_y, \, \sigma_z)$$

is ascribed, where $\sigma_x, \, \sigma_y, \sigma_z$ are Pauli's spin matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; ; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; ; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \, ,$$

represented in the eigen-basis of σ_z.

A spin-1/2 particle in a homogeneous magnetic field $\mathbf{B} = B\,\mathbf{e}_z$ ($\mathbf{e}_z$: unit vector in z-direction) is described by the Hamiltonian

$$H = \hbar\,\omega\,\sigma_z\,; \quad \omega = \frac{q\,B}{2\,m}$$

($q(m)$: charge (mass) of the particle). The initial state at the time $t = 0$ reads in the eigen-basis of σ_z:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\,.$$

Calculate the expectation values of the spins $\langle\sigma_{x,y,z}\rangle$ at the times $t_1 = 0$, $t_2 = \frac{\pi\,m}{q\,B}$.

Exercise 3.4.3 Calculate with the Hamilton operator

$$\begin{aligned} H &= \hbar\,\omega(\mathbf{e}\cdot\boldsymbol{\sigma})\,,\\ \mathbf{e} &= (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)\,,\\ \boldsymbol{\sigma} &= (\sigma_x,\,\sigma_y,\,\sigma_z) : \text{Pauli spin operator} \end{aligned}$$

the time-dependence of the density matrix:

$$\rho(t) = \frac{1}{2}\,(\mathbb{1} + \mathbf{P}\cdot\boldsymbol{\sigma})$$

(**P**: polarization vector, see Exercises 3.3.8, 3.3.9).

Exercise 3.4.4 For a closed system ($\partial H/\partial t = 0$) let A be an observable in the Schrödinger picture and A_H the corresponding observable in the Heisenberg picture. Let both pictures coincide at the time $t_0 = 0$. Let the initial state $|\psi(0)\rangle$ be an eigen-state of A. Show that for $t > 0$ $|\psi(t)\rangle$ is an eigen-state of $A_H(-t)$ with the same eigen-value.

Exercise 3.4.5 The linear harmonic oscillator is described by the Hamilton operator:

$$H = \frac{p^2}{2\,m} + \frac{1}{2}\,m\,\omega^2 q^2\,.$$

Show that the momentum operator p and the position operator q fulfill the following equations of motion in the Heisenberg picture:

$$\begin{aligned} \frac{d^2}{dt^2}\,q_H(t) + \omega^2\,q_H(t) &= 0\,,\\ \frac{d^2}{dt^2}\,p_H(t) + \omega^2\,p_H(t) &= 0\,. \end{aligned}$$

Exercise 3.4.6 Consider the force-free one-dimensional motion of a particle of the mass m:

$$H = \frac{1}{2m} p^2 \, .$$

1. Solve the equation of motion of the position operator $q_H(t)$ and of the momentum operator $p_H(t)$ in the Heisenberg picture.
2. Calculate the commutators:

$$[q_H(t_1),\, q_H(t_2)]_- \, ; [p_H(t_1),\, p_H(t_2)]_- \, ; [q_H(t_1),\, p_H(t_2)]_- \, .$$

Exercise 3.4.7 A particle of the mass m may possess the potential energy

$$V(q) = -\alpha q \quad (\alpha > 0)$$

1. Calculate the time-dependences of the observables *position* $q(t)$ and *momentum* $p(t)$ in the Heisenberg picture, where $q(0) = q_0$ and $p(0) = p_0$ are the initial conditions.
2. Calculate the following commutators:

$$[q(t_1), q(t_2)]_- \, , \quad \left[q(t_1), p^2(t_2)\right]_- \, , \quad \left[p(t_1), q^2(t_2)\right]_- \qquad \text{for } t_1 \neq t_2 !$$

Exercise 3.4.8 Derive the equation of motion of the expectation value $\langle A \rangle$ of the observable A for pure as well as mixed states, in the

1) Schrödinger picture, 2) Heisenberg picture, 3) Dirac picture

(Ehrenfest's theorem (3.211)).

Exercise 3.4.9 Let a particle of the mass m perform a one-dimensional motion under the influence of a constant force F. Show that the expectation value of the momentum increases linearly with time.

Exercise 3.4.10

1. The classical Hamilton function of the linear harmonic oscillator reads:

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 = H(p, q) \, .$$

   Calculate the classical equations of motion for $q(t)$ and $p(t)$.
2. In the classical Hamilton function we replace the variables q and p by the position operator $\hat{q}$ and the momentum operator $\hat{p}$ getting therewith the Hamilton

operator $\widehat{H}$ of the linear harmonic oscillator. Show that the equations of motion of the expectation values $\langle\hat{q}\rangle$, $\langle\hat{p}\rangle$ are identical to the classical equations of the particle from part 1) (*Ehrenfest's theorem*).

3. Is the statement of part 2) correct also for a potential of the form:

$$V(q) = \alpha\, q^4\,?$$

3.5 Principle of Correspondence

Already several times we have tried to demonstrate analogies between Classical Mechanics and Quantum Mechanics. That started in Sect. 1.5.3 with Bohr's considerations about a *super-ordinate* theory, which we call today *Quantum Mechanics*, and which incorporates the macroscopically correct Classical Mechanics as that limiting case, for which *quantizations* and *quantum jumps* become unimportant ('$\hbar \to 0$-*limiting case*'). Bohr's postulates still testify even today to the ingenious physical intuition of the author, since they had been the leading viewpoint for the discovery of the *correct* quantum laws.

In Sect. 2.3.3 we have developed, in the framework of wave mechanics, a practical recipe (*rule of correspondence*) for the formulation of the Schrödinger equation as the equation of motion of the wave function $\psi(\mathbf{r}, t)$ of a physical system. This recipe resulted, in the final analysis, out of considerations to express the momentum operator in the position space, i.e., by $\psi(\mathbf{r}, t)$.

In this section we now want to discuss analogies between Classical Mechanics and Quantum Mechanics in an essentially more abstract, representation-independent manner. For this purpose we pick up a thought, with which we already dealt in Vol. 2 (Analytical Mechanics) of this ground course in Theoretical Physics. This can be given in a general form as follows:

A formal analogy exists between Classical Physics and Quantum Mechanics! The relations between classical dynamical variables can be adopted in similar form in Quantum Mechanics as relations between Hermitian operators (principle of correspondence)!

The next section is devoted to the derivation of the corresponding translation code.

3.5.1 Heisenberg Picture and Classical Poisson Bracket

Dynamical variables of Classical Mechanics,

$$A = A(\mathbf{q}, \mathbf{p}, t)\ ; \quad B = B(\mathbf{q}, \mathbf{p}, t)\ ,$$

are phase-space functions. Each pair of such variables can be combined to a new phase-space function ((2.104), Vol. 2):

Poisson bracket

$$\{A,\, B\} = \sum_{i=1}^{S} \left(\frac{\partial A}{\partial q_i}\,\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\,\frac{\partial B}{\partial q_i} \right) . \tag{3.224}$$

Some important properties can be directly read off from this definition:

1. The Poisson bracket is a *canonical invariant*, i.e., it is independent of the set of canonical-conjugate variables $\mathbf{q}, \mathbf{p}$ which are applied for its calculation (see Sect. 2.4.2, Vol. 2):

   $$\{A,\, B\}_{\mathbf{q},\mathbf{p}} = \{A,\, B\}_{\mathbf{Q},\mathbf{P}} .$$

   This holds for the case that the sets of variables $(\mathbf{q}, \mathbf{p})$ and $(\mathbf{Q}, \mathbf{P})$ emerge from one another by a canonical transformation ((2.134)–(2.136), Vol. 2), i.e., by a transformation that keeps Hamilton's equations of motion form-invariant.
2. $\{A, B\} = -\{B, A\}$.
3. $\{A, \text{const}\} = 0$.
4. $\{A, B + C\} = \{A, B\} + \{A, C\}$.
5. $\{A, B\, C\} = B\,\{A, C\} + \{A, B\}\, C$.
6. Jacobi identity:

   $$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 .$$

7. Fundamental Poisson brackets:

   $$\{q_i, p_j\} = \delta_{ij} ; \quad \{q_i, q_j\} = \{p_i, p_j\} = 0 . \tag{3.225}$$

8. Equation of motion:

   $$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t} . \tag{3.226}$$

Especially:

$$\dot{q}_j = \{q_j, H\} ; \quad \dot{p}_j = \{p_j, H\} . \tag{3.227}$$

Instead of deriving the properties 2) to 8) from the concrete definition (3.224) of the classical Poisson bracket one can also proceed inversely by interpreting them as

axioms of an abstract mathematical structure, independently of a special definition of the bracket-symbol $\{\ldots,\ldots\}$.

The classical Poisson bracket, built according to (3.224) with classical dynamical variables, is then one, but not the only, realization of this abstract structure. We establish, as further realization, a

quantum-mechanical bracket $\left\{\widehat{A},\,\widehat{B}\right\}_{\mathrm{QM}}$

built up by

observables $\widehat{A},\,\widehat{B}$ **in the Heisenberg picture.**

We assume that it exhibits the properties 2) to 8). In particular, the bracket itself shall again be an observable.

The following correspondence exists between these two realizations of the abstract bracket-symbol:

$$\begin{array}{ccc} \textit{classical dynamical variable} & & \textit{observable, i.e., Hermitian} \\ A, B, C & \Longleftrightarrow & \textit{operators } \widehat{A}, \widehat{B}, \widehat{C} \end{array}$$

$$\{A, B\} = C \Longleftrightarrow \left\{\widehat{A}, \widehat{B}\right\}_{\mathrm{QM}} = \widehat{C}\,. \tag{3.228}$$

For a practical evaluation we still need, though, detailed information about the quantum-Poisson bracket. Since both exhibit the same properties we suppose:

$$\left\{\widehat{A}, \widehat{B}\right\}_{\mathrm{QM}} \sim \left[\widehat{A}, \widehat{B}\right]_{-} = \widehat{A}\,\widehat{B} - \widehat{B}\,\widehat{A}\,.$$

That the commutator fulfills the properties 2) to 4) is immediately clear; 5) and 6) are the matter of Exercise 3.2.13. We can justify the supposed proportionality also as follows:

Let $\widehat{A}_1,\,\widehat{A}_2;\,\widehat{B}_1,\,\widehat{B}_2$ be Hermitian operators. Furthermore, let $\widehat{A}_1$ and $\widehat{A}_2$ as well as $\widehat{B}_1$ and $\widehat{B}_2$ commute, in order to guarantee that also $\widehat{A}_1\,\widehat{A}_2$ and $\widehat{B}_1\,\widehat{B}_2$ are Hermitian:

$$\begin{aligned} \left\{\widehat{A}_1\,\widehat{A}_2,\,\widehat{B}_1\,\widehat{B}_2\right\}_{\mathrm{QM}} &\overset{(5)}{=} \widehat{A}_1\,\left\{\widehat{A}_2,\,\widehat{B}_1\,\widehat{B}_2\right\}_{\mathrm{QM}} + \left\{\widehat{A}_1,\,\widehat{B}_1\,\widehat{B}_2\right\}_{\mathrm{QM}}\,\widehat{A}_2 = \\ &= \widehat{A}_1\,\widehat{B}_1\,\left\{\widehat{A}_2, \widehat{B}_2\right\}_{\mathrm{QM}} + \widehat{A}_1\,\left\{\widehat{A}_2, \widehat{B}_1\right\}_{\mathrm{QM}}\,\widehat{B}_2 + \\ &+ \widehat{B}_1\,\left\{\widehat{A}_1, \widehat{B}_2\right\}_{\mathrm{QM}}\,\widehat{A}_2 + \left\{\widehat{A}_1, \widehat{B}_1\right\}_{\mathrm{QM}}\,\widehat{B}_2\,\widehat{A}_2\,. \end{aligned}$$

One can disentangle the bracket in another sequence also:

$$\begin{aligned} \left\{\widehat{A}_1\,\widehat{A}_2, \widehat{B}_1\,\widehat{B}_2\right\}_{\mathrm{QM}} &= \widehat{B}_1\,\left\{\widehat{A}_1\,\widehat{A}_2, \widehat{B}_2\right\}_{\mathrm{QM}} + \left\{\widehat{A}_1\,\widehat{A}_2, \widehat{B}_1\right\}_{\mathrm{QM}}\,\widehat{B}_2 = \\ &= \widehat{B}_1\,\widehat{A}_1\,\left\{\widehat{A}_2, \widehat{B}_2\right\}_{\mathrm{QM}} + \widehat{B}_1\,\left\{\widehat{A}_1, \widehat{B}_2\right\}_{\mathrm{QM}}\,\widehat{A}_2 + \\ &+ \widehat{A}_1\,\left\{\widehat{A}_2, \widehat{B}_1\right\}_{\mathrm{QM}}\,\widehat{B}_2 + \left\{\widehat{A}_1, \widehat{B}_1\right\}_{\mathrm{QM}}\,\widehat{A}_2\,\widehat{B}_2\,. \end{aligned}$$

When we subtract these two expressions from each other then we are left with:

$$\left[\widehat{A}_1, \widehat{B}_1\right]_- \left\{\widehat{A}_2, \widehat{B}_2\right\}_{\mathrm{QM}} = \left\{\widehat{A}_1, \widehat{B}_1\right\}_{\mathrm{QM}} \left[\widehat{A}_2, \widehat{B}_2\right]_- \ .$$

Since $\widehat{A}_i$, $\widehat{B}_i$ are *almost arbitrarily* chosen operators, this result indeed suggests the proportionality between the commutator and the quantum-Poisson bracket:

$$\left\{\widehat{A}, \widehat{B}\right\}_{\mathrm{QM}} = i\alpha \left[\widehat{A}, \widehat{B}\right]_- \ ; \qquad \alpha \in \mathbb{R} \ .$$

The proportionality constant must be purely imaginary since for Hermitian operators $\widehat{A}$ and $\widehat{B}$ the bracket shall also be Hermitian, whilst the commutator ($[\widehat{A}, \widehat{B}]_-^+ = -[\widehat{A}, \widehat{B}]_-$) is anti-Hermitian. The real constant α has to be fitted to the experiment. The choice $\alpha = -\hbar^{-1}$ turns out to be the only unambiguous one so that finally the following prescription of translation results from (3.228):

$$\begin{array}{ll} \textbf{Classical Mechanics} & \Longleftrightarrow \textbf{Quantum Mechanics} \\ \{A, B\} = C & \Longleftrightarrow \left\{\widehat{A}, \widehat{B}\right\}_{\mathrm{QM}} = \widehat{C} = \frac{1}{i\hbar}\left[\widehat{A}, \widehat{B}\right]_- \ . \end{array} \tag{3.229}$$

All equations of motion of the Classical Mechanics can be expressed by Poisson brackets. The corresponding relations of the Quantum Mechanics are then fixed by the principle of correspondence (3.228) and (3.229). So it follows from (3.226) immediately the equation of motion (3.191) for time-dependent Heisenberg operators with the important special cases:

$$i\hbar\, \dot{\hat{q}}_i = \left[\hat{q}_i, \widehat{H}\right]_- \ , \tag{3.230}$$

$$i\hbar\, \dot{\hat{p}}_i = \left[\hat{p}_i, \widehat{H}\right]_- \ , \tag{3.231}$$

$$\frac{d}{dt}\widehat{H} = \frac{\partial}{\partial t}\widehat{H} \ . \tag{3.232}$$

For simplicity we have omitted here the index 'H' for the operator-symbols, since it is clear from the context that here exclusively *Heisenberg operators* are meant. For the same reason of simplicity, we will cut down on the sign '$\widehat{\ }$', which we introduced to distinguish operators from classical variables, because confusion is to be no longer feared.

The rule of quantization, developed in this section, turns out to be a thorough generalization of the rule of correspondence which we drew up in Sect. 2.3.3 for the special case of the position (spatial) representation. A quantum-mechanical problem is solved taking the first step, which is converting the classical Hamilton function into the Hamilton operator by declaring the coordinates $\mathbf{q} = (q_1, q_2, \ldots, q_s)$ and

momenta $\mathbf{p} = (p_1, p_2, \ldots, p_s)$ to be operators, which fulfill with (3.229) the fundamental brackets (3.225). The possible ambiguity appearing, because of the non-commutability of these operators, is avoided by additional prescriptions like (2.113) (*symmetrization*). With a known Hamilton operator the time-dependence of each Heisenberg-observable can in principle be calculated by the use of the equation of motion (3.226) with the translation code (3.229).

3.5.2 Position and Momentum Representation

Let us try to bring, at the end of this section, the general theory, developed so far, into contact with the wave mechanics of Chap. 2. The rule of correspondence for the translation of classical quantities and relations into the quantum-mechanical formalism, developed in Sect. 2.3.3 especially for wave mechanics, shall be retraced and justified here in a more abstract manner. As a result, we will then have identified the Schrödinger's wave mechanics as a special realization of the abstract Dirac-formalism. For the explicit evaluation of quantum-mechanical problems we can then apply the one or the other representation, according to expedience.

By the principle of correspondence in Sect. 3.5.1, we have carried out the transition from the classical Hamilton function $H(q, p)$ to the quantum-mechanical Hamilton operator

$$H(\hat{q}, \hat{p}) = T(\hat{p}) + V(\hat{q}) = \frac{1}{2m}\hat{p}^2 + V(\hat{q}) \; . \tag{3.233}$$

In order to keep the issue so well-arranged as possible, we restrict ourselves here to the one-dimensional motion of a particle of the mass m in the potential V. The generalization to more-dimensional systems will not create substantial problems.

$\hat{q}$ and $\hat{p}$ are observables,

$$\begin{aligned} \hat{q} = \hat{q}^+ \; &: \quad \text{position operator} \; , \\ \hat{p} = \hat{p}^+ \; &: \quad \text{momentum operator} \; , \end{aligned}$$

with the eigen-value equations:

$$\hat{q}|q\rangle = q|q\rangle \; , \tag{3.234}$$

$$\hat{p}|p\rangle = p|p\rangle \; . \tag{3.235}$$

q and p are the precisely measured values of position and momentum, which can vary through continuous regions. Therefore

$$|q\rangle, \; |p\rangle \; : \quad \text{are improper (Dirac-)states} \; ,$$

as we have discussed them in Sect. 3.2.4. They represent a complete system so that each state $|\psi\rangle$ can be expanded in them :

$$|\psi(t)\rangle = \int dq|q\rangle\langle q|\psi(t)\rangle \,, \tag{3.236}$$

$$|\psi(t)\rangle = \int dp|p\rangle\langle p|\psi(t)\rangle \,. \tag{3.237}$$

The expansion coefficients are scalar functions of the variables q and p, respectively. We denote as *wave functions* both the scalar products, built by the position-eigen states and $|\psi\rangle$ as well as by the momentum-eigen states and $|\psi\rangle$:

$$\text{position space:} \qquad \psi(q,t) = \langle q|\psi(t)\rangle \,, \tag{3.238}$$

$$\text{momentum space:} \qquad \overline{\psi}(p,t) = \langle p|\psi(t)\rangle \,. \tag{3.239}$$

At first we want to deal with the position-space function $\psi(q,t)$. The time-dependence of $|\psi(t)\rangle$ points to the Schrödinger picture, in which $|\psi(t)\rangle$ obeys the fundamental equation of motion (3.165)

$$i\hbar|\dot{\psi}\rangle = H|\psi\rangle \,.$$

When we multiply scalarly this equation from the left with the bra-state $\langle q|$ then we get:

$$i\hbar\,\frac{\partial}{\partial t}\,\psi(q,t) = \langle q|H|\psi(t)\rangle \,. \tag{3.240}$$

This equation does not help us before we know what $\langle q|H|\psi\rangle$ actually means. For this purpose we look at the somewhat more general expression

$$\langle q|A(\hat{q},\hat{p})|\psi\rangle \,,$$

where $A(\hat{q},\hat{p})$ is an operator function in the sense of Sect. 3.2.7 (power series, polynomial). Some preparing considerations are necessary!

Definition 3.5.1 (Translation Operator)

$$T(a)|q\rangle = |q+a\rangle \,; \quad a \in \mathbb{R} \,. \tag{3.241}$$

We will investigate several important properties of this operator as Exercise 3.5.6. It is clear that the application of $T(a)$ solely means the shift of the system of coordinates by the constant distance a. This operation of course can not change *the physics* of the system. In particular, the norm of the position states must be conserved:

$$\langle q+a|q+a\rangle \stackrel{!}{=} \langle q|q\rangle \Longrightarrow T(a) \text{ unitary} \,. \tag{3.242}$$

If one performs at first a translation by the distance a_1 and then another one by the distance a_2, then the sequence of the partial steps should not matter. Furthermore, in the final result what comes out should be nothing else but the result of a single translation by the total distance $a_1 + a_2$:

$$T(a_1)\,T(a_2) = T(a_2)\,T(a_1) = T(a_1 + a_2)\ . \tag{3.243}$$

We first differentiate this expression with respect to the parameter a_1, then with respect to a_2:

$$\frac{dT\,(a_1)}{da_1}\,T(a_2) = \frac{dT\,(a_1 + a_2)}{d\,(a_1 + a_2)} = \frac{dT\,(a_2)}{da_2}\,T(a_1)\ .$$

This means also:

$$\frac{dT\,(a_1)}{da_1}\,T^{-1}\,(a_1) = \frac{dT\,(a_2)}{da_2}\,T^{-1}\,(a_2)\ .$$

The left-hand side depends only on a_1, the right-hand side only on a_2. This is possible only if each side itself is independent of a_1 and a_2, respectively. We therefore write

$$\frac{dT\,(a)}{da}\,T^{-1}\,(a) \equiv i\,K\ ,$$

where the operator K is independent of the parameter a. The imaginary unit i is included here only because of reasons of convenience. With $T(a = 0) = \mathbb{1}$ the integration yields:

$$T\,(a) = \exp(i\,a\,K)\ . \tag{3.244}$$

It follows from the unitarity of T ($T^{-1} = T^{+}$) that K is an Hermitian operator. For a further fixing of K we now investigate an infinitesimal translation $a = dq$, for which it must hold because of (3.241) and (3.244):

infinitesimal translation operator

$$\begin{aligned} T_{dq}|q\rangle &= |q + dq\rangle\ , \\ T_{dq} &= \mathbb{1} + i\,dq\,K\ . \end{aligned} \tag{3.245}$$

As introduced generally in (3.94), T_{dq} represents an *infinitesimal unitary transformation*.

The operators T_{dq} and $\hat{q}$ **do not** commute:

$$\begin{aligned} T_{dq}\,\hat{q}|q\rangle &= q|q + dq\rangle\ , \\ \hat{q}\,T_{dq}|q\rangle &= (q + dq)|q + dq\rangle\ . \end{aligned}$$

We subtract these two equations:

$$[\hat{q},\, T_{dq}]_-|q\rangle = dq|q+dq\rangle = dq\,(\mathbb{1} + i\,dq\,K)|q\rangle = dq\mathbb{1}|q\rangle + \mathcal{O}(dq^2)\ .$$

This holds for all $|q\rangle$, which otherwise build a closed system. We therefore recognize the operator identity:

$$[\hat{q},\, T_{dq}]_- = dq\mathbb{1} \Longrightarrow i\,[\hat{q}, K]_- = \mathbb{1}\ .$$

The comparison with the fundamental bracket (3.225) $[\hat{q}, \hat{p}]_- = i\hbar\mathbb{1}$ forces us to the conclusion:

$$[\hat{q},\, \hbar\,K + \hat{p}]_- = 0 \Longleftrightarrow [\hat{q}^n,\, \hbar\,K + \hat{p}]_- = 0\ .$$

In the next step we exploit the commutability of momentum operator and translation operator (see part 5) of Exercise 3.5.6). It is clear that the momentum of the particle does not change when the spatial system of coordinates is shifted. As a matter of course, it has therefore to be assumed

$$[\hat{p},\, T_{dq}]_- = 0 \Longrightarrow [\hat{p}, K]_- = 0$$

and therewith also:

$$[\hat{p}^m,\, \hbar\,K + \hat{p}]_- = 0\ .$$

The two intermediate results can be combined to

$$[\hat{q}^n\,\hat{p}^m,\, \hbar\,K + \hat{p}]_- = 0\ .$$

We know that any arbitrary operator function $A(\hat{q}, \hat{p})$ is representable as polynomial or power series (Sect. 3.2.7). By applying the commutator-relation $[\hat{q}, \hat{p}]_- = i\hbar\mathbb{1}$ all position operators can be gathered to the left, all momentum operators to the right, so that always the following representation is achievable:

$$A(\hat{q}, \hat{p}) = \sum_{n,m} \alpha_{nm}\,\hat{q}^n\,\hat{p}^m\ . \tag{3.246}$$

But therewith it is clear that any arbitrary operator function $A(\hat{q}, \hat{p})$ commutes with the operator $\hbar\,K + \hat{p}$:

$$[A(\hat{q}, \hat{p}), \hbar\,K + \hat{p}]_- = 0\ .$$

Since this should be valid for all A, the operator on the right part of the commutator must be equal to $(c\mathbb{1})$ with a real constant c, which we put to zero, because only this choice will not pose any contradictions later:

$$K = -\frac{1}{\hbar}\hat{p}\ . \tag{3.247}$$

The momentum operator $\hat{p}$ turns out therewith, according to (3.245), as the *generator of an infinitesimal translation*, in the same way as we found in (3.164) the Hamilton operator to be the generator of the time translation:

$$T_{dq} = \mathbb{1} - \frac{i}{\hbar}\,dq\,\hat{p}\ , \tag{3.248}$$

$$T(a) = \exp\left(-\frac{i}{\hbar}\,a\,\hat{p}\right)\ . \tag{3.249}$$

When we now multiply the following derivative of the bra-vector $\langle q|$,

$$\frac{d}{dq}\langle q| = \frac{\langle q+dq| - \langle q|}{dq} = \frac{1}{dq}\langle q|\left(\mathbb{1} + \frac{i}{\hbar}dq\,\hat{p} - \mathbb{1}\right) = \frac{i}{\hbar}\langle q|\hat{p}\ ,$$

from the right by the ket $|\psi(t)\rangle$, then we obtain the important intermediate result:

$$\langle q|\hat{p}|\psi(t)\rangle = \frac{\hbar}{i}\frac{\partial}{\partial q}\psi(q,t)\ . \tag{3.250}$$

We further obtain recursively on $\hat{p}^n$:

$$\begin{aligned}
\langle q|\hat{p}^n|\psi(t)\rangle &= \langle q|\hat{p}\mathbb{1}\hat{p}^{n-1}|\psi(t)\rangle = \\
&= \langle q|\hat{p}\left(\int dq'|q'\rangle\langle q'|\right)\hat{p}^{n-1}|\psi(t)\rangle = \\
&= \frac{\hbar}{i}\frac{\partial}{\partial q}\int dq'\,\underbrace{\langle q|q'\rangle}_{\delta(q-q')}\langle q'|\hat{p}^{n-1}|\psi(t)\rangle = \\
&= \frac{\hbar}{i}\frac{\partial}{\partial q}\langle q|\hat{p}^{n-1}|\psi(t)\rangle = \\
&\ \ \vdots \\
&= \left(\frac{\hbar}{i}\frac{\partial}{\partial q}\right)^n\psi(q,t)\ .
\end{aligned} \tag{3.251}$$

It follows further, since $\hat{q}$, as observable, is Hermitian:

$$\langle q|\hat{q}^m\hat{p}^n|\psi(t)\rangle = q^m\langle q|\hat{p}^n|\psi(t)\rangle = q^m\left(\frac{\hbar}{i}\frac{\partial}{\partial q}\right)^n\psi(q,t)\ .$$

The general operator relation

$$A(\hat{q},\hat{p})|\psi(t)\rangle = |\varphi(t)\rangle \ ,$$

where A is an arbitrary operator function of the type (3.246), becomes therewith in the representation with spatial wave functions:

$$A\left(q,\ \frac{\hbar}{i}\frac{\partial}{\partial q}\right)\psi(q,t) = \varphi(q,t) \ . \tag{3.252}$$

In the end we have derived the following assignment:

position representation

$$\begin{aligned} |\psi(t)\rangle &\longrightarrow \psi(q,t) \ , \\ \hat{p} &\longrightarrow \tfrac{\hbar}{i}\tfrac{\partial}{\partial q} \ , \\ \hat{q} &\longrightarrow q \ , \\ A(\hat{q},\hat{p}) &\longrightarrow A\left(q,\ \tfrac{\hbar}{i}\tfrac{\partial}{\partial q}\right) \ . \end{aligned} \tag{3.253}$$

It holds in particular for the Hamilton operator in the position representation:

$$H(\hat{q},\hat{p}) \longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V(q) \ . \tag{3.254}$$

The time-dependent Schrödinger Eq. (3.240) reads with this H:

$$i\hbar\frac{\partial}{\partial t}\psi(q,t) = H\,\psi(q,t) \ . \tag{3.255}$$

This result is identical to (2.107) and (2.108). The *position representation* (3.253) developed here is thus completely equivalent to that in Sect. 2.3.1. The latter we had *'justified'*, starting from the action wave concept of the classical Hamilton-Jacobi theory, more or less by plausibility considerations and conclusions by analogy. That these were obviously correct, is documented by the stricter and more general method of conclusion, which led in this section to (3.253).

A completely analogous train of thought, which we will not reconstruct here in detail, recommending it instead as Exercise 3.5.9, yields the

momentum representation

$$\begin{aligned} |\psi(t)\rangle &\longrightarrow \overline{\psi}(p,t) \ , \\ \hat{p} &\longrightarrow p \ , \\ \hat{q} &\longrightarrow -\tfrac{\hbar}{i}\tfrac{\partial}{\partial p} \ , \\ B(\hat{q},\hat{p}) &\longrightarrow B\left(-\tfrac{\hbar}{i}\tfrac{\partial}{\partial p},\ p\right) \ . \end{aligned} \tag{3.256}$$

Even this result agrees with the statements in Sect. 2.3.1!

3.5.3 Exercises

Exercise 3.5.1

1. Calculate for the classical angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

the Poisson brackets:

a) $\{L_i, L_j\}, \{L_i, \mathbf{L}^2\}$,
b) $\{L_i, x_j\}, \{L_i, \mathbf{r}^2\}$,
c) $\{L_i, p_j\}, \{L_i, \mathbf{p}^2\}$.

The indexes i, j denote the Cartesian components!

2. Which commutation relations follow herefrom for the corresponding quantum-mechanical operators?

Exercise 3.5.2 Prove by the use of the equation of motion for Heisenberg-observables the following rules of differentiation:

1. $\frac{d}{dt}(A + B) = \frac{d}{dt}A + \frac{d}{dt}B$,
2. $\frac{d}{dt}(A\,B) = \left(\frac{d}{dt}A\right) B + A \left(\frac{d}{dt}B\right)$,
3. $\frac{d}{dt}(\alpha\,A) = \dot{\alpha}\,A + \alpha \left(\frac{d}{dt}A\right)$; $\quad \alpha$ time-independent c-number

Exercise 3.5.3 Express the operator of acceleration $\frac{d^2}{dt^2}q$ by the position operator q and the Hamilton operator H.

Exercise 3.5.4 Let a particle of the mass m move in a potential $V = V(\mathbf{r})$, which is a homogeneous function of degree n:

$$V(\alpha\,\mathbf{r}) = \alpha^n\,V(\mathbf{r}) \qquad \forall \alpha \in \mathbb{R}^+, n \in \mathbb{N}\,.$$

It possesses therewith the Hamiltonian:

$$H = T(\mathbf{p}) + V(\mathbf{r})\,; \qquad T(\mathbf{p}) = \frac{\mathbf{p}^2}{2\,m}\,.$$

The observable

$$A = \frac{1}{2}(\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r})$$

will lead us to the quantum-mechanical analog of the classical virial theorem ((3.33), Vol. 1).

1. Verify the relations:

$$A = \mathbf{r} \cdot \mathbf{p} + \frac{3}{2} \frac{\hbar}{i} \mathbb{1} \,,$$

$$\sum_{i=1}^{3} x_i \frac{\partial V}{\partial x_i} = n\, V \,.$$

2. Prove the virial theorem:

$$\dot{A} = 2\, T - n\, V \,.$$

3. Let the system be in the pure state $|E\rangle$, which is an eigen-state of H. Show that then

$$2\langle T \rangle = n \langle V \rangle \,.$$

What does that mean for the Coulomb potential and the potential of the harmonic oscillator, respectively?

Exercise 3.5.5 Calculate the position-space wave functions

$$\psi_p(q) = \langle q|p \rangle \,,$$

which are ascribed to the eigen-states $|p\rangle$ of the momentum operator,

$$\hat{p}|p\rangle = p|p\rangle \,.$$

Exercise 3.5.6 According to (3.241) the translation operator $T(a)$ for the one-dimensional particle motion is defined by

$$T(a)|q\rangle = |q + a\rangle \,; \qquad a \in \mathbb{R} \,,$$

where $|q\rangle$ is an (improper) eigen-state of the position operator. Prove the following relations:

$$\begin{aligned}
&1)\ T^{-1}(a) = T(-a) \,, \\
&2)\ T^{+}(a) = T^{-1}(a) \,, \\
&3)\ T(a)\, T(b) = T(a + b) \,, \\
&4)\ T(a)\, \hat{q}\, T^{+}(a) = \hat{q} - a\mathbb{1} \,, \\
&5)\ T(a)\, \hat{p}\, T^{+}(a) = \hat{p} \,.
\end{aligned}$$

Exercise 3.5.7 The so-called *parity operator* Π is defined by

$$\Pi|q\rangle = |-q\rangle \,; \qquad q \in \mathbb{R} \,.$$

$|q\rangle$ is an (improper) eigen-state of the position operator for the one-dimensional particle motion.

1. Show that Π is Hermitian and unitary!
2. Calculate the eigen-values π of the parity operator!
3. One calls A an *odd* operator if

$$\Pi A \Pi^{+} = -A \ .$$

Let $|\alpha\rangle$, $|\beta\rangle$ be eigen-states of Π with the same eigen-value π. Verify

$$\langle \alpha | A | \beta \rangle = 0 \ .$$

4. Show that the position operator $\hat{q}$ is an *odd* operator!
5. Does the momentum operator $\hat{p}$ also possess odd parity?

Exercise 3.5.8 Which boundary conditions for the wave function of a particle in one dimension guarantee that the momentum operator

$$\hat{p} \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial q}$$

is a Hermitian operator?

Exercise 3.5.9 Give reasons for the momentum-representation (3.256):

$$\begin{aligned} |\psi\rangle &\longrightarrow \overline{\psi}(p) = \langle p | \psi \rangle \ , \\ \hat{p} &\longrightarrow p \ , \\ \hat{q} &\longrightarrow -\frac{\hbar}{i} \frac{\partial}{\partial p} \ , \\ B(\hat{q}, \hat{p}) &\longrightarrow B\left(-\frac{\hbar}{i} \frac{\partial}{\partial p}, p \right) \ . \end{aligned}$$

Use a procedure which is analogous to the method which was applied for the derivation of the position-representation (3.253).

Exercise 3.5.10 The Hamilton operator for the one-dimensional particle motion has the general form:

$$H = \frac{1}{2m} \hat{p}^2 + V(\hat{q}) \ .$$

Let E_n, $|E_n\rangle$ be the eigen-values and eigen-states of H:

$$H|E_n\rangle = E_n |E_n\rangle \ ; \quad \langle E_n | E_{n'} \rangle = \delta_{nn'} \ .$$

1. Calculate the double-commutator

$$[[H, \hat{q}]_-, \hat{q}]_- \ .$$

2. Use the result of part 1) for the proof of the *sum rule*:

$$\sum_n |\langle E_{n'}|\hat{q}|E_n\rangle|^2 \, (E_n - E_{n'}) = \frac{\hbar^2}{2\,m} \ .$$

3.6 Self-Examination Questions

To Section 3.1

1. How does Classical Physics define the term *state*?
2. Why can the classical definition of state not be directly adopted by Quantum Mechanics?
3. What does one understand by a *pure state* in Quantum Mechanics?
4. Is the state of a system directly measurable?
5. How do the measuring results change by the transition $|\psi\rangle \rightarrow \alpha|\psi\rangle$, where α is an arbitrary complex number?
6. How does one prepare a pure state?
7. Describe the modes of action of a *separator* $T(A)$ and a *filter* $P\,(a_i)$.
8. When are the properties of A and B denoted as *compatible*?
9. Which gedanken-experiment is hidden behind the formula $P(b_j)\,P(a_i)|\varphi\rangle$?
10. What is to be understood by $P(a_i) + P(a_j)$?
11. How is a classical dynamical variable defined?
12. Do you know of quantum-mechanical variables **without** a classical analog?
13. How is an observable defined in Quantum Mechanics?

To Section 3.2

1. Which axioms define the Hilbert space?
2. When does an ensemble of elements build a linear vector space?
3. When are the state vectors $|\varphi_1\rangle, |\varphi_2\rangle, \ldots, |\varphi_n\rangle$ linearly independent?
4. How is the dimension of a vector space defined?
5. When is a vector space called unitary?
6. Which properties define a scalar product?
7. When are state vectors $|\alpha_i\rangle$ called orthonormal?
8. What does one understand by *strong* convergence?
9. What is a Cauchy sequence?

10. What does separability of the Hilbert space mean?
11. How does the expansion law read? Which conditions guarantee its convergence?
12. What does one understand by a CON-system?
13. How does one conveniently define a scalar product for square integrable functions?
14. Explain the notations *bra*- and *ket*-vector!
15. By what is the bra-vector $\langle\varphi|$ uniquely defined?
16. When does the introduction of Dirac vectors become important and unavoidable, respectively?
17. How is a Dirac vector defined?
18. How does the expansion law read for improper states?
19. How is the *orthonormalization* of improper (Dirac) states to be understood?
20. What does one understand by the *eigen-differential* of a Dirac vector?
21. By which data is an operator uniquely defined?
22. When are two operators A_1 and A_2 considered as equal?
23. When do we speak of commutable operators?
24. How is the operator adjoint to A defined?
25. When is an operator called linear, Hermitian, bounded, and continuous?
26. What does one understand by the eigen-value problem of the operator A?
27. When is an eigen-value *degenerate*?
28. Which states belong to the eigen-space to the eigen-value a?
29. Which general statements can be made about eigen-values and eigen-states of Hermitian operators?
30. What does one denote as the *spectral representation* of the Hermitian operator A?
31. Formulate the completeness relation for the unit operator $\mathbb{1}$!
32. Which calculation trick is meant by the *insertion of intermediate states*?
33. How can one express the expectation value of the Hermitian operator A $\langle\psi|A|\psi\rangle$ in the state $|\psi\rangle$ by its eigen-values a_i and the eigen-states $|a_i\rangle$?
34. What can be said about the eigen-states of two commuting Hermitian operators A and B?
35. How can operators be built up with states?
36. What is a dyadic product? How does the corresponding adjoint operator look like?
37. When is a dyadic product also a projection operator?
38. What is to be understood by the idempotence of the projection operator? Does it also hold for improper vectors?
39. Let P_M project onto the subspace $M \subset \mathcal{H}$. Which eigen-values and eigen-states does P_M possess? Which degrees of degeneracy are present?
40. When is the inverse operator A^{-1} Hermitian?
41. How do the eigen-values and eigen-states of A^{-1} follow from those of A?
42. When is an operator unitary?
43. What is characteristic for unitary transformations?
44. Under which pre-conditions can functions of operators be defined?

45. When is $\exp A \cdot \exp B = \exp(A + B)$?
46. How does one differentiate an operator with respect to a real parameter?
47. How does one differentiate an operator function $f(A)$ with respect to the operator A?
48. Which characteristics does the matrix of an Hermitian operator have?
49. What can be said about rows and columns of a unitary matrix?
50. How does the unitary transformation, which brings the matrix of an operator A into a diagonal form look like?
51. What is the trace of a matrix?
52. How does the trace of a matrix depend on the applied CON-basis?

To Section 3.3

1. By what is an observable represented in Quantum Mechanics?
2. Which statements can in principle be delivered by a quantum-mechanical measurement?
3. Which physical components participate in a measuring process?
4. What is the essential difference between a classical and a quantum-mechanical measurement?
5. Let the system be in any state $|\psi\rangle$ **before** the measurement of the observable A. What can be said about the state of the system **after** the measurement?
6. Which statements are possible, when the initial state is already an eigen-state of A?
7. Under which conditions does the mean square deviation ΔA_ψ vanish?
8. What is to be understood by the expectation value of the observable A in the state $|\psi\rangle$?
9. When are observables called (non-) compatible?
10. What do we understand by a complete or maximal set of commuting observables?
11. Let the eigen-state $|a_i\rangle$ be prepared by measuring of A. What can be said about the state of the system when subsequently the observable B, which does not commute with A, is measured?
12. What is an anti-Hermitian operator?
13. Does there exist a connection between the uncertainty in quantum-mechanical measurements and the non-commutability of Hermitian operators?
14. What do we understand by the generalized Heisenberg uncertainty relation?
15. When is a physical system in a mixed state?
16. Comment on the two conceptually different types of averaging, which are necessary for the calculation of the expectation value of an observable A in a mixed state!
17. How is the density matrix defined?
18. With a given density matrix, how can one calculate the expectation values of observables?

19. Let the density matrix ρ be represented in the CON-eigen basis $\{|a_i\rangle\}$ of the observable A. Which physical meaning do the diagonal elements have?
20. Let $|\varphi\rangle$ be a normalized pure state. What does $\langle\varphi|\rho|\varphi\rangle$ mean?
21. What can be said about the trace of the density matrix?
22. Which form does the density matrix for pure states have?
23. How can one decide from the density matrix ρ whether a pure or a mixed state is given?

To Section 3.4

1. Why does the time evolution operator $U(t, t_0)$ have to be unitary?
2. Which quantity is regarded as *generator of the time translation*?
3. What is the equation of motion for state vectors in the Schrödinger picture?
4. What is the equation of motion of the density matrix in the Schrödinger picture?
5. Characterize the Schrödinger picture!
6. What justifies the fact that several, different *pictures* exist for the description of the dynamics of quantum systems?
7. How does the equation of motion of the time evolution operator read in the Schrödinger picture?
8. How does the formal solution for the time evolution operator look like?
9. What is a stationary state?
10. Which form does the time evolution operator of a closed system have?
11. Which are the characteristics of the Heisenberg picture?
12. Which connection exists between the observables of the Heisenberg picture and those of the Schrödinger picture?
13. How does the equation of motion of the observables read in the Heisenberg picture?
14. What is an integral of motion?
15. How does the Dirac picture differ from the Schrödinger picture and the Heisenberg picture, respectively?
16. In which way are Schrödinger's and Dirac's time evolution operator connected to one another?
17. What is the equation of motion of an observable in the Dirac picture?
18. Which equation determines the time-dependence of the pure (mixed) states in the Dirac picture?
19. What is the statement of Ehrenfest's theorem?
20. On which physical processes can the energy-time uncertainty relation be applied?
21. Is the energy-time uncertainty relation a special case of the generalized uncertainty relation (3.155)?
22. What follows from the energy-time uncertainty relation for stationary states?

To Section 3.5

1. What is the definition of the classical Poisson bracket?
2. List the most important properties of the Poisson bracket!
3. Which relationship exists between the classical Poisson bracket, built with classical dynamic variables, and the commutator, built by the corresponding quantum-mechanical observables?
4. How are the scalar wave functions $\psi(q,t)$ and $\overline{\psi}(p,t)$, respectively, of an abstract state $|\psi(t)\rangle$ defined?
5. What is the mode of action of the translation operator $T(a)$? Why must it be an unitary operator?
6. How is $T(a)$ connected to the momentum operator?
7. What does one have to understand by an *infinitesimal translation operator*?
8. Which operator is considered as the generator of an infinitesimal translation?
9. How can the matrix element $\langle q|\hat{q}^m\,\hat{p}^n|\psi(t)\rangle$ be expressed by the wave function $\psi(q,t)$?
10. How does $\langle p|\hat{p}^m\,\hat{q}^n|\psi\rangle$ read in the momentum representation?

Chapter 4
Simple Model Systems

Having worked out the abstract theoretical framework of Quantum Mechanics in the preceding chapter, we will now interrupt these general considerations and discuss some special applications. Thereby, we will restrict ourselves to the discussion of the *course of motion in one dimension*, i.e., to one-dimensional potentials $V(q)$. On the one hand, we do this because of mathematical simplicity, in order to practice the formalism learned so far as directly as possible, and that, too, without being distracted too much by purely mathematical difficulties, which are somewhat irrelevant at the present stage. On the other hand, many of the typically quantum-mechanical phenomena are indeed practically of one-dimensional nature. Physical processes in the three-dimensional space can very often be described, as we will discuss extensively, by the use of a so-called *separation ansatz* for the required wave function, resulting in effectively one-dimensional equations of motion. The variable, that appears then, need not necessarily have the dimension *'length'*; it can be, for instance, an angle or some such quantity. In order to indicate the somewhat more general aspect, we will therefore in this chapter use for the variable of the potential always the letter q as it is usually done for *generalized coordinates*.

In transferring the abstract formalism to concrete quantum-mechanical problems, we will get to know some characteristic phenomena, which are unexplainable by Classical Physics. An especially striking consequence of the wave nature of matter is the tunnel effect (Sect. 4.3.3) with important consequences, such as, for instance, the α*-radioactivity* (Sect. 4.3.4), the so-called *cold emission* (*field emission*) of electrons out of metals (Exercise 4.3.5), and the *energy-band structure of solids* (Sect. 4.3.5, Exercises 4.3.6 and 4.3.7).

We start, however, in Sect. 4.1 with some already rather far-reaching conclusions, which can be derived directly from the general formalism, without the need of a detailed specification of the potential $V(q)$. These considerations will turn out to be very helpful when we solve the Schrödinger equation in Sect. 4.2 (*'potential well'*) and in Sect. 4.3 (*'potential barrier'*), for special piecewise constant potential curves. In Sect. 4.4 we then deal with the *harmonic oscillator* ($V(q) \sim q^2$), one of the most frequently discussed and applied model systems of Theoretical Physics. On

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the one hand, it is mathematically rigorously tractable, and, on the other hand, many realistic potential curves can indeed be, within certain limits, well approximated by the parabola of the harmonic oscillator. In forthcoming chapters, this model system will serve us, again and again, as test and illustration of new abstract concepts of Quantum Mechanics.

In this fourth chapter, we will use for most of our considerations the position representation (*Schrödinger's wave mechanics*, Chap. 2), which turns out to be convenient for the simple potentials which we discuss. Only for the harmonic oscillator, the abstract Dirac formalism (Chap. 3) also can actually be recommendable. Indeed, we are in the meantime in the fortunate situation to be capable of choosing between different, but equivalent representations.

4.1 General Statements on One-Dimensional Potential Problems

The concrete form of the solution of the Schrödinger equation is of course determined by the special structure of the potential V, in which the system or the particle moves. Beyond that, there are, however, also some generally valid properties, which **each** solution must fulfill, independently of V, in order to satisfy, e.g., the statistical character of the wave function (Sect. 2.2.1). These properties can become eminently important when one is obliged to select out of a set of mathematical solutions of the fundamental equations of motion, the physically relevant ones. Such aspects are in the focus of this section, where we will exclusively use the position representation (3.253).

4.1.1 Solution of the One-Dimensional Schrödinger Equation

We restrict our considerations to a one-dimensional conservative system. *'Conservative'* means that the classical Hamilton function is not explicitly time-dependent. According to the principle of correspondence, this property transfers to the Hamilton operator:

$$\frac{\partial H}{\partial t} = 0 : \; H = H(\hat{q}, \hat{p}) = \frac{\hat{p}^2}{2\,m} + V(\hat{q}) = -\frac{\hbar^2}{2\,m}\,\frac{\partial^2}{\partial q^2} + V(q) \; . \tag{4.1}$$

The central task consists of solving the time-dependent Schrödinger equation,

$$i\,\hbar\,\frac{\partial}{\partial t}\,\psi(q,t) = H\,\psi(q,t) \; ,$$

where, because of the absence of time-dependence, a separation ansatz appears to be recommendable:

$$\psi(q,t) = \varphi(q)\, X(t) \ .$$

Inserting this into the Schrödinger equation one gets, after division by $\psi(q,t) \neq 0$, an expression,

$$\frac{1}{X(t)}\, i\hbar\, \frac{\partial}{\partial t} X(t) = \frac{1}{\varphi(q)}\, H\, \varphi(q) \ ,$$

whose left-hand side depends only on the variable t, while the right-hand side is solely determined by the position-variable q. Each of both the sides must therefore be equal to a constant:

$$\begin{aligned} i\hbar\, \frac{\partial}{\partial t} X(t) &= E\, X(t) \ , \\ H\, \varphi(q) &= E\, \varphi(q) \ . \end{aligned} \tag{4.2}$$

The time-dependence is now very easily calculable:

$$X(t) \sim \exp\left(-\frac{i}{\hbar}\, E\, t\right) \ .$$

Here we need not worry about an integration constant since, if there is one, it can be incorporated into the second factor $\varphi(q)$:

$$\psi(q,t) = \varphi(q)\, \exp\left(-\frac{i}{\hbar}\, E\, t\right) \ . \tag{4.3}$$

The wave function, we are looking for, represents a stationary state (3.179). The remaining task consists of solving the time-independent Schrödinger Eq. (4.2), which itself is an eigen-value equation of the Hamilton operator H. Since H is a Hermitian operator, the constant E must be real. With the abbreviation

$$k^2(q) = \frac{2\, m}{\hbar^2}\, \big(E - V(q)\big) \tag{4.4}$$

equation (4.2) can be brought into the compact form

$$\varphi''(q) + k^2(q)\varphi(q) = 0 \ . \tag{4.5}$$

An explicit solution is of course possible only if the potential $V(q)$ is known. A few general properties, however, can already be found without a precise knowledge of the potential. To begin with, we recognize that, in the case of a real $V(q)$, if $\varphi(q)$

is a solution, then the conjugate-complex function $\varphi^*(q)$ and therewith also the real combinations $\varphi(q) + \varphi^*(q)$ and $-i\big(\varphi(q) - \varphi^*(q)\big)$ are also always solutions. We thus can presume for the following considerations $\varphi(q)$ to be already real. The next statements are, though, more important:

1) φ (q) is finite everywhere!

This is a requirement of the statistical interpretation of the wave function (Sect. 2.2.1). According to (2.26) we have to understand $|\varphi(q)|^2$ $(= \varphi^2(q))$ as probability density.

2) φ (q) and φ'(q) are everywhere continuous!

As a rule, we can assume that $V(q)$ is continuous or, if not, has only finite discontinuities. That transfers directly to the second derivative of the wave function,

$$\varphi''(q) = -k^2(q)\varphi(q) \ ,$$

which is therefore integrable. $\varphi'(q)$ is hence continuous and therewith, in any case, also $\varphi(q)$. Note that, if $V(q)$ exhibits at certain q-values infinite jumps, the continuity of $\varphi'(q)$ can not be presumed anymore.

The conditions 1) and 2) can be very helpful in what concerns the explicit solution of potential problems. Often it is so that the term $k^2(q)$ in the differential Eq. (4.5) is of quite a different form in different q-regions. The approaches in the various regions can therefore differ substantially from one another. Free parameters in the respective ansatz functions are then fixed by the requirement that the partial solutions are to be fitted at the *'links'* in such a way that the conditions of continuity are fulfilled.

It is reasonable to split the q-axis into the following regions:

a) Classically allowed region

$$V(q) < E \iff k^2(q) > 0 \ . \tag{4.6}$$

Since the kinetic energy can not be negative, classically, motion is possible only when the potential energy is smaller than the total energy. Quantum-mechanically, however, this statement has to be modified.

Because of $k^2(q) > 0$, φ'' and φ have always opposite signs. That means that in the region $\varphi > 0$ φ is concave as function of q and in the region $\varphi < 0$ it is convex (see (4.32), Vol. 5). In any case, φ is always inflected towards the q-axis (Fig. 4.1). Zero-crossings represent inflection points ($\varphi'' = 0$). An

oscillatory behavior of the wave function

is therefore typical for the *classically allowed region*. For the simplified situation that we have in the classically allowed region $V(q) = V_a = \text{const}$ the general

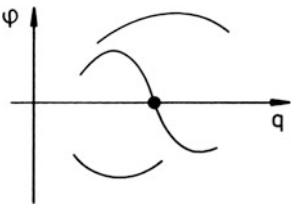

Fig. 4.1 Qualitative behavior of the wave function in the classically allowed region

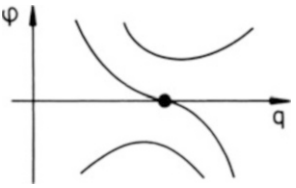

Fig. 4.2 Qualitative behavior of the wave function in the classically forbidden region

solution of (4.5) reads:

$$\varphi(q) = \alpha_+ \, e^{i k_\mathrm{a} q} + \alpha_- \, e^{-i k_\mathrm{a} q} \, ,$$
$$k_\mathrm{a} = \sqrt{\frac{2\,m}{\hbar^2}(E - V_\mathrm{a})} \, . \tag{4.7}$$

k_a is real. The oscillatory behavior of φ as function of q is obvious. α_+ and α_- are constants to be fixed by boundary conditions.

b) Classical turning points

$$V(q^*) = E \iff k^2(q^*) = 0 \, . \tag{4.8}$$

At these positions the wave function $\varphi(q)$ has, because of $\varphi''(q^*) = 0$, an inflection point, which, of course, has not necessarily to be located on the q-axis.

c) Classically forbidden region

$$V(q) > E \iff k^2(q) < 0 \, . \tag{4.9}$$

The fact that a quantum-mechanical particle can have a finite spatial probability density even in such a region, leads to very characteristic phenomena (e.g., tunnel effect), which we will encounter in the course of this chapter.

$\varphi''(q)$ and $\varphi(q)$ have the same sign everywhere in the classically forbidden region. For $\varphi > 0$, the wave function is therefore convex and for $\varphi < 0$ concave. It is always *inflected away* from the q-axis (Fig. 4.2).

Let us now investigate a bit more carefully the not so untypical situation that for all $q \geq q_0$ *classically forbidden region* is present. Figure 4.3 shows three possibilities. In the *classically allowed region* $q < q_0$ the wave function oscillates.

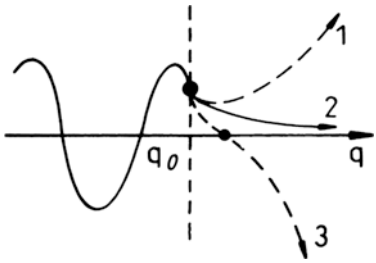

Fig. 4.3 Asymptotic behavior of the wave function in the classically forbidden region $q \geq q_0$

In the *classically forbidden region*, in the case 1, a too strong curvature leads to $\varphi(q \to +\infty) \to \infty$, in the case 3, a too weak curvature, after a further zero crossing, leads to $\varphi(q \to \infty) \to -\infty$. Both the situations are not acceptable because of the probability interpretation of the wave function. So we are left with possibility 2, according to which $\varphi(q)$ asymptotically approaches the q-axis.

For a simple estimation, let us assume for the moment that $V(q) \equiv V_c = \text{const}$ for $q \geq q_0$. Then the formal solution of (4.5) reads in this region:

$$\varphi(q) = \beta_+ \, e^{\kappa q} + \beta_- \, e^{-\kappa q} \, ,$$
$$\kappa = \sqrt{\frac{2m}{\hbar^2} (V_c - E)} \, . \tag{4.10}$$

κ is positive-real. The first summand would therefore diverge for $q \to \infty$ and therewith also $\varphi(q)$, unless we chose $\beta_+ = 0$. An

exponential decay of the wave function

is thus typical for $q \to \infty$ in the *classically forbidden region*, and that is very general and valid not only for the example $V(q) \equiv \text{const}$. The conclusions for $q \to -\infty$ are of course completely analogous.

4.1.2 Wronski Determinant

We try to get further general statements about the solution $\varphi(q)$ of the time-independent, one-dimensional Schrödinger Eq. (4.5). We thereby presume for the following considerations only that the potential $V(q)$ is bounded below and has, at most, discontinuous jumps of finite sizes.

Let $\varphi_1(q)$ and $\varphi_2(q)$ be two real solutions of the Schrödinger equation with the energies E_1 and E_2:

$$\varphi_1''(q) + k_1^2(q)\varphi_1(q) = 0 \, ,$$
$$\varphi_2''(q) + k_2^2(q)\varphi_2(q) = 0 \, ,$$
$$k_i^2 = \frac{2m}{\hbar^2} \big(E_i - V(q)\big) \, ; \quad i = 1, 2 \, .$$

We multiply the first of the two differential equations by $\varphi_2(q)$, the second equation by $\varphi_1(q)$ and take the difference:

$$\varphi_1''(q)\,\varphi_2(q) - \varphi_2''(q)\,\varphi_1(q) = \left(k_2^2(q) - k_1^2(q)\right)\varphi_1(q)\,\varphi_2(q) = \\ = \frac{2\,m}{\hbar^2}\,(E_2 - E_1)\,\varphi_1(q)\,\varphi_2(q)\ .$$

We integrate this equation with respect to q from q_0 to $q_1 > q_0$. For the left-hand side, we then perform an integration by parts:

$$\int_{q_0}^{q_1} dq\left(\varphi_1''(q)\,\varphi_2(q) - \varphi_2''(q)\,\varphi_1(q)\right) =$$

$$= \left(\varphi_1'(q)\,\varphi_2(q) - \varphi_2'(q)\,\varphi_1(q)\right)\Big|_{q_0}^{q_1} - \int_{q_0}^{q_1}\left(\varphi_1'(q)\,\varphi_2'(q) - \varphi_2'(q)\,\varphi_1'(q)\right)dq\ .$$

When we introduce at this stage the so-called

Wronski determinant

$$W(\varphi_1,\varphi_2;q) = \begin{vmatrix}\varphi_1(q) & \varphi_2(q)\\ \varphi_1'(q) & \varphi_2'(q)\end{vmatrix} = \varphi_1(q)\,\varphi_2'(q) - \varphi_2(q)\,\varphi_1'(q)\ , \tag{4.11}$$

it remains:

$$W(\varphi_1,\varphi_2;q)\Big|_{q_0}^{q_1} = \frac{2\,m}{\hbar^2}\,(E_1 - E_2)\int_{q_0}^{q_1}\varphi_1(q)\,\varphi_2(q)\,dq\ . \tag{4.12}$$

This is a relation, which can often be exploited advantageously. Let us assume, for instance, that φ_1 and φ_2 are two wave functions with the same energy-eigen value $E = E_1 = E_2$. Then we argue from (4.12) that the Wronski determinant must be q-independent:

$$E = E_1 = E_2: \qquad W(\varphi_1,\varphi_2;q) = \text{const}\ . \tag{4.13}$$

If, in addition, the two solutions have a common zero q^*,

$$\varphi_1(q^*) = \varphi_2(q^*) = 0\ ,$$

then the constant in (4.13) is equal to zero. φ_1 and φ_2 have therefore the same logarithmic derivatives:

$$W = 0 \iff \frac{\varphi_2'(q)}{\varphi_2(q)} = \frac{\varphi_1'(q)}{\varphi_1(q)} \iff 0 = \frac{d}{dq} \ln \frac{\varphi_2(q)}{\varphi_1(q)}$$
$$\iff \varphi_2(q) = c\,\varphi_1(q)\,; \quad c \in \mathbb{C}\,. \tag{4.14}$$

If both the eigen-solutions can be assumed to be normalized, then φ_1 and φ_2 can at most differ only by an unimportant phase factor of the magnitude 1. The energy-eigen value E is thus not degenerate! We prove further statements of this kind as Exercises 4.1.1 and 4.1.2. They are of interest, in particular, because of the fact that they are valid independent of the special form of the potential $V(q)$.

4.1.3 Eigen-Value Spectrum

By some qualitative considerations, we now want to get a general idea of the possible structures of the eigen-value spectrum. These are of course determined by the actual form of $V(q)$. We therefore review here some typical potential curves. Our qualitative statements can of course be proven also mathematically rigorously. That we will demonstrate in the following parts on some special potentials.

1) $V(q) \to \infty$ for $q \to \pm\infty$

We know from Classical Mechanics (Sect. 2.3.6, Vol. 1) that such a potential leads to a periodic motion with two finite turning points (Fig. 4.4). For $E < V_{\min}$ it is always $k^2(q) < 0$, i.e., the whole q-region is *classically forbidden*. It is then easy to realize that only $\varphi \equiv 0$ can come into question as a solution.

For each energy $E > V_{\min}$ there are two classical turning points q_1 and q_2, which divide the q-axis into three relevant regions (Fig. 4.4):

$$\begin{aligned} -\infty < q \le q_1 &: \quad \text{classically forbidden:} \quad k^2(q) < 0\,, \\ q_1 \le q \le q_2 &: \quad \text{classically allowed:} \quad k^2(q) > 0\,, \\ q_2 \le q < +\infty &: \quad \text{classically forbidden:} \quad k^2(q) < 0\,. \end{aligned}$$

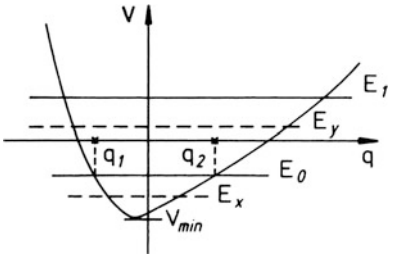

Fig. 4.4 Typical potential curve, which guarantees for each energy $E > V_{\min}$ the existence of two finite classical turning points

In order to carry on the following discussion in a concrete manner, we assume that the solution function $\varphi(q)$ exhibits for $q \leq q_1$ already the correct exponential decay (Figs. 4.5, and 4.6). We inspect therefore only the behavior of the wave function in the (classically forbidden) region $q \geq q_2$. The further assumption that $\varphi(q)$ for $q \to -\infty$, coming from the positive side, approaches zero exponentially, does not mean a restriction, either.

We first inspect the energy $E = E_x$ (Fig. 4.5). Between the two classical turning points q_1 and q_2, φ is concave. The *allowed region* $q_1 \leq q \leq q_2$ is, though, not sufficiently extended, in order to prevent the divergence of $\varphi(q \to +\infty)$ in the region $q \geq q_2$, caused by the convexity of φ. The energy $E = E_x$ therewith does not permit an acceptable solution of the Schrödinger Eq. (4.5).

We now increase the energy E shifting therewith the classical turning points q_1 and q_2 further outwards. At a certain energy E_0, the concave bending in the classically allowed region $q_1 \leq q \leq q_2$ is just sufficient to ensure the correct exponential decay of the wave function for $q \to \infty$ (Fig. 4.6). We have found therewith a first solution of the eigen-value problem (4.2). E_0 is obviously the lowest energy-eigen value. It is the so-called *ground-state energy*.

If we continue to enhance the energy to E_y (Fig. 4.4), the *classically allowed* region grows accordingly. There will appear a first zero-crossing. The bending towards the q-axis is, however, for $q > q_2$ not yet strong enough to prevent the divergence of the wave function for $q \to +\infty$. E_y is therefore as energy-eigen value out of the question (Fig. 4.7).

For getting the next solution of the eigen-value problem, the *classically allowed region* must reach a certain width as is the case at $E = E_1$ (Figs. 4.4, and 4.8).

The procedure can be continued in this way. It is quite clear that the next eigen-function $\varphi_2(q)$ is marked by two zero-crossings, $\varphi_3(q)$ by three zero-crossings, and so on. The fact that the wave function has to convert its oscillatory behavior in the

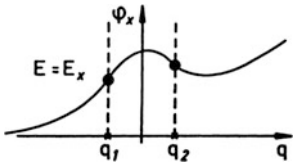

Fig. 4.5 Behavior of the wave function at an energy E_x (Fig. 4.4), which does not allow a physically correct connection at q_2. E_x can therefore not be a physical solution

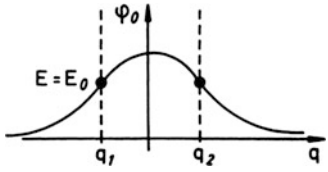

Fig. 4.6 Behavior of the ground state wave function with the correct exponential decay in the classically forbidden regions

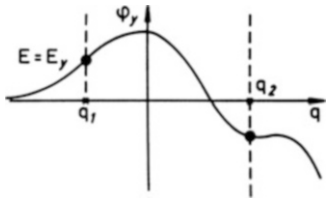

Fig. 4.7 Behavior of the wave function at an energy E_y, for which no physically acceptable connection at q_2 is possible. E_y is therewith not a physical solution

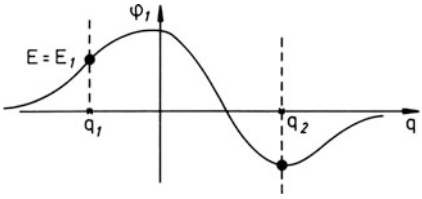

Fig. 4.8 Behavior of the wave function of the first excited state with the correct exponential decay in the classically forbidden regions and with the correct oscillatory behavior in the classically allowed region

classically allowed region $q_1 \leq q \leq q_2$ to the left at q_1 and to the right at q_2 to an *exponential decay* for $q \to \pm\infty$, together with the requirement that the *piecing together* at q_1 and q_2 for φ and φ' has to take place continuously, is the reason for the fact that only

$$\textbf{discrete energy-eigen values } E_n \; ; \quad n = 0, 1, 2, \ldots$$

are allowed. Ultimately, it turns out to be crucial for the *discreteness* that the *classically allowed region* is confined by two finite *classical turning points*. Classically seen, the particle can not move up to infinity, being rather confined to a finite space region. One therefore speaks of

$$\textbf{bound states } \varphi_n(q) \; ; \quad n = 0, 1, 2, \ldots .$$

If in the discrete energy spectrum the eigen-values are ordered by magnitude,

$$E_0 < E_1 < E_2 < \ldots < E_n < \ldots \; ,$$

then the index n corresponds to the so-called

number of nodes=number of zeros of $\varphi(q)$ on the finite q-axis.

This is the statement of the *'law of nodes'*, which we have made plausible here, but which of course can also be proven in a mathematically rigorous manner. Let us add some remarks for its justification:

Let $\varphi_n(q)$ and $\varphi_m(q)$ be two (real) eigen-functions with eigen-values $E_n > E_m$. We denote by q_0, q_1 two neighboring zeros (nodes) of $\varphi_m(q)$. Between these, $\varphi_m(q)$

has a fixed sign. It may be, for instance, that $\varphi_m(q) > 0$ for $q_0 < q < q_1$. But then it must also be $\varphi'_m(q_0) > 0$ and $\varphi'_m(q_1) < 0$, and the Wronski determinant (4.12) leads to the following relation:

$$\varphi_n(q)\,\varphi'_m(q)\big|_{q_0}^{q_1} = \frac{2\,m}{\hbar^2}\,(E_n - E_m)\int_{q_0}^{q_1} \varphi_n(q)\,\varphi_m(q)\,dq\,.$$

If $\varphi_n(q)$ likewise did not change its sign in the interval $[q_0, q_1]$, the right-hand side of this equation would have the same sign as $\varphi_n(q)$, the left-hand side, however, exactly the opposite sign. The assumption that $\varphi_n(q)$ does not change its sign in the interval $q_0 \le q \le q_1$, thus must be wrong. Between each of two nodes of $\varphi_m(q)$ there is therefore at least one node of $\varphi_n(q)$!

The eigen-functions $\varphi_n(q)$, $\varphi_m(q)$ both vanish exponentially for $q \to \pm\infty$. When $\varphi_m(q)$ has m nodes then the q-axis will be divided by it into $(m + 1)$ partial pieces. In each of these partial pieces there is at least one node of $\varphi_n(q)$. Accordingly, $\varphi_n(q)$ has at least (!) $(m+1)$ nodes. It is strictly proven therewith that the number of nodes is the larger the higher the discrete energy E_n is. This statement is an essential part of the law of nodes.

We can derive a further important statement with the aid of the Wronski determinant:

The energies E_n of the discrete spectrum are *are non-degenerate*!

To prove this let us assume that there are two different eigen-functions $\varphi_n(q)$, $\overline{\varphi}_n(q)$ with the same eigenvalue E_n. Then, according to (4.13), the corresponding Wronski determinant would be a constant and therefore independent of q. Since $\varphi_n(q)$ as well as $\overline{\varphi}_n(q)$ vanish for $q \to \pm\infty$, φ_n and $\overline{\varphi}_n$ are, according to (4.14), identical. E_n is thus not degenerate. That holds, however, only for the one-dimensional systems discussed here.

2) $V(q) \to \infty$ for finite $q = q_0$ and $q \to +\infty$

For $q \le q_0$ only $\varphi(q) \equiv 0$ can be a solution ($\kappa = \infty$ in (4.10)!) (Fig. 4.9). For $q > q_0$ the same conclusions are valid as in 1). Because of the continuity of $\varphi(q)$ all the discrete eigen-functions $\varphi_n(q)$ have to fulfill as boundary condition $\varphi_n(q_0) = 0$. Apart from that, the same statements are valid as in 1).

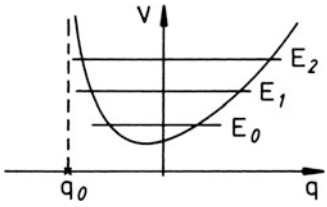

Fig. 4.9 Example of a potential, which diverges at a finite q_0 as well as for $q \to +\infty$

3) $V(q \to \pm\infty) = V_{\pm\infty} < \infty$

The behavior of the wave function depends now very decisively on the energy E. We have to distinguish different situations:

3a) $E < V_{\min}$

We argued in part 1) that in such a case no solution exists.

3b) $V_{\min} \leq E \leq V_{+\infty}$

This is the region of the discrete spectrum which explains itself exactly as in the case 1). The number of the really existing eigen-values essentially depends on the structure of the potential $V(q)$. Numbers between 0 and ∞ are thinkable. Classically, the particle is confined to a finite space region. The eigen-functions therefore represent bound states.

3c) $V_{+\infty} < E \leq V_{-\infty}$

Now there exists for each eigen-value E the possibility to find an eigen-solution. This must, for $q \to -\infty$, approach exponentially the q-axis. The *classically allowed region* to the right is unrestricted (Fig. 4.10). There, the wave function oscillates. The *fitting* to the left, to the *classically forbidden region*, is always realizable. A

continuous spectrum

is therefore typical which is, because of the *fitting*, not degenerate. Since the oscillatory behavior persists up to $q \to +\infty$, the eigen-solutions are not anymore normalizable. On the other hand, they do not diverge, either (see improper Dirac states, Sect. 3.2.4).

3d) $E > V_{-\infty}$

In this case, the eigen-solutions show oscillatory behavior over the whole q-region. The spectrum of the eigen-values is continuous and doubly degenerate. The latter is true because for each energy E, two linearly independent solutions of the differential Eq. (4.5) exist!

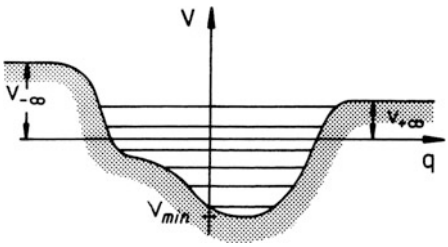

Fig. 4.10 Example of a potential which is finite over the whole q-axis

4.1.4 *Parity*

The action of the parity operator Π on the wave functions $\varphi(q)$ or the spatial eigen-states $|q\rangle$ consists of replacing the position coordinate q by $(-q)$ (space inflection!):

$$\Pi\,\varphi(q) = \varphi(-q)\ . \tag{4.15}$$

In Exercise 3.5.7 we have derived a series of important properties of this operator, for instance, that it is a Hermitian and unitary operator:

$$\Pi = \Pi^{+} = \Pi^{-1}\ . \tag{4.16}$$

As eigen-values ($\Pi\,\psi = \pi\,\psi$) only

$$\pi = +1,\ -1 \tag{4.17}$$

come into question:

$$\Pi^2\,\psi(q) \quad \begin{array}{l} \nearrow \\ \searrow \end{array} \quad \begin{array}{l} \pi\,\Pi\,\psi(q) = \pi^2\,\psi(q) \\ \Pi\,\psi(-q) = \psi(q)\ . \end{array}$$

The even wave functions are eigen-functions with the eigen-value
$\pi = +1$: even parity

$$\Pi\,\psi(q) = \psi(q) \stackrel{!}{=} \psi(-q)\ , \tag{4.18}$$

and the odd wave functions with the eigen-value
$\pi = -1$: odd parity

$$\Pi\,\psi(q) = -\psi(q) \stackrel{!}{=} \psi(-q)\ . \tag{4.19}$$

Any arbitrary wave function can be split into a part with even parity and a part with odd parity:

$$\chi(q) = \chi_{+}(q) + \chi_{-}(q)\ , \tag{4.20}$$

$$\chi_{+}(q) = \frac{1}{2}\big(\chi(q) + \chi(-q)\big) = \chi_{+}(-q)\ , \tag{4.21}$$

$$\chi_{-}(q) = \frac{1}{2}\big(\chi(q) - \chi(-q)\big) = -\chi_{-}(-q)\ . \tag{4.22}$$

That corresponds, by the way, to the expansion law (3.66), according to which any arbitrary state can be expanded in the eigen-states of a Hermitian operator.

Π conveys a unitary transformation (3.90). We have shown in Exercise 3.5.7 that it holds for position and momentum operator:

$$\Pi\,\hat{q}\,\Pi^{+} = -\hat{q}\,; \quad \Pi\,\hat{p}\,\Pi^{+} = -\hat{p}\,. \tag{4.23}$$

Thus, both operators are odd. Since, according to the general agreement (Sect. 3.2.7), each operator function $A(\hat{q}, \hat{p})$ can be understood as polynomial or power series with respect to $\hat{q}$ and $\hat{p}$, it is:

$$\Pi\,A(\hat{q},\hat{p})\,\Pi^{+} = A(-\hat{q},-\hat{p})\,. \tag{4.24}$$

The Hamilton operator H (4.1) is an even operator only if $V(\hat{q}) = V(-\hat{q})$. Let us assume that this is the case:

$$V(\hat{q}) = V(-\hat{q}) \implies \Pi\,H\,\Pi^{+} = H\,. \tag{4.25}$$

This property of invariance of the Hamilton operator leads to certain symmetry conditions for the eigen-functions (eigen-states) and can therefore very often be conveniently exploited. If one multiplies (4.25) from the right by Π, it follows because of (4.16):

$$[\Pi,\,H]_{-} = 0\,. \tag{4.26}$$

The Hermitian operators Π and H thus have a common set of eigen-functions (eigen-states). One can therefore choose the eigen-states of H always so that they have a definite parity. If the respective energy-eigen value is not degenerate, the corresponding wave function has a well-defined parity. If it is, however, degenerate, then the eigen-space can be built with basis states which are of well-defined, but of different parity.

4.1.5 Exercises

Exercise 4.1.1 Let $\varphi_1(q)$ and $\varphi_2(q)$ be two real solutions of the one-dimensional Schrödinger equation with different eigen-values E_1, E_2 from the discrete part of the energy spectrum. Show, with the aid of the Wronski determinant, the orthogonality of the two eigen-functions.

Exercise 4.1.2 The solutions $\varphi_1(q)$, $\varphi_2(q)$ of the one-dimensional Schrödinger equation are linearly dependent in the interval $q_0 \le q \le q_1$, if the Wronski determinant $W(\varphi_1, \varphi_2; q)$ in this interval is *identically equal to zero*. Prove this statement!

Exercise 4.1.3 Let the Hamilton operator of a particle of mass m in a one-dimensional potential

$$V(q) = V(-q) \; ; \qquad q \in \mathbb{R}$$

have discrete energy-eigen values E_n with $E_0 < E_1 < \ldots < E_n < \ldots$. According to the law of nodes, the index n is identical to the number of zeros of the corresponding eigen-function $\varphi_n(q)$ in the interval $-\infty < q < +\infty$. What is the parity of the $\varphi_n(q)$?

Exercise 4.1.4 The eigen-functions $p(q)$ of the parity operator Π are, of course, as the eigen-functions of a Hermtian operator, orthogonal. Justify this fact directly from the properties of the functions $p(q)$!

4.2 Potential Well

We want to test the general considerations of the last section by a first concrete example of application. The rectangular one-dimensional potential well can serve as a simple model for short-range attractive forces, as they are experienced by electrons in solids, for instance, due to imperfections, i.e. due to the deviations from the ideal periodic lattice structure. In the position-representation, the potential is given by

$$V(q) = \begin{cases} -V_0 & \text{for } |q| < q_0 \; , \\ 0 & \text{otherwise} \end{cases} \; . \tag{4.27}$$

The one-dimensional Schrödinger equation leads to the differential Eq. (4.5), in which $k^2(q)$ is piecewise constant (Fig. 4.11):

$$\begin{aligned} &\text{regions A and C:} \quad k^2(q) = \tfrac{2m}{\hbar^2} E \; , \\ &\text{region B:} \qquad\qquad k^2(q) = \tfrac{2m}{\hbar^2} (E + V_0) \; . \end{aligned} \tag{4.28}$$

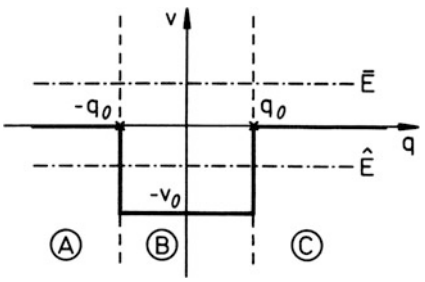

Fig. 4.11 Space dependence of the simple potential well

4.2.1 Bound States

At first we investigate the discrete spectrum of the Hamiltonian (4.1); that means we presume

$$-V_0 < E < 0\,. \tag{4.29}$$

According to our preliminary considerations in Sect. 4.1, we know that the levels of the discrete spectrum are not degenerate. The functions, that we seek, namely $\varphi_n(q)$, $n = 0, 1, 2, \ldots$, must have a definite parity, since the Hamilton operator H is an even operator (4.25) because $V(q) = V(-q)$. The index n corresponds to the number of nodes of the wave function $\varphi_n(q)$ in the region B, in which we have to expect oscillatory behavior and which is matched to an asymptotically exponential decay in the regions A and C (Fig. 4.12). We have therewith, qualitatively, already quite a precise idea about the system of solutions, which is to be expected. This we want to confirm now by an explicit calculation. For this purpose, we first solve the differential Eq. (4.5) separately for the three regions A, B, and C, in order to match the three partial solutions at $\pm q_0$ in compliance with the continuity conditions. The latter will serve to fix free parameters in the partial solutions.

Region A

Here we have:

$$k^2(q) \longrightarrow -\kappa^2 = -\frac{2\,m}{\hbar^2}|E|\,. \tag{4.30}$$

Therewith, the differential Eq. (4.5), to be solved, reads:

$$\varphi''(q) - \kappa^2\,\varphi(q) = 0\,. \tag{4.31}$$

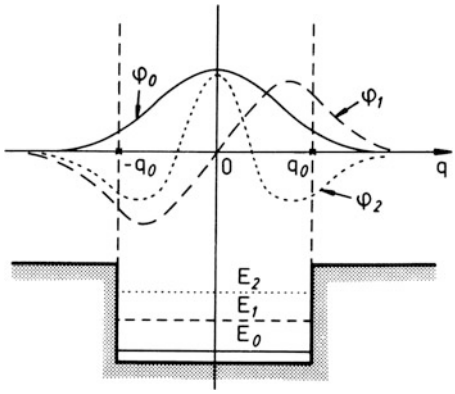

Fig. 4.12 Qualitative behavior of the wave functions of the ground state and the first two excited states of the potential-well problem

It is a *classically forbidden* region, in which the general solution,

$$\varphi_{\mathrm{A}}(q) = \alpha_+ \, e^{\kappa q} + \alpha_- \, e^{-\kappa q} \, ,$$

must exponentially approach the q-axis for $q \to -\infty$. That works only with $\alpha_- = 0$:

$$\varphi_{\mathrm{A}}(q) = \alpha_+ \, e^{\kappa q} \, . \tag{4.32}$$

Region B

This represents a *classically allowed region*:

$$k^2(q) = \frac{2\,m}{\hbar^2} \, (V_0 - |E|) > 0 \, . \tag{4.33}$$

The wave function oscillates:

$$\varphi_{\mathrm{B}}(q) = \beta_+ \, e^{ikq} + \beta_- \, e^{-ikq} \, . \tag{4.34}$$

Region C

It is again a *classically forbidden region*, for which (4.31) is to be solved with the same κ as that in (4.30). As solution with correct exponential decay for $q \to +\infty$, we get:

$$\varphi_{\mathrm{C}}(q) = \gamma_- \, e^{-\kappa q} \, . \tag{4.35}$$

For fixing the still unknown coefficients in the three partial solutions (4.32)–(4.35) we now exploit the fitting conditions at $\pm q_0$. The continuity of $\varphi(q)$ at $\pm q_0$ leads to the following conditional equations:

$$\alpha_+ \, e^{-\kappa q_0} \stackrel{!}{=} \beta_+ \, e^{-ikq_0} + \beta_- \, e^{ikq_0} \, , \tag{4.36}$$

$$\beta_+ \, e^{ikq_0} + \beta_- \, e^{-ikq_0} \stackrel{!}{=} \gamma_- \, e^{-\kappa q_0} \, . \tag{4.37}$$

Two further conditional equations are due to the continuity of $\varphi'(q)$:

$$\kappa \, \alpha_+ \, e^{-\kappa q_0} = i\,k\big(\beta_+ \, e^{-ikq_0} - \beta_- \, e^{+ikq_0}\big) \, , \tag{4.38}$$

$$i\,k\big(\beta_+ \, e^{ikq_0} - \beta_- \, e^{-ikq_0}\big) = -\kappa \, \gamma_- \, e^{-\kappa q_0} \, . \tag{4.39}$$

These are four equations for four unknowns. However, the system of equations simplifies further essentially when we exploit the symmetry, i.e., when we exploit the fact that the eigen-functions must have a well-defined parity.

1) Symmetric solutions (even parity)

It follows immediately from $\varphi(q) = \varphi(-q)$:

$$\alpha_+ = \gamma_- = \alpha \; ; \quad \beta_+ = \beta_- = \beta \; .$$

Each two of the four Eqs. (4.36)–(4.39) are therewith identical:

$$\begin{aligned} \alpha \, e^{-\kappa q_0} &= 2 \, \beta \cos k \, q_0 \; , \\ \kappa \, \alpha \, e^{-\kappa q_0} &= 2 \, \beta \, k \sin k \, q_0 \; . \end{aligned}$$

This is a homogeneous system of equations for the unknown parameters α and β, which has a non-trivial solution if the secular determinant vanishes. That leads to the transcendental conditional equation,

$$k \tan k q_0 = \kappa \; , \tag{4.40}$$

of which we will read off at a later stage the discrete energy-eigen values. But at first we fix the coefficients α, β:

$$\beta = \frac{e^{-\kappa q_0}}{2 \cos k q_0} \, \alpha = \frac{1}{2} \sqrt{1 + \frac{\kappa^2}{k^2}} \, e^{-\kappa q_0} \, \alpha \; .$$

This leads to the following symmetric wave function:

$$\varphi_+(q) = \alpha \begin{cases} \exp(\kappa q) & \text{for } -\infty < q \leq -q_0 \; , \\ \dfrac{\exp(-\kappa q_0)}{\cos k q_0} \cos k q & \text{for } -q_0 < q < +q_0 \; , \\ \exp(-\kappa q) & \text{for } +q_0 \leq q < +\infty \; . \end{cases} \tag{4.41}$$

The still remaining constant α is fixed by the normalization condition

$$1 \stackrel{!}{=} \int_{-\infty}^{+\infty} dq |\varphi_+(q)|^2 \; .$$

It follows, if one, in particular, uses (4.40) and assumes α to be real:

$$\alpha = e^{\kappa q_0} \left[\left(1 + \frac{\kappa^2}{k^2} \right) \left(q_0 + \frac{1}{\kappa} \right) \right]^{-\frac{1}{2}} \; . \tag{4.42}$$

2) Antisymmetric solutions (odd parity)

Because of $\varphi(q) = -\varphi(-q)$, we can now use in (4.36)–(4.39)

$$\alpha_+ = -\gamma_- = a\,; \quad \beta_+ = -\beta_- = b\,.$$

It then results the homogeneous system of equations:

$$\begin{aligned} a\,e^{-\kappa q_0} &= -2ib\sin kq_0\,, \\ \kappa a\,e^{-\kappa q_0} &= 2ikb\cos kq_0\,. \end{aligned}$$

The requirement that the secular determinant has to vanish, now leads to:

$$k\cot kq_0 = -\kappa\,. \tag{4.43}$$

The antisymmetric solution function is now easily calculated:

$$\varphi_-(q) = a\begin{cases} \exp(\kappa q) & \text{for } -\infty < q \le -q_0\,, \\ \dfrac{-\exp(-\kappa q_0)}{\sin kq_0}\sin kq & \text{for } -q_0 < q < +q_0\,, \\ -\exp(-\kappa q) & \text{for } q_0 \le q < +\infty\,. \end{cases} \tag{4.44}$$

The coefficient a is again found from the normalization. It turns out that it is identical with α from (4.42).

We now want to analyze the energy conditions (4.40) and (4.43). These are transcendental equations, which do not allow for an analytical solution. The computational evaluation, though, does not pose any difficulties. But let us here try to get a certain overview of the system of solution (Fig. 4.13). For this purpose, we multiply (4.40) and (4.43) both by q_0 and write for abbreviation:

$$\eta = \kappa q_0\,; \qquad \xi = kq_0\,. \tag{4.45}$$

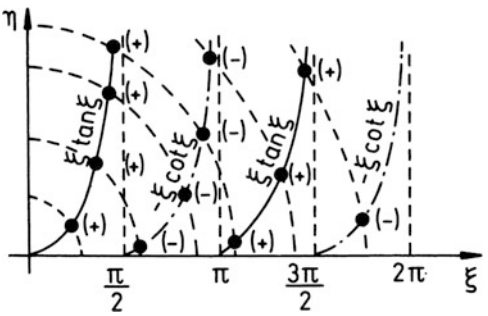

Fig. 4.13 Graphical solution of the energy conditions for the potential well

We then have to solve the following system of equations:

$$\eta = \xi \tan \xi \; ; \qquad \eta = -\xi \cot \xi \; . \tag{4.46}$$

ξ and η are not independent of each other:

$$\xi^2 = k^2 q_0^2 = \frac{2\,m\,q_0^2}{\hbar^2}\,(V_0 - |E|) \; ,$$

$$\eta^2 = \kappa^2 q_0^2 = \frac{2\,m\,q_0^2}{\hbar^2}\,|E| \; .$$

The sum $\xi^2 + \eta^2$ is independent of the energy E describing a circle with the radius R (Fig. 4.13):

$$R^2 = \xi^2 + \eta^2 = \frac{2\,m}{\hbar^2}\,q_0^2\,V_0 \; . \tag{4.47}$$

The radius R of the circle is determined by the product $q_0^2\,V_0$, i.e., by the width and the depth of the potential well. Since η and ξ must be positive, the solutions can be found exclusively in the upper right quadrant of the η–ξ-coordinate axes. The intersection points of the curves (4.46) with the circles (4.47) represent the solutions. The sketch (Fig. 4.13) makes clear that for arbitrarily small parameters at least one symmetric solution always exists, while for solution with odd parity the product $q_0^2\,V_0$ has to exceed a minimal value. We recognize further that for a *finite* potential well ($q_0^2\,V_0 < \infty \iff R < \infty$) also only finitely many energy-eigen values exist and therewith only finitely many bound states. Their number can be related to R in a simple manner. If N is the number of intersection points and therewith the number of solutions, then it must obviously hold:

$$(N-1)\,\frac{\pi}{2} < R < N\,\frac{\pi}{2} \implies N = \left[\frac{2\,R}{\pi}\right] \; . \tag{4.48}$$

The sign $[x]$ means the smallest integer greater than x. We still can break down the number of solutions with respect to parities. The number N_+ of the solutions with even parity comes out as follows:

$$(N_+ - 1)\,\pi < R < N_+\pi \implies N_+ = \left[\frac{R}{\pi}\right] .$$

For the number N_- of odd solutions, we read off from the sketch in Fig. 4.13:

$$(2\,N_- - 1)\,\frac{\pi}{2} < R < (2\,N_- + 1)\,\frac{\pi}{2} \implies N_- = \left[\frac{R}{\pi} - \frac{1}{2}\right] \; .$$

One recognizes that a symmetric solution exists even for an arbitrarily small well, while for the antisymmetric solution $R > \pi/2$ must be fulfilled. The potential well thus must be of such a size that

$$q_0^2 V_0 > \frac{\pi^2 \hbar^2}{8\, m} \tag{4.49}$$

is guaranteed, in order that at least one antisymmetric bound state exists.

These explicit calculations agree with our preliminary qualitative considerations, by which we could indicate right at the beginning of this chapter, the structure of the solutions.

4.2.2 Scattering States

We now analyze the situation $E > 0$ for the potential well, introduced at the beginning of the Sect. 4.2. *Classically seen*, the particle can propagate to both sides up to infinity. Bound states thus can not exist. Since for $E > 0$, the whole q-axis represents *classically allowed region*, the wave function, we are looking for, will exhibit everywhere oscillatory behavior (Fig. 4.14), being therewith not any longer normalizable. The de Broglie-wave length will be different, though, inside and outside the *region of the well*. Our considerations in Sect. 4.1 allows us to expect a continuous energy spectrum.

Starting point is of course now also the Schrödinger equation in the form (4.5), whose structure of solution is known qualitatively by the analysis performed in Sect. 4.1. We use the abbreviations

$$k_0^2 = \frac{2\, m}{\hbar^2} E\,; \quad k^2 = \frac{2\, m}{\hbar^2} (E + V_0)\,;$$
$$y = \frac{k}{k_0} = \sqrt{\frac{E + V_0}{E}} \tag{4.50}$$

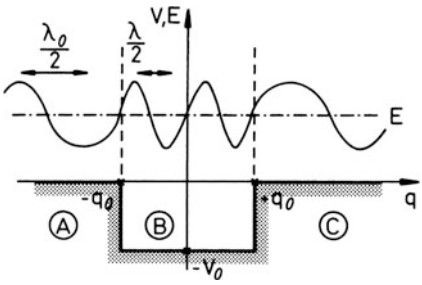

Fig. 4.14 Qualitative behavior of a scattering state at the potential well

and choose the following ansatz for the solution:

$$\varphi(q) = \begin{cases} \varphi_0(q) + \varphi_\mathrm{r}(q) : & -\infty < q \le -q_0 \,, \\ \beta_+ \, e^{ikq} + \beta_- \, e^{-ikq} : & -q_0 < q < +q_0 \,, \\ \varphi_\mathrm{t}(q) : & +q_0 \le q < +\infty \,. \end{cases} \tag{4.51}$$

Without loss of generality, we can assume the particle wave, which comes from the negative infinite, to be of intensity 1:

$$\varphi_0(q) = e^{ik_0 q} \,. \tag{4.52}$$

A part of the wave is possibly reflected by the potential well at $-q_0$ (Fig. 4.14):

$$\varphi_\mathrm{r}(q) = \alpha_- \, e^{-ik_0 q} \,. \tag{4.53}$$

The transmitted wave, on the other hand, will not be reflected at the positive infinite:

$$\varphi_\mathrm{t}(q) = \gamma_+ \, e^{ik_0 q} \,. \tag{4.54}$$

With these partial waves, probability-current densities (2.27) are connected,

$$j_{0,\mathrm{r,t}} = \frac{\hbar}{2\,m\,i} \left(\varphi^*_{0,\mathrm{r,t}} \frac{d}{dq} \varphi_{0,\mathrm{r,t}} - \varphi_{0,\mathrm{r,t}} \frac{d}{dq} \varphi^*_{0,\mathrm{r,t}} \right) \,,$$

which can be calculated easily here to be

$$j_0 = \frac{\hbar\, k_0}{m} \,; \quad j_\mathrm{r} = -\frac{\hbar\, k_0}{m} |\alpha_-|^2 \,; \quad j_\mathrm{t} = \frac{\hbar\, k_0}{m} |\gamma_+|^2 \,. \tag{4.55}$$

Physically important quantities are the *transmission coefficient* T and the *reflection coefficient* R, which are a measure of, which part of the wave will traverse the *region of the well* and which part is reflected by the potential well:

$$T = \left| \frac{j_\mathrm{d}}{j_0} \right| = |\gamma_+|^2 \,, \tag{4.56}$$

$$R = \left| \frac{j_\mathrm{r}}{j_0} \right| = |\alpha_-|^2 \,. \tag{4.57}$$

From a *classical view point*, the particle wave can be for $E > 0$ at most slowed down by the potential, but not reflected at all. The following calculation, however, will show that normally $R \neq 0$, wherein, once more, a typical quantum-mechanical phenomenon manifests itself, which has its origin in the classically not explainable

wave nature of matter. The particle-number conservation of course requires

$$T + R = 1 \tag{4.58}$$

For the explicit calculation of T and R we need the still unknown coefficients of the ansatz functions (4.51)–(4.54). These we again get by the continuity conditions for φ and φ' at the discontinuity positions $\pm q_0$ of the potential. At $q = -q_0$ it must be:

$$\begin{aligned} e^{-ik_0q_0} + \alpha_- \, e^{ik_0q_0} &= \beta_+ \, e^{-ikq_0} + \beta_- \, e^{ikq_0} \,, \\ i\,k_0 \left(e^{-ik_0q_0} - \alpha_- \, e^{ik_0q_0}\right) &= i\,k \left(\beta_+ \, e^{-ikq_0} - \beta_- \, e^{ikq_0}\right) \end{aligned}$$

and at $q = +q_0$:

$$\begin{aligned} \beta_+ \, e^{ikq_0} + \beta_- \, e^{-ikq_0} &= \gamma_+ \, e^{ik_0q_0} \,, \\ i\,k \left(\beta_+ \, e^{ikq_0} - \beta_- \, e^{-ikq_0}\right) &= i\,k_0 \, \gamma_+ \, e^{ik_0q_0} \,. \end{aligned}$$

We divide the second and the fourth equation both by $i\,k_0$ and then add the second to the first, and subtract the fourth from the third conditional equation:

$$\begin{aligned} 2\,e^{-ik_0q_0} &= \beta_+ \,(1+y)\, e^{-ikq_0} + \beta_-(1-y)\, e^{ikq_0} \,, \\ 0 &= \beta_+(1-y)\, e^{ikq_0} + \beta_-(1+y)\, e^{-ikq_0} \,. \end{aligned}$$

That is a linear inhomogeneous system of equations for the amplitudes β_+ and β_-. The determinant of the matrix of coefficients

$$\begin{aligned} \det A &= \det \begin{pmatrix} (1+y)\, e^{-ikq_0} & (1-y)\, e^{ikq_0} \\ (1-y)\, e^{ikq_0} & (1+y)\, e^{-ikq_0} \end{pmatrix} = \\ &= (1+y)^2 \, e^{-2ikq_0} - (1-y)^2 \, e^{2ikq_0} \end{aligned} \tag{4.59}$$

is in any case unequal zero. According to the Cramer's rule ((1.349), Vol. 1), there exists for each $E > 0$ a unique solution of the inhomogeneous system of equations. That confirms that for $E > 0$ the eigen-value spectrum is continuous.

For the concrete solutions, we need the Cramer's rule once more:

$$\begin{aligned} \beta_+ \, \det A &= \det \begin{pmatrix} 2\,e^{-ik_0q_0} & (1-y)\, e^{ikq_0} \\ 0 & (1+y)\, e^{-ikq_0} \end{pmatrix} = 2(1+y)\, e^{-i(k+k_0)q_0} \,, \\ \beta_- \, \det A &= \det \begin{pmatrix} (1+y)\, e^{-ikq_0} & 2\,e^{-ik_0q_0} \\ (1-y)\, e^{ikq_0} & 0 \end{pmatrix} = -2(1-y)\, e^{i(k-k_0)q_0} \,. \end{aligned}$$

The amplitudes α_- and γ_+, which determine reflection and transmission, are more interesting than β_+ and β_-. When we insert the results for β_+ and β_- into the initial

system of equations, after simple rearrangements we get:

$$\gamma_+ = \frac{4\,y}{\det A}\, e^{-2ik_0 q_0} \;, \tag{4.60}$$

$$\alpha_- = -2\,i \sin(2\,k\,q_0)\, \frac{1-y^2}{\det A}\, e^{-2ik_0 q_0} \;. \tag{4.61}$$

If we eventually still use (4.59) for the evaluation of

$$|\det A|^2 = 16\,y^2 + 4(1-y^2)^2 \sin^2(2\,k\,q_0) \;, \tag{4.62}$$

then we get, after insertion of (4.60) and (4.61) into (4.56) and (4.57), the following expressions for the transmission and the reflection coefficient:

$$T = \frac{16\,y^2}{|\det A|^2} = T(E) \;, \tag{4.63}$$

$$R = \frac{4(1-y^2)^2 \sin^2(2\,k\,q_0)}{|\det A|^2} = R(E) \;. \tag{4.64}$$

The condition (4.58) is obviously fulfilled. We recognize that, in general, the particle wave experiences, quantum-mechanically, a reflection at the potential well. More precisely, R shows an oscillatory behavior. At certain values of $2\,k\,q_0$, i.e., at certain energies, the value of the sine-function becomes equal to zero:

$$2\,k\,q_0 = n\,\pi \iff 2\,q_0 = n\,\frac{\lambda}{2}\;; \qquad n = 1, 2, 3 \ldots \;. \tag{4.65}$$

That is therefore always the case when an integral multiple of half the de Broglie wave length λ just fits the potential well. One speaks of *resonances*, which, according to (4.65), appear at the energies

$$E_n^{(\mathrm{R})} = -V_0 + \frac{\hbar^2 \pi^2}{8 m q_0^2}\, n^2 \tag{4.66}$$

($n \geq n_0$, therewith $E_n^{(\mathrm{R})} > 0$). Interestingly, these are just the energy-eigen values of the infinitely high potential well, which we calculate as Exercise 4.2.1. At these resonance energies, the potential well becomes *totally transparent*:

$$T\big(E = E_n^{(\mathrm{R})}\big) = 1\;; \qquad R\big(E = E_n^{(\mathrm{R})}\big) = 0\;. \tag{4.67}$$

These resonance can be illustratively understood by destructive interference of the partial waves, which are reflected at $-q_0$ and $+q_0$. At $q = -q_0$, the directly reflected wave and the wave, which *comes back* from $q = +q_0$, have a path difference of $4kq_0 = 2\pi n$. In addition, there is a phase jump by π for the direct reflection, so that

finally the two partial waves, reflected at $-q_0$ and $+q_0$, cancel each other. On the other hand, maxima of the reflection and minima of the transmission, respectively, can be expected at

$$2kq_0 = (2n+1)\,\frac{\pi}{2}\,,$$

because it is then in (4.64)

$$\sin^2 2kq_0 = 1\,.$$

For $E \gg V_0$ one finds $y^2 \approx 1$ and therewith $R \approx 0$, $T \approx 1$. That is quite plausible since for high incident energies the particle does *'hardly feel'* the potential well.

For very low energies $E \to 0$, i.e., $y \to \infty$,, the reflection dominates ($R \to 1$, $T \to 0$). Qualitatively, it results in an energy-dependence of transmission and reflection coefficient as schematically plotted in Fig. 4.15. The oscillations of T and R will be the sharper, and the corresponding amplitudes the larger, the deeper the potential well is.

4.2.3 Exercises

Exercise 4.2.1 A particle of mass m moves in a one-dimensional infinitely high potential well:

$$V(q) = \begin{cases} 0\,, & \text{if } |q| < q_0 \quad (q_0 > 0)\,, \\ \infty\,, & \text{if } |q| \geq q_0\,. \end{cases}$$

1. Formulate the time-independent Schrödinger equation together with the boundary conditions.
2. Calculate the discrete energy-eigen values and the corresponding eigenfunctions.
3. How large is the probability to find the particle in the space interval

$$-\frac{q_0}{2} \leq q \leq +\frac{q_0}{2}\ ?$$

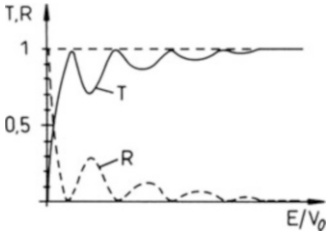

Fig. 4.15 Energy-dependence of the transmission (T)- and the reflection coefficient (R) for scattering states at the potential well

Exercise 4.2.2 Determine once more for the same one-dimensional, infinitely high potential well as in Exercise 4.2.1, the wave function $\varphi(q)$ and the energy-eigen value E, but now by the use of *periodic boundary conditions* (Sect. 2.2.5):

$$\varphi(q + 2q_0) = \varphi(q) \; .$$

Compare the results with those of the preceding exercise, which have been derived with *homogeneous boundary conditions* $\varphi(\pm q_0) = 0$.

Exercise 4.2.3 A particle of mass m moves in a one-dimensional, piecewise constant potential (Fig. 4.16):

$$V(q) = \begin{cases} V_1 > 0 & \text{for } -\infty < q \leq -q_0 \; , \\ 0 & \text{for } -q_0 < q < +q_0 \; , \\ V_3 > 0 & \text{for } +q_0 \leq q < +\infty \; . \end{cases}$$

1. Formulate the Schrödinger equation and find the fitting conditions for the wave function at $\pm q_0$. Thereby use the abbreviations:

$$k^2 = \frac{2m}{\hbar^2} E \; ; \quad \kappa_{1,3}^2 = \frac{2m}{\hbar^2} (V_{1,3} - E) \; .$$

2. Show that the discrete eigen-energies are to be determined from the transcendental equation:

$$1 = e^{-4ikq_0} \frac{V_3}{V_1} \left(\frac{k + i\kappa_1}{k - i\kappa_3} \right)^2$$

3. Bring the conditional equation of part 2. into the form:

$$f(E) = \arcsin \sqrt{\frac{E}{V_1}} + \arcsin \sqrt{\frac{E}{V_3}} = n\pi - 2q_0 k \; ; n = 1, 2, 3, \ldots \; .$$

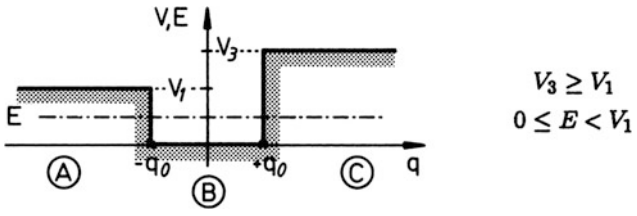

Fig. 4.16 Example of an asymmetric potential

Hint: Use for the complex wave number combinations their polar representations!

4. By the use of a *'graphical discussion'* show that the eigen-value spectrum is discrete.
5. Compare the eigen-values for $V_3 = V_1$ with those for $V_3 = 2V_1$. How does the eigen-value spectrum change?

Exercise 4.2.4 Inspect the following one-dimensional potential (Fig. 4.17):

$$V(q) = \begin{cases} \infty & \text{for } q \leq 0 \quad \text{(A)}\,, \\ -V_0 & \text{for } 0 < q < q_0 \quad \text{(B)}\,, \\ 0 & \text{for } q_0 \leq q < \infty \text{ (C)}\,. \end{cases}$$

1. By which equation are the energy-eigen values for the bound states of a particle of mass m determined? Use for the interval $0 < q < q_0$ the ansatz:

$$\varphi(q) = \alpha \sin(kq + \overline{\varphi})\,.$$

2. Derive a necessary condition for the appearance of bound states!
3. Are there bound states for $V_0 = \hbar^2/(mq_0^2)$?

Exercise 4.2.5 Consider the one-dimensional motion of a particle of mass m in a δ-potential (Fig. 4.18):

$$V(q) = -V_0\delta(q)\,; \quad V_0 > 0\,.$$

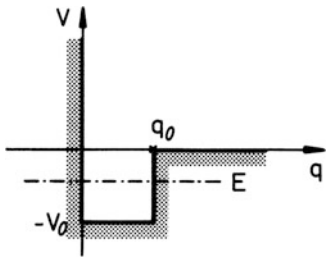

Fig. 4.17 Asymmetric potential well with an infinitely high wall from the left

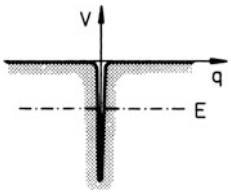

Fig. 4.18 Limiting case of a δ-function like potential

Calculate the normalized eigen-functions of the bound states! How many bound states exist in dependence of V_0?

For the solution presume that the wave function $\varphi(q)$, looked for, behaves, in spite of the *unphysical* potential, *physically reasonably* everywhere, i.e. for instance, that it permits the important statistical interpretation (Chap. 2).

Exercise 4.2.6 A particle of mass m moves in the potential

$$V(q) = \begin{cases} +\infty & \text{for } |q| \geq q_0 > 0 \\ \dfrac{\hbar^2}{2m} V_0 \delta(q) & \text{if } \quad 0 \leq |q| < q_0 \, . \end{cases}$$

1. What can be said about the parity of the solution $\varphi(q)$ of the time-independent Schrödinger equation?
2. Presume that the wave function is continuous everywhere. How do the wave function and its derivative $\varphi'(q)$ behave at the point $q = 0$?
3. Formulate the physical boundary conditions, which must be fulfilled by $\varphi(q)$ at the points $q = 0, \pm q_0$.
4. Find conditional equations for the possible energy-eigen values!
5. Derive the eigen-function $\varphi(q)$, except for a normalization constant!

Exercise 4.2.7

1. Write down the time-independent, one-dimensional Schrödinger equation for a potential $V(q)$ in the momentum representation, i.e., for the wave function $\overline{\psi}(p)$.
2. Look at the special case

$$V(q) = V_0 \delta(q) \qquad (V_0 < 0) \, .$$

Determine the eigen-energy of the bound state and compare the result with that from Exercise 4.2.5. How does the normalized wave function $\overline{\psi}(p)$ read?

Exercise 4.2.8 Investigate the same problem as in Exercise 4.2.5, but now for the double-δ-potential (Fig. 4.19):

$$V(q) = -V_0 \delta(q + q_0) - V_0 \delta(q - q_0) \, ; \quad V_0 > 0 \, .$$

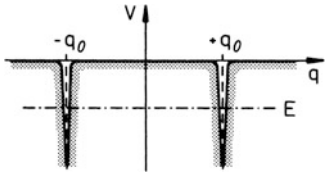

Fig. 4.19 Combination of two delta-function-like potentials

Exercise 4.2.9 A particle of mass m moves in the potential of Exercise 4.2.3:

$$V(q) = \begin{cases} V_1 > 0 & \text{for } -\infty < q \le -q_0 \,, \\ 0 & \text{for } -q_0 < q < +q_0 \,, \\ V_3 > V_1 & \text{for } +q_0 \le q < +\infty \,. \end{cases}$$

For the scattering states ($E > V_3$) calculate the reflection coefficient R and the transmission coefficient T.

Exercise 4.2.10 Consider a particle in an infinitely high potential well (see Exercise 4.2.1):

$$V(q) = \begin{cases} 0 & \text{if } |q| < q_0 \,, \\ \infty & \text{if } |q| \ge q_0 \,. \end{cases}$$

Let the particle be in a non-stationary state $\psi(q)$:

$$\psi(q) = \begin{cases} A(q^2 - q_0^2) & \text{for } -q_0 < q < +q_0 \,, \\ 0 & \text{otherwise} \,. \end{cases}$$

1. Calculate the (real) normalization constant A.
2. With which probability does a measurement of the energy of the particle yield the energy $E_n^{(-)}$ of the stationary state

$$\varphi_n^{(-)}(q) = \frac{1}{\sqrt{q_0}} \sin\left(\frac{\pi}{q_0} n q\right)$$

   (see Exercise 4.2.1) $\left(\varphi_n^{(-)}(q) \equiv 0 \text{ for } |q| \ge q_0\right)$?
3. With which probability does the measurement of energy yield the value $E_n^{(+)}$ of the stationary state

$$\varphi_n^{(+)}(q) = \frac{1}{\sqrt{q_0}} \cos\left(\frac{\pi}{2q_0}(2n+1) q\right)$$

   $\left(\varphi_n^{(+)}(q) \equiv 0 \text{ for } |q| > q_0\right)$?

4.3 Potential Barriers

In this subsection we will discuss some more simple examples of one-dimensional motion, on the one hand, in order to get the quantum-mechanical formalism, i.e., the *'calculation tools'*, under still better control. On the other hand, we want to describe some examples of typical quantum-mechanical phenomena (tunnel effect, energy bands in solids, ...), which are classically not explainable, in which, in particular, the wave nature of matter manifests itself.

4.3.1 Potential Step

The simplest form of a potential barrier is the step (Fig. 4.20):

$$V(q) = \begin{cases} 0 & \text{for } q < 0\,, \\ V_0 & \text{for } q \geq 0\,. \end{cases} \tag{4.68}$$

We again imagine (*gedanken-experiment*) that a suitably dimensioned particle-current density($\cong$ particle wave $\varphi_0(q)$) with the energy E impinges from the left on the potential step. Qualitatively different results are to be expected for $E > V_0$ and $E < V_0$. We start with the case

1) $E > V_0$,

which realizes a *classically allowed region* for the whole q-axis. Our general considerations in Sect. 4.1 help us to an already rather detailed solution-ansatz. So we know that the required wave function $\varphi(q)$ will exhibit everywhere an oscillatory behavior. The energy spectrum will be continuous and doubly degenerate. Discrete solutions are not be expected:

$$\varphi(q) = \begin{cases} \varphi_0(q) + \varphi_r(q) & \text{for } q \leq 0\,, \\ \varphi_t(q) & \text{for } q \geq 0\,. \end{cases} \tag{4.69}$$

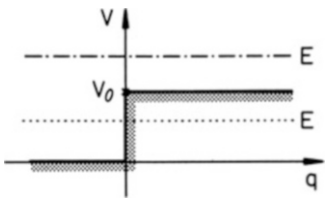

Fig. 4.20 The step as the simplest case of a potential barrier

$\varphi_0(q)$ is the incoming particle wave,

$$\varphi_0(q) = \exp(ik_0 q) \; ; \quad k_0^2 = \frac{2m}{\hbar^2} E \; , \tag{4.70}$$

which we have again, for simplicity, dimensioned such that its amplitude is equal to 1. Without the potential step, this would already be the complete solution of the Schrödinger equation. The step splits the incident wave into a reflected partial wave,

$$\varphi_\mathrm{r}(q) = \alpha \, \exp(-ik_0 q) \; , \tag{4.71}$$

and a partial wave which traverses the full region $q > 0$,

$$\varphi_\mathrm{t}(q) = \gamma \, \exp(ikq) \; ; \quad k^2 = \frac{2m}{\hbar^2} (E - V_0) \; . \tag{4.72}$$

Since the particle does not return from the positive infinite, a e^{-ikq}-term can not appear in φ_t. This would have represented a particle wave which runs from the right towards the step.

The various partial waves correspond, according to (2.27) and (4.55), to the following current densities:

$$j_0 = \frac{\hbar \, k_0}{m} \; ; \quad j_\mathrm{r} = -\frac{\hbar \, k_0}{m} |\alpha|^2 \; ; \quad j_\mathrm{t} = \frac{\hbar k}{m} |\gamma|^2 \; . \tag{4.73}$$

The coefficients of reflection and transmission are of special physical interest here. The following calculation therefore aims at the determination of these terms:

$$R = \left| \frac{j_\mathrm{r}}{j_0} \right| = |\alpha|^2 \; ; \quad T = \left| \frac{j_\mathrm{t}}{j_0} \right| = \frac{k}{k_0} |\gamma|^2 \; . \tag{4.74}$$

The requirement of continuity of $\varphi(q)$ and $\varphi'(q)$ at the point of discontinuity $q = 0$ of the potential serves to fix the still unknown coefficients α and γ:

$$\begin{aligned} \varphi(0) &= 1 + \alpha = \gamma \; , \\ \varphi'(0) &= ik_0(1 - \alpha) = ik\,\gamma \; . \end{aligned}$$

This can of course easily be solved for α and γ:

$$\alpha = \frac{k_0 - k}{k_0 + k} \; ; \quad \gamma = \frac{2k_0}{k_0 + k} \; . \tag{4.75}$$

The wave function is therewith completely determined. The real part

$$\mathrm{Re}\, \varphi(q) = \frac{2k_0}{k + k_0} \begin{cases} \cos k_0 q & \text{for } q \le 0 \; , \\ \cos kq & \text{for } q \ge 0 \end{cases} \tag{4.76}$$

oscillates with a shorter wavelength $\lambda_0 = 2\pi/k_0$ for $q < 0$ than for $q > 0$ where $\lambda = 2\pi/k$. The amplitude of the oscillation, however, does not change at $q = 0$. With respect to the wavelengths, the same statements are valid for the imaginary part of the wave function:

$$\operatorname{Im} \varphi(q) = \frac{2k_0}{k + k_0} \begin{cases} \dfrac{k}{k_0} \sin k_0 q & \text{for } q \leq 0 \,, \\ \sin kq & \text{for } q \geq 0 \,. \end{cases} \tag{4.77}$$

The amplitude, however, is now smaller in the region $q < 0$ by the factor k/k_0 than in the region $q > 0$.

In the region on the left side of the potential step the probability of finding the particle exhibitsan oscillatory space-dependence due to interference of incident and reflected waves, while it is constant for $q > 0$ (Fig. 4.21):

$$|\varphi(q)|^2 = \frac{4k_0^2}{(k + k_0)^2} \begin{cases} 1 - \left(1 - \dfrac{k^2}{k_0^2}\right) \sin^2 k_0 q & \text{for } q \leq 0 \,, \\ 1 & \text{for } q \geq 0 \,. \end{cases} \tag{4.78}$$

For the reflection and transmission coefficient we find with (4.74) and (4.75):

$$R = \left(\frac{k_0 - k}{k_0 + k}\right)^2 \,; \qquad T = \frac{4kk_0}{(k + k_0)^2} \,. \tag{4.79}$$

The physically self-evident relation $T+R = 1$, which, ultimately, expresses particle-number conservation, is obviously fulfilled. R is the probability for the particle to be reflected at the step. As already stated in the last section in connection with the potential well, a finite reflection coefficient in the case of $E > 0$ is *classically completely incomprehensible* and must be ascribed to the wave nature of matter. We know that for the propagation of light an abrupt change of the index of refraction brings about a partial reflection of the wave. An analogous situation is obviously present here.

For high particle energies $E \gg V_0$, the relative jump of the wave vector at $q = 0$ becomes less and less important ($k_0 \to k$), and the reflection, at the cost of the transmission, is therefore weaker. In the opposite case $E \overset{>}{\to} V_0$ ($k \to 0$) the reflection prevails more and more: $R \to 1$, $T \to 0$.

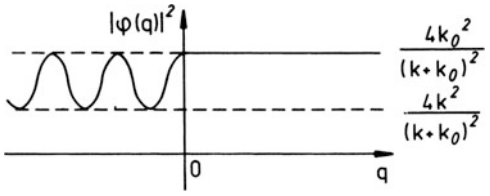

Fig. 4.21 Space-dependence of the square of the absolute value of the wave function for the scattering at the potential step ($E > V_0$)

It is remarkable that,according to (4.79), R as well as T are symmetric with respect to k and k_0. Obviously they are independent of the direction of motion of the particle. We could have let it run with the same energy E also from right to left, i.e., from $q = +\infty$ to $q = -\infty$.

We now come to a somewhat different case

2) $E < V_0$

Let the energy of the incident particle be now smaller than the height of the potential step. Hence, only the region $q < 0$ is still *classically allowed* with an oscillatory behavior of the wave function, while for $q > 0$ an exponential decay of the wave function is to be expected. The energy spectrum will be continuous, but non-degenerate.

We write the solution-ansatz as in (4.69) with formally unchanged $\varphi_0(q)$ and $\varphi_r(q)$, but now have to assume for the transmitted partial wave

$$\varphi_t(q) = \gamma\, e^{-\kappa q}\ ; \quad \kappa^2 = \frac{2m}{\hbar^2}(V_0 - E)\ . \tag{4.80}$$

That corresponds now, however, to a vanishing current density

$$j_t = \frac{\hbar}{2mi}|\gamma|^2 \left(e^{-\kappa q}\,\frac{d}{dq}\,e^{-\kappa q} - e^{-\kappa q}\,\frac{d}{dq}\,e^{-\kappa q} \right) = 0 \tag{4.81}$$

and therewith to a transmission coefficient $T = 0$. On the other hand, the probability to find the particle in the region to the right of the step ($q > 0$) is definitely not equal to zero. This will now be investigated in some more detail. The continuity conditions,

$$\begin{aligned} \varphi(0) &= 1 + \alpha = \gamma\ , \\ \varphi'(0) &= ik_0(1-\alpha) = -\kappa\,\gamma\ , \end{aligned}$$

immediately lead to the coefficients α and γ:

$$\alpha = \frac{k_0 - i\kappa}{k_0 + i\kappa}\ ; \quad \gamma = \frac{2k_0}{k_0 + i\kappa}\ . \tag{4.82}$$

For the complex number $k_0 + i\kappa$, if we utilize its polar representation,

$$\begin{aligned} k_0 + i\kappa &= \sqrt{k_0^2 + \kappa^2}\; e^{i\overline{\varphi}} = \frac{\sqrt{2mV_0}}{\hbar}\; e^{i\overline{\varphi}}\ , \\ \tan\overline{\varphi} &= \frac{\kappa}{k_0} \qquad \left(-\frac{\pi}{2} \le \overline{\varphi} \le +\frac{\pi}{2}\right)\ , \end{aligned}$$

then we recognize that $\alpha = \exp(-2i\overline{\varphi})$ is a pure phase factor of the magnitude 1. The wave is thus completely reflected at the step,

$$R = \left|\frac{j_r}{j_0}\right| = |\alpha|^2 = 1\,; \qquad T = \left|\frac{j_t}{j_0}\right| = 0\,, \tag{4.83}$$

in agreement with the *classical expectation* for a particle of mass m, which impinges on the step at $q = 0$ with the momentum $p = \hbar k_0/(2m)$, and travels back, after elastic reflection, with the same momentum in the opposite direction.

In contrast, the result for the position probability of the particle is *classically completely incomprehensible*, namely that this probability, because of $\gamma \neq 0$, is different from zero (Fig. 4.22) even in the *classically forbidden region* $q > 0$:

$$|\varphi(q)|^2 = \begin{cases} 4\cos^2(k_0 q + \overline{\varphi}) & \text{for } q \leq 0\,, \\ \dfrac{4k_0^2}{\kappa^2 + k_0^2}\exp(-2\kappa q) & \text{for } q \geq 0\,. \end{cases} \tag{4.84}$$

The *quantum-mechanical particle* is therefore able to penetrate the *classically forbidden region* up to a certain distance, although, according to (4.81), actually no particle flow takes place. In the next section, this phenomenon explains the important tunnel effect. The intersection point with the ordinate, i.e., the position-probability density at the potential jump, shifts with increasing height of the step V_0 towards zero:

$$|\varphi(0)|^2 = \frac{4k_0^2}{\kappa^2 + k_0^2} = 4\frac{E}{V_0} \tag{4.85}$$

For the special case of an infinitely high step ($V_0 \to \infty$) we therefore get $\varphi(q) \equiv 0$ for $q \geq 0$. The interference (Sect. 1.4.1) of incident and reflected waves takes care for an oscillatory behavior of the position probability (Fig. 4.22) in the *classically allowed region* $q < 0$:

$$\begin{aligned} |\varphi_0(q) + \varphi_r(q)|^2 &= \left|e^{ik_0 q} + \alpha e^{-ik_0 q}\right|^2 = \left|e^{ik_0 q} + e^{-2i\overline{\varphi}} e^{-ik_0 q}\right|^2 \\ &= \left|e^{-i\overline{\varphi}}\left(e^{i(k_0 q + \overline{\varphi})} + e^{-i(k_0 q + \overline{\varphi})}\right)\right|^2 \\ &= 4\cos^2(k_0 q + \overline{\varphi})\,. \end{aligned}$$

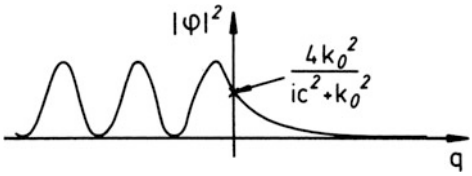

Fig. 4.22 Position probability for the particle which is reflected at the potential step ($E < V_0$)

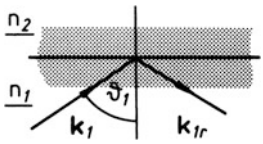

Fig. 4.23 Reflection of electromagnetic radiation at the interface of two insulators with different indexes of refraction

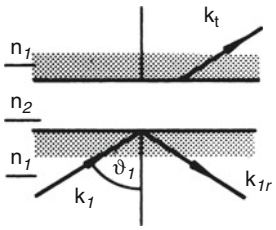

Fig. 4.24 Reflection and transmission of electromagnetic radiation by a layer system of insulators with different indexes of refraction

We want to close this section with a retrospection of an analogous situation in Classical Electrodynamics, which is observed with the reflection and refraction of electromagnetic waves at the interface of two insulators with different indexes of refraction. If a wave falls in an optically denser medium 1 (index of refraction n_1) on the interface with an optically rarer medium 2 ($n_2 < n_1$) (Fig. 4.23), then one observes total internal reflection (Sect. 4.3.10, point G, Vol. 3), as soon as the angle of incidence ϑ_1 exceeds a certain limiting angle. There does not take place any energy flow into the medium 2. Nevertheless, the amplitude of the electric field strength does not at all go abruptly to zero at the interface, but decreases only exponentially with the distance from the interface. The reason for this is a complex wave vector, which causes the damping of the amplitude and prevents the wave propagation within the medium 2. This corresponds exactly to the behavior of the quantum-mechanical particle wave at the potential step.

These analogy observations can be expanded still further. Strictly speaking, the wave will be totally reflected only when medium 2 is infinitely extended. If it is only a relatively thin layer, to which is again medium 1 attached from above (Fig. 4.24), then the amplitude of the field does not possibly completely decay at the next interface. In such a case, the wave is no longer totally reflected at the first interface. In the upper medium 1 (Fig. 4.24), a transmitted propagating wave is observed, whose amplitude corresponds to the *residue amplitude*, which survives after the exponential decay in medium 2. The in principle *optically opaque* interlayer has partially been *tunneled through* by the wave. In the next section, we will get to know the quantum-mechanical analog suitable to this.

4.3.2 Potential Wall

A logical continuation of the considerations to the potential step discussed in the last subsection is offered by the potential wall of finite height V_0 and finite width

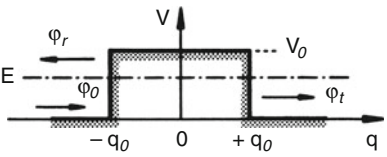

Fig. 4.25 Space-dependence of a one-dimensional potential wall

$2q_0$ (Fig. 4.25). In the corresponding *gedanken-experiment* we send a particle of the mass m with the velocity $\hbar k_0/m$ and energy $E < V_0$ from the left, i.e., from $q = -\infty$, towards the potential

$$V(q) = \begin{cases} V_0 > 0 & \text{for } |q| \le q_0 \,, \\ 0 & \text{otherwise} \end{cases} \tag{4.86}$$

This particle is again described by a plane wave:

$$\varphi_0(q) = \exp(ik_0 q) \,; \quad k_0^2 = \frac{2m}{\hbar^2} E \,.$$

From a *classical viewpoint* it can not permeate the wall but instead has to be reflected:

$$\varphi_\mathrm{r}(q) = \alpha_- \, \exp(-ik_0 q) \,.$$

But as we already know, a *quantum-mechanical particle* can enter, to a certain degree, even the *classically forbidden region*. If on the right-hand side of the wall the exponential decay of the position-probability density $|\varphi(q)|^2$ is not fully completed, then the particle should indeed be capable to traverse the wall, in order to move then without further perturbations in the direction to $q = +\infty$:

$$\varphi_\mathrm{t}(q) = \gamma_+ \, \exp(ik_0 q) \,.$$

This we now want to analyze in more detail, where the explicit calculation, however, goes completely analogously to that in Sect. 4.2.2 for the (unbounded) scattering states of the potential well, and therefore need not be repeated here in all details. So we can choose, formally, the same ansatz for the wave function as in (4.51). We have only to take into consideration that in the *classically forbidden region* $-q_0 < q < +q_0$ the wave number k is purely imaginary:

$$k^2 = \frac{2m}{\hbar^2}(E - V_0) = -\kappa^2 \implies k = i\kappa \,. \tag{4.87}$$

This also means:

$$y = \frac{k}{k_0} = ix \,; \quad x = \frac{\kappa}{k_0} = \sqrt{\frac{V_0 - E}{E}} \,. \tag{4.88}$$

With these substitutions and

$$\sin ix = i \sinh x$$

all the results from Sect. 4.2.2 can be adopted. So it follows, according to (4.63) and (4.64), for the coefficients of transmission and reflection, respectively:

$$T(E) = \frac{4x^2}{4x^2 + (1+x^2)^2 \sinh^2 2\kappa q_0} , \tag{4.89}$$

$$R(E) = \frac{(1+x^2)^2 \sinh^2 2\kappa q_0}{4x^2 + (1+x^2)^2 \sinh^2 2\kappa q_0} . \tag{4.90}$$

Since $T(E)$ is in any case unequal zero, always there exists a transmission which is *classically not allowed*. One says that the particle *'tunnels through'* the potential wall. Many basically as well as technically important applications are based on this so-called *tunnel effect*, which again represents a typical quantum-mechanical wave phenomenon. (See also the analogies to the refraction and the reflection of electromagnetic waves as qualitatively worked out at the end of the preceding subsection!). Special examples for the consequences of the tunnel effect are the α-radioactivity (Sect. 4.3.4), the field-induced emission of electrons out of metals (Exercise 4.3.5) and the existence of energy bands in solids (Sect. 4.3.5, Exercise 4.3.6).

The *tunnel-probability* $T(E)$ takes an especial clear form when

$$\kappa q_0 = \frac{1}{\hbar} \sqrt{2m(V_0 - E)} q_0 \gg 1 \tag{4.91}$$

can be assumed. Then the hyperbolic sine-function dominates in (4.89) in the form of

$$\sinh^2 2\kappa q_0 \approx \frac{1}{4} e^{4\kappa q_0} ,$$

and $T(E)$ is of the following relatively simple form:

$$\begin{aligned} T(E) &\approx \frac{16(\kappa k_0)^2}{(k_0^2 + \kappa^2)^2} e^{-4\kappa q_0} = \\ &= \frac{16E(V_0 - E)}{V_0^2} \exp\left(-\frac{4}{\hbar} \sqrt{2m(V_0 - E)}\, q_0 \right) . \end{aligned} \tag{4.92}$$

The tunnel probability therefore decreases exponentially with the width $2q_0$ of the potential wall and with the root of the *effective* potential barrier $V_0 - E$.

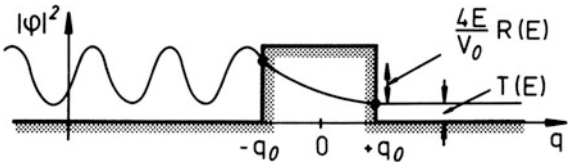

Fig. 4.26 Position-probability density for the scattering at the potential wall

In the other limit $\kappa q_0 \ll 1$, which is realized, for instance, as $E \to V_0$, one can estimate with $\sinh x \approx x$:

$$T(E) \approx \frac{1}{1 + k_0^2 q_0^2} \,. \tag{4.93}$$

In this section we have restrict ourselves, when evaluating the potential wall, to that what is really new, as for instance the tunnel effect. The complete and explicit calculation of the wave function $\varphi(q)$ (Exercise 4.3.2) leads to a density $|\varphi(q)|^2$ of the position probability as it is qualitatively plotted in Fig. 4.26. For $q < -q_0$ incident and reflected waves take care by interference for an oscillatory space-dependence of the probability density. In the region of the potential wall, this decreases exponentially, and then remains constant for $q > q_0$. The latter results from the fact that to the right of $q = q_0$, there is only a partial wave $\varphi_t(q)$ which proceeds to $+\infty$. From positive infinity no wave is reflected, with which φ_t could interfere.

4.3.3 *Tunnel Effect*

For the description of realistic tunnel processes the rectangular shape of the potential wall is of course over-idealized. In the practically interesting cases, the potential V is a continuous function of q. By a *trick* the results of the last section can be transferred, at least approximately, to such continuous potential curves.

At first we presume the validity of the formula (4.92) for the transmission coefficient:

$$T(E) \approx \exp\left[-\frac{4}{\hbar}\sqrt{2m(V_0 - E)}q_0 + \ln\left(\frac{16E(V_0 - E)}{V_0^2}\right)\right] \,.$$

For all situations, which come into question, the first summand in the exponent can be seen to be the dominant one, so that one can further simplify:

$$T(E) \approx \exp\left[-\frac{4}{\hbar}\sqrt{2m(V_0 - E)}q_0\right] \,. \tag{4.94}$$

This is an indeed strongly simplified formula, which, however, turns out to be very useful for estimations, and to be even reasonably accurate. As indicated in Fig. 4.27, we now decompose the area below the continuous potential curve into N number

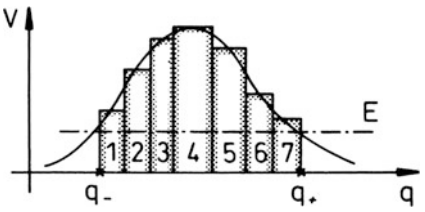

Fig. 4.27 Approximation of a general potential wall by small potential boxes

of rectangles, where we are interested only in the region between the *classical turning points* $q_\pm$ ($V(q_\pm) \stackrel{!}{=} E$). If the curve is smooth, then it can be rather well approximated by such steps. We now replace the actual tunnel process through the continuous potential wall, the mathematical treatment of which is rather difficult, by an N-fold tunneling through rectangular walls. If the transmission is not too strong, then we can consider the tunneling processes through the various partial walls as statistically independent events. For the current, which tunnels through all the N walls, we then have:

$$j_\mathrm{t}^{(N)} = T_N j_\mathrm{t}^{(N-1)} = T_N T_{N-1} j_\mathrm{t}^{(N-2)} = \ldots = T_N T_{N-1} \cdots T_2 T_1 j_0 \; .$$

The transmission coefficient for the whole set up $\left(T = j_\mathrm{t}^{(N)}/j_0\right)$ should therefore be multiplicatively composed of all the individual contributions:

$$T = T_1 T_2 \cdots T_N \; .$$

Of course, only the rectangles between the classical turning points q_- and q_+ can come into consideration, since the particle penetrates the potential wall at q_- and leaves it again at q_+. Let the i-th rectangular wall be centered at q_i with a width of Δq_i. Then it holds with (4.94):

$$T(E) \approx \prod_i \exp\left[-\frac{2}{\hbar}\sqrt{2m\big(V(q_i) - E\big)}\,\Delta q_i\right] =$$

$$= \exp\left[-\frac{2}{\hbar}\sum_i \sqrt{2m\big(V(q_i) - E\big)}\,\Delta q_i\right] \; .$$

When we now perform the transition to infinitely small intervals ($\Delta q \to dq$), then we can replace the sum by an integral:

$$T(E) \approx \exp\left[-\frac{2}{\hbar}\int_{q_-}^{q_+} \sqrt{2m\big(V(q) - E\big)}\,dq\right] \; . \tag{4.95}$$

It is clear that what is done here is an altogether very rough approximation, since, for instance, the presumptions for the estimation (4.94) become surely questionable

in the limit $\Delta q \to dq$. That is true, in particular, for the rectangles very close to the turning points. Nevertheless, (4.95) yields a qualitatively correct picture of the tunnel effect, as it is demonstrated in the next section for the example of α-radioactivity. The expression (4.95) can be justified, incidentally, mathematically a bit more convincingly by the use of the so-called WKB-method (**W**entzel-**K**ramers-**B**rillouin), a method, which will be discussed in more detail in a forthcoming section (*Methods of Approximation*, Sect. 7.4, Vol. 7).

Equation (4.95) shows that the tunneling probability increases with increasing particle energy E, because of two reasons; first, because the effective tunnel barrier $(V - E)$ becomes smaller, and second, because the region of integration (distance between q_- and q_+) is diminished. The transmission coefficient, however, decreases with the increasing particle mass m.

Furthermore, one can convince oneself by insertion of realistic numerical values that the tunnel effect will be observable only in regions of atomic dimensions.

4.3.4 Example: α-Radioactivity

Many radioactive elements disintegrate by emission of α-particles and change thereby their nuclear charge from $Z'e$ to Ze. Since the α-particle itself is twofold positively charged, the atomic number changes from the mother to the daughter nucleus from Z' to $Z = Z' - 2$. The decay happens *spontaneously*, i.e., it can not be influenced by external parameters like, e.g., pressure, temperature, electromagnetic fields, ... A quantitative measure of the spontaneous decay is the half-life. This is the time, after which from the original number N_0 of identical particles, the half decays radioactively. Apart from the rather involved explanation of the basic effect, a special difficulty lies in understanding the huge range of orders of magnitude of the half-lives of different radioactive elements:

$$
\begin{aligned}
{}^{212}_{84}\mathrm{Po}: \quad & \tau_{1/2} = 3 \cdot 10^{-7} s \,, \\
{}^{228}_{90}\mathrm{Th}: \quad & \tau_{1/2} = 1.91 a \,, \\
{}^{238}_{92}\mathrm{U}: \quad & \tau_{1/2} = 4.5 \cdot 10^{9} a \,.
\end{aligned}
$$

It is further typical for the α-decay that the emitted α-particle exhibits an energy, which is characteristic of the emitter, and the experimental findings show to a strong correlation between this energy and the half-life.

In order to understand these observations, at least qualitatively, we use a simple theoretical model: Because of its great stability, we assume that the twofold positively charged α-particle does exist even within the nucleus as a self-reliant entity, which is of course not at all strictly proven. The α-particle is exposed to two different types of forces (Fig. 4.28). There is at first the *normal* Coulomb repulsion

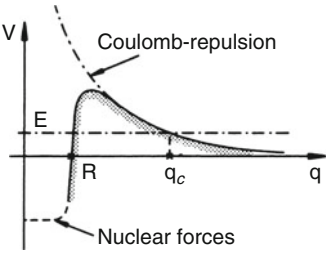

Fig. 4.28 Qualitative behavior of the potential of the α-particle in the immediate proximity of the nucleus

between the α-particle and the also positively charged nucleus (charge: Ze):

$$V(q) = \frac{2Ze^2}{4\pi\varepsilon_0 q} \,. \tag{4.96}$$

In addition to this, there are the very short range and very strongly attractive nuclear forces, about the true nature of which there do not exist clear concepts even today. In any case, however, they must take care for a potential minimum, since otherwise the long life time of the α-particle in the proximity of the nucleus, or of the nucleons by which it is built up, would be unexplainable.

To leave the region of the nucleus, the α-particle has to tunnel through the potential hill, which divides the attractive from the repulsive region (see Fig. 4.28). *Classically*, we have to provide the α-particle with sufficient energy to overcome the potential hill. *Quantum-mechanically* the tunneling, discussed in the last two sections, comes into consideration, however only then, when the α-particle occupies a state with an energy $E > 0$ inside the nucleus. For $E < 0$, the particle is in a bound state; an escaping is then impossible. In radioactive elements, it must therefore be $E > 0$.

Let us estimate, at first, the tunneling probability, using for that purpose the relation (4.95). The classical turning points are R and q_c, where we assume that within the potential hill, $R < q < q_c$, the potential is sufficiently well approximated by (4.96). For q_c we get then:

$$q_c = \frac{\gamma}{E} \,; \quad \gamma = \frac{2Ze^2}{4\pi\varepsilon_0} \,.$$

The *radius of the nucleus* R is known only rather approximately. The following formula, however, has proven to be rather helpful (A_r: relative atomic mass):

$$R \approx 1.5 \cdot 10^{-13} A_r^{1/3} \,\text{cm} \approx 2 \cdot 10^{-13} Z^{1/3} \,. \tag{4.97}$$

To evaluate (4.95) we have to determine the following integral (m: mass of the α-particle):

$$I = \frac{2}{\hbar} \int_R^{q_c} \sqrt{2m\left(\frac{\gamma}{q} - E\right)}\, dq = \frac{2}{\hbar}\sqrt{2mE} \int_R^{q_c} \sqrt{\frac{q_c}{q} - 1}\, dq \,.$$

The integral can be solved elementarily. For this purpose we substitute:

$$\frac{q}{q_c} = \sin^2 u \implies dq = 2q_c \sin u \cos u\, du \,.$$

With $u_c = \arcsin\sqrt{R/q_c}$ it then remains to be calculated:

$$I = \frac{4q_c}{\hbar}\sqrt{2mE} \int_{u_c}^{\pi/2} \cos^2 u\, du = \frac{4q_c}{\hbar}\sqrt{2mE}\,\frac{1}{2}(u + \sin u \cos u)\Big|_{u_c}^{\pi/2} =$$

$$= \frac{2q_c}{\hbar}\sqrt{2mE}\left(\frac{\pi}{2} - \arcsin\sqrt{\frac{R}{q_c}} - \sqrt{\frac{R}{q_c}\left(1 - \frac{R}{q_c}\right)}\right) \,.$$

We can now assume $R/q_c \ll 1$ and therefore further estimate with $\arcsin x \approx x$:

$$I \approx \frac{2q_c}{\hbar}\sqrt{2mE}\left(\frac{\pi}{2} - 2\sqrt{\frac{R}{q_c}}\right) \,.$$

That eventually yields the α-tunneling probability:

$$T(E) \approx \exp\left[-\frac{\beta_1}{\sqrt{E}} + \beta_2\right] \,. \tag{4.98}$$

The constants β_1 and β_2 are determined, especially, by the atomic number Z of the daughter-nucleus:

$$\beta_1 = \frac{\sqrt{2m}\,e^2}{2\hbar\varepsilon_0} Z = \overline{\beta}_1 Z \,, \tag{4.99}$$

$$\beta_2 = \frac{4e}{\hbar}\sqrt{\frac{mZR}{\pi\,\varepsilon_0}} \approx \overline{\beta}_2 Z^{2/3} \,. \tag{4.100}$$

We now have to think about how from the expression (4.98) for the tunneling probability we can draw conclusions on the lifetime of the radioactive nucleus. For that purpose, we imagine—surely a bit naively—that the α-particle jumps back and forth between the walls of the potential with the velocity v, and at each collision

against them permeates it with the probability $T(E)$. The time between two wall collisions can be estimated to

$$t_0 = \frac{2R}{v} \quad \left(v \approx \sqrt{\frac{2E}{m}} \right) ,$$

where, in nuclear physics, the velocity v is only a very vague term. The α-particle needs, on average, $1/T$ collisions, in order to actually tunnel through the potential hill. It makes therefore sense to define:

$$\textit{lifetime} \quad \tau \approx \frac{t_0}{T} . \tag{4.101}$$

If one takes the logarithm of τ, then $(\ln t_0)$ whose E-dependence being anyway not really clear for substances which come into question, carries hardly any weight compared to the first term in (4.98):

$$\ln \tau = \overline{\beta}_1 \frac{Z}{\sqrt{E}} - \overline{\beta}_2 Z^{2/3} + \ln t_0 . \tag{4.102}$$

This characteristic connection between the energy of the α-particle, which, as mentioned initially, is a characteristic quantity for a radioactive element, and the lifetime of the nucleus is brilliantly confirmed by the experiment. If one plots the logarithms (mostly one takes to the base 10: $\log \tau = (\log e) \ln \tau \approx 0.434 \cdot \ln \tau$) of the lifetimes of the nuclei, which differ by many decimal powers, against $(\beta_1/\sqrt{E} - \beta_2)$, then one obtains a uniquely linear behavior. For further details the reader is referred to the special literature on nuclear physics.

The lifetime of the radioactive nucleus is closely related to its own law of decay, by which one ultimately determines the lifetime. dt/τ is the probability that in the time interval dt a nucleus decays α-radioactively. The number dN of the N present nuclei, which decay in the time dt, is then given by

$$dN = -N \frac{1}{\tau} dt .$$

That can easily be integrated if one chooses as initial condition the number N_0 of the nuclei present at the time $t = 0$:

$$N = N_0 \, e^{-t/\tau} . \tag{4.103}$$

One denotes $\lambda = 1/\tau$ also as *decay constant*. Via (4.103), we can eventually still bring into contact the lifetime τ with the previously mentioned *half-life* $\tau_{1/2}$:

$$\frac{N}{N_0} \stackrel{!}{=} \frac{1}{2} = e^{-\tau_{1/2}/\tau} \curvearrowright \tau_{1/2} = \ln 2 \, \tau \approx 0.693 \cdot \tau .$$

4.3.5 Kronig-Penney Model

An extraordinary characteristic of solids with their periodic lattice structure must be seen in the fact that electrons in them can occupy only discrete energy levels, which are very densely gathered into *energy bands*. Between the various energy bands there appear *forbidden zones (energy gaps)*, which do not contain any stationary electronic states of the solid. This arrangement of *allowed* and *forbidden* energy regions explains why solids are classified into insulators, semiconductors, and metals. The *Pauli principle*, which is still to be discussed in a forthcoming chapter, requires that each energy level can be occupied by at most two electrons of opposite spin (Chap. 5, Vol. 7). In the ground state, all energy levels are filled with electrons up to a limiting energy, the so-called *Fermi energy*. It is typical for an insulator that each energy band is either completely occupied or totally empty. The electrons therefore can not be *excited* by normal electric fields into other unoccupied levels, and for this reason do not contribute to a current flow. In metals, in contrast, the Fermi energy lies within a band, which is thus not completely filled. The electrons can be accelerated (*excited*) by electric fields. Semiconductors take an intermediate position. The energy-band structure is in principle the same as for insulators, but with an energetic distance between the highest occupied and the lowest empty band being so small that electrons can be *excited*, e.g. thermally, into free states and then can be accelerated by an electric field.

The physical reason for the appearance of energy bands is, on the one hand, the strictly periodic arrangement of the atoms of the crystal, and on the other side, the quantum-mechanical tunnel process, which enables electrons of the solid to *tunnel* with a certain probability from lattice site to lattice site. We will illustrate this issue by a simple, but rather revealing, one-dimensional model. The Kronig-Penney model presumes in one dimension a periodic arrangement of δ-potentials:

$$V(q) = D \sum_{n=-\infty}^{+\infty} \delta(q - na) \; . \tag{4.104}$$

a is the lattice constant and therewith, along with the coupling parameter D, a firmly preset constant ($D > 0$). One can consider (4.104) as to be result of a limiting process $q_0 \to 0$ from a periodic arrangement of potential walls of the height V_0 and width $2q_0$, where the product $D = 2q_0V_0$ remains constant. The potential walls express the fact that *classically* the electrons can reach the neighboring atom only after overcoming a potential hill (see Exercise 4.3.6). In the following we intend to derive with the potential (4.104) an eigen-value condition for the possible electron energies. For that purpose we of course use again the time-independent Schrödinger equation in the form of (4.5), whose general structure of the solution is already, from the preliminary considerations in Sect. 4.1, familiar to us. However, we have to bear in mind that δ-potentials, like the one in (4.104), give rise to certain peculiarities, to which we still have to be responsive separately (see Exercises 4.2.5, 4.2.8, 4.3.5).

In the regions

$$B_n = \{q\,;\; na < q < (n+1)a\}\,; \quad n \in \mathbb{Z}$$

we have $V(q) = 0$. For $E > 0$ they thus represent *classically allowed regions*. (The case $E < 0$ is uninteresting for the model (4.104), since it leads to an *identically vanishing* wave function.) In B_n the solution functions exhibit an oscillatory behavior. A proper ansatz is therefore:

$$\varphi(q) = a_n e^{ik(q-na)} + b_n\, e^{-ik(q-na)}\,, \qquad k = \sqrt{\frac{2m}{\hbar^2}\,E}\,; \quad q \in B_n\,. \tag{4.105}$$

The fact that we drew out of the coefficients a_n, b_n explicitly the terms exp $(\pm ikna)$, is due to pure convenience, and is not at all mandatory.

How do the fitting conditions at the critical points $q = na$ now look like? At first, the resulting wave function as probability amplitude has to be uniquely defined at all space points, and has to be finite. Hence, it has to be continuous:

$$\begin{aligned} \varphi(na+\eta) \;&=\; \varphi(na-\eta) = \varphi(na) \\ &\text{for}\;\; \eta \to 0^+ \;\;\text{and}\;\; \forall n \in \mathbb{Z}\,. \end{aligned} \tag{4.106}$$

In the regions B_n, besides φ, of course also φ' and φ'' are continuous. Only at the discrete points $q = na$, discontinuities may appear. But in any case, the Schrödinger Eq. (4.5) can be integrated over a small interval around $q = na$:

$$\eta \to 0^+ : \quad \int\limits_{na-\eta}^{na+\eta} \varphi''(q)dq - \frac{2m}{\hbar^2}\,D \int\limits_{na-\eta}^{na+\eta} \delta(q-na)\,\varphi(q)\,dq = -\frac{2m}{\hbar^2}\,E \int\limits_{na-\eta}^{na+\eta} \varphi(q)\,dq\,.$$

Because of the continuity of the wave function, the term on the right-hand side of the equation vanishes for $\eta \to 0^+$. Then what is left is:

$$\varphi'(na+\eta) - \varphi'(na-\eta) = \frac{2m}{\hbar^2}\,D\,\varphi(na)\,. \tag{4.107}$$

The first derivative thus exhibits a finite jump at the critical points.

Equations (4.106) and (4.107) are the required fitting conditions, by which we can fix the coefficients a_n and b_n in our ansatz (4.105). But before we do that, we still want to exploit, at first, the periodicity of the problem, which manifests itself in the potential by

$$V(q) = V(q+a)\,. \tag{4.108}$$

Since the kinetic energy $-(\hbar^2/2m)\,(d^2/dq^2)$, too, does not change with the shift $q \to q + a$, the total Hamilton operator is invariant with respect to translations by the period a. That holds then also for all the other observable, measurable quantities. The wave function itself is not measurable, so that $\varphi(q)$ and $\varphi(q + a)$ may be definitely different. In contrast, the square of the absolute value of the wave function is, as the density of the position probability, observable. We have to therefore require:

$$|\varphi(q + a)|^2 \stackrel{!}{=} |\varphi(q)|^2 \,.$$

That means, however, that $\varphi(q)$ and $\varphi(q + a)$ can differ only by a pure phase factor:

$$\varphi(q + a) = e^{iKa}\,\varphi(q)\,; \quad -\pi < Ka \leq +\pi \,. \tag{4.109}$$

The inequality on the right does not mean any restriction, since by that all points of the unit circle in the complex number plane are involved. The solution-function is therewith marked by an additional wave number K:

$$\varphi_K(q + na) = e^{iKna}\,\varphi_K(q) \,. \tag{4.110}$$

One can therefore cast the wave function, we are looking for, into the form

$$\varphi_K(q) = u_K(q)\,e^{iKq}\,; \quad u_K(q + a) = u_K(q) \,, \tag{4.111}$$

with a *lattice-periodic* amplitude function $u_K(q)$. That is the message of the **Bloch theorem**, which is fundamental for solid state physics. The $u_K(q)$ incorporate the whole influence of the lattice potential. In the special case of a vanishing potential (*empty lattice*), $u_K(q) \equiv$ const, and the solution functions (4.111) become plane waves.

After these general considerations it is already clear that, because of

$$|\varphi_K(q + na)|^2 = |\varphi_K(q)|^2$$

for arbitrarily large n, the wave function can not be normalizable in the original sense. On the other hand, each solid is of course finite. In the case of our one-dimensional model, this can be accounted for, for instance, by periodic boundary conditions (Sect. 2.2.5) on a chain of $N < \infty$ *'building blocks'*:

$$\varphi_K(q + Na) \stackrel{!}{=} \varphi_K(q) \,.$$

This means, because of $\exp(iKNa) \stackrel{!}{=} 1$, a discretization of the K-values comes into consideration:

$$K = \frac{2\pi}{Na}\,m\,; \quad m = 0, \pm 1, \pm 2, \ldots, \pm\left(\frac{N}{2} - 1\right), +\frac{N}{2} \,. \tag{4.112}$$

The number of different K-values thus corresponds to the (even) number N of periodicity intervals of the linear lattice.

What does the Bloch theorem (4.110) now mean for our general ansatz of solution (4.105)? By insertion,

$$\varphi_K(q+na) = e^{iKna}\varphi(q) = e^{iKna}\left(a_0\, e^{ikq} + b_0\, e^{-ikq}\right) \stackrel{!}{=} a_n\, e^{ikq} + b_n\, e^{-ikq}\ ,$$

one finds that only two coefficients are to be determined, e.g. a_0 and b_0. All the others are then already known:

$$a_n = a_0\, e^{iKna}\ ; \quad b_n = b_0\, e^{iKna}\ . \tag{4.113}$$

For fixing a_0 and b_0 we use the continuity conditions (4.106) and (4.107) for the point $q = a$:

$$(4.106) \implies \varphi_K(q=a) = a_0\, e^{ika} + b_0\, e^{-ika} \stackrel{!}{=} a_1 + b_1 = e^{iKa}\,(a_0 + b_0)\ ,$$

$$(4.107) \implies ik\,(a_1 - b_1) - ik\left(a_0\, e^{ika} - b_0\, e^{-ika}\right) = \frac{2m}{\hbar^2}\,D\, e^{iKa}\,(a_0 + b_0)\ .$$

That yields a homogeneous system of equations:

$$\begin{pmatrix} \left(e^{ika} - e^{iKa}\right) & \left(e^{-ika} - e^{iKa}\right) \\ \left(ik\left(e^{iKa} - e^{ika}\right) - \frac{2m}{\hbar^2}\,D\, e^{iKa}\right) & \left(ik\left(-e^{iKa} + e^{-ika}\right) - \frac{2m}{\hbar^2}\,D\, e^{iKa}\right) \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}\ .$$

The determinant of the matrix of coefficients,

$$\Delta = 2i\, e^{iKa}\left(2k\cos Ka - 2k\cos ka - \frac{2m}{\hbar^2}\,D\,\sin ka\right)\ ,$$

must vanish, for the system of equations to have a unique solution. That leads, eventually, to the decisive condition for possible electron energies:

$$\cos Ka = \cos ka + \frac{mD}{\hbar^2 k}\sin ka\ . \tag{4.114}$$

From this relation, several important conclusions can be drawn:

1. Only those energies

$$E = \frac{\hbar^2 k^2}{2m}$$

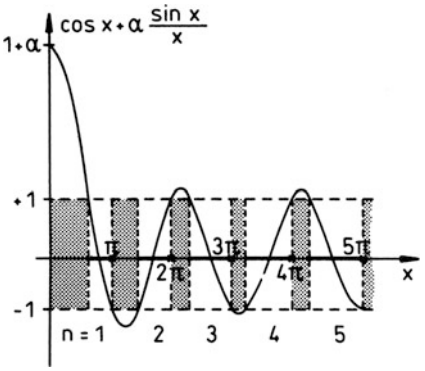

Fig. 4.29 Graphic solution of the Eq. (4.114). In the hatched regions, the equation has no solution

are obviously possible, for which the magnitude of the right-hand side of (4.114) does not exceed the value 1. That divides the energy axis into *allowed* and *forbidden* regions, i.e., into *energy bands* and *energy gaps*. The latter are recognizable in Fig. 4.29 as hatched regions.

$$x = ka = \sqrt{\frac{2m}{\hbar^2}E}\,a\ ,$$

$$\alpha = \frac{mDa}{\hbar^2}$$

2. The begin of a forbidden zone is always given by

$$ka = n\pi\ ; \qquad n = 1, 2, 3, \ldots\ ,$$

because then $\sin ka = 0$ and $\cos ka = (-1)^n$. The upper band edges therefore lie, independently of the strength D of the potential, always at the energies

$$E_n = \frac{\hbar^2\pi^2}{2ma^2}\,n^2\ . \tag{4.115}$$

This allows to number the bands sequentially by a band index n with respect to increasing energy.

3. One obtains the discrete energy values, belonging to a given wave number $K\left(-\frac{\pi}{a} < K \leq +\frac{\pi}{a}\right)$,

$$E_n(K)\ ,$$

by an explicit solving of the Eq. (4.114) for the corresponding energy band n. The K-dependence of the band energies is called the *band dispersion*, and the whole set of $E_n(K)$-curves is called the *band structure* (Fig. 4.30). According to (4.112), the wave number K can assume N different values. Each energy band contains therefore N discrete, but densely placed energy levels.

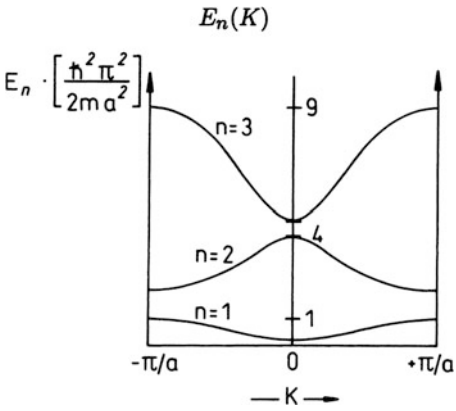

Fig. 4.30 Band structure according to the Kronig-Penney model

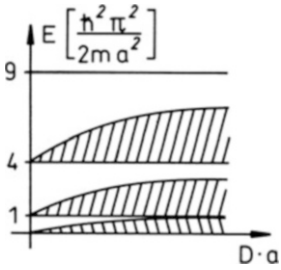

Fig. 4.31 *Upper and lower* band edges of the Kronig-Penney model as functions of the product of the strength of the potential D and the lattice constant a. The hatched regions correspond to the energy gaps

4. With increasing Da the energy gaps become broader, where, however, the respective opening of a gap is, according to (4.115), independent of Da (Fig. 4.31).

   For $Da \to \infty$ the bands shrink to levels (Fig. 4.31). All the N dispersion energies $E_n(K)$ then become equal to the energy E_n from (4.115).

   For $D \to 0$ (a fix), the interaction of the electrons with the lattice is *switched off*. All energies E are then allowed.
5. For fixed D and a, the energy bands become broader and broader with increasing band index n.

4.3.6 Exercises

Exercise 4.3.1 A particle wave, coming from the left ($E > V_0$), impinges on a double-step potential (Fig. 4.32):

$$V(q) = \begin{cases} 0 & \text{for } q \le 0\,, \\ \dfrac{V_0}{2} & \text{for } 0 < q < q_0\,, \\ V_0 & \text{for } q_0 \le q\,. \end{cases}$$

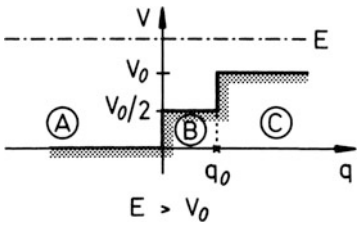

Fig. 4.32 Sketch of a double-step potentional

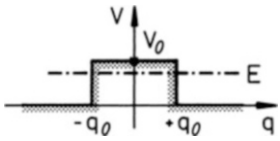

Fig. 4.33 Potential wall of width $2q_0$ and the height V_0. The particle energy E is smaller than the height of the wall

Determine the reflection coefficient for the partial wave reflected at $q = 0$! Is it larger or smaller than that for the simple potential step (Sect. 4.3.1)?

Exercise 4.3.2 For the potential step, which we discussed in Sect. 4.3.2,

$$V(q) = V_0\,\Theta(q_0 - |q|)$$

calculate the density of the position probability $|\varphi(q)|^2$ for the whole q-axis for a particle energy $0 < E < V_0$ (Fig. 4.33). Verify the following expressions:

1. $q \geq q_0$

$$|\varphi(q)|^2 = \text{const} = T(E)\ ,$$

2. $q_0 \geq q \geq -q_0$

$$|\varphi(q)|^2 = T(E) + \frac{4ER(E)}{V_0 \sinh^2 2\kappa q_0} \sinh^2 \kappa(q_0 - q)\ ,$$

3. $-q_0 \geq q$

$$|\varphi(q)|^2 = 1 + R(E) + \frac{2E}{V_0} R(E) \left[\left(1 - \frac{\kappa^2}{k_0^2}\right) \cos 2k_0(q_0 + q) - \right.$$
$$\left. -2\frac{\kappa}{k_0} \coth 2\kappa q_0 \, \sin 2k_0(q_0 + q) \right]$$

Thereby it is:

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}\ ; \quad k_0 = \sqrt{\frac{2m}{\hbar^2}E}\ .$$

Exercise 4.3.3 A particle wave, coming from $q = -\infty$, travels towards the asymmetric potential wall (Fig. 4.34):

$$V(q) = \begin{cases} 0 & \text{for } -\infty < q \le -q_0 \\ V_0 & \text{for } |q| < q_0 \\ \frac{1}{2}V_0 & \text{for } +q_0 \le q \end{cases}$$

What are the reflection and transmission coefficients ($R(E)$ and $T(E)$), if the particle energy is given by

$$\frac{1}{2}V_0 < E < V_0 \,?$$

Compare $R(E)$ and $T(E)$ with the results (4.89) and (4.90) for the symmetric potential wall!

Exercise 4.3.4 A (free) particle wave

$$\varphi_0(q) = \exp(ik_0 q)$$

comes from $q = -\infty$ and travels towards the one-dimensional potential:

$$V(q) = \begin{cases} \dfrac{\hbar^2 v_0}{2m}\delta(q + q_0) & \text{for } q \le 0;\ q_0 > 0\,, \\ +\infty & \text{for } q > 0\,. \end{cases}$$

1. Formulate suitable solution ansatzes of the wave function $\varphi(q)$ for the regions A, B and C (Fig. 4.35) (particle energy $E > 0$; $k_0^2 = (2m/\hbar^2)E$).
2. Which are the fitting conditions at $q = 0$, $-q_0$? Fix therewith $\varphi(q)$!
3. Determine and discuss the reflection coefficient for the region A!

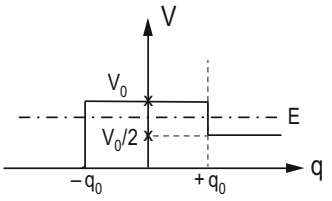

Fig. 4.34 Potential of an asymmetric double-step for a particle wave, which comes from $q = -\infty$ with the energy E ($V_0/2 < E < V_0$)

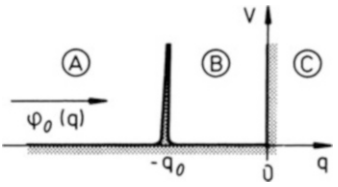

Fig. 4.35 Delta-potential in front of an infinitely high potential wall

4. Investigate, for which values of the wave vector k_0 the position-probability density of the particle in the region B becomes independent of v_0 and q_0.

Exercise 4.3.5 The quasi-free conduction electrons of a metallic solid have a smaller potential energy within the solid than outside the solid. They are therefore, under normal conditions, not able to leave the metal. Because of the Pauli principle each energy level can be occupied by at most two electrons (of opposite spin). At $T = 0$ they fill the so-called *conduction band* up to the *Fermi energy* ε_F. The energetic distance to the exterior potential V_0 is called *electronic work function* W $(= V_0 - \varepsilon_F)$ (Fig. 4.36).

When one applies perpendicular to the metal surface a homogeneous electric field E, then it can hardly at all enter the metal, but it changes the potential outside the metal from $V_0 = \text{const}$ to

$$V(q) = V_0 - eEq$$

(e: elementary charge). Quantum-mechanical tunneling then becomes possible (*field emission, cold emission*).

Which current j_t is observed outside the metal after switching on the field? For the answer assume that, because of the shortest tunneling distance, mainly the electrons at the Fermi edge will come into question for a tunneling process.

Exercise 4.3.6 Given is the following one-dimensional potential $V(q)$ with the period length $l = a + b$ (Fig. 4.37):

$$V(q) = \begin{cases} 0 & \text{for } q \in \mathrm{B}_n \,, \\ V_0 & \text{for } q \in \mathrm{C}_n \,, \end{cases} \qquad n = 0, \pm 1, \pm 2, \ldots$$

$$\mathrm{B}_n = \{q;\ n\,l < q < n\,l + a\} \,,$$
$$\mathrm{C}_n = \{q;\ n\,l - b < q < n\,l\} \,,$$

A particle (electron) of mass m moves with the energy E in this periodic potential.

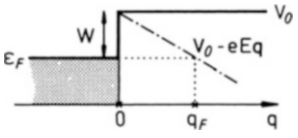

Fig. 4.36 Schematic plot of the course of the potential for the explanation of field emission from a metal

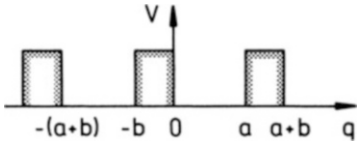

Fig. 4.37 Simple model for the periodic lattice potential of a solid

1. Find for $0 < E < V_0$ a suitable ansatz for the wave function!
2. Reduce the number of determinants to four, by application of the Bloch theorem (4.110)!
3. Introduce periodic boundary conditions:

$$\varphi(q + Nl) \stackrel{!}{=} \varphi(q) \; .$$

4. For the derivation of a conditional equation for the possible energy-eigen values E exploit the continuity conditions for φ and φ', for instance at $q = 0$ and $q = a$.
5. Compare the result in 4. with that of the Kronig-Penny model (4.114). Use therefore the limiting transition:

$$V_0 \to \infty \; , \; b \to 0 \; ; \quad bV_0 \to D \; (< \infty) \; .$$

6. Discuss, whether the conditional equation in 4. is solvable for all energies E. Give an example for forbidden energy values.
7. Investigate the limiting case $E \ll V_0$ and comment qualitatively on the connection between the widths of the energy bands and the magnitude of E.

Exercise 4.3.7 Show for the periodic potential $V(q)$ from Exercise 4.3.6 that, for the case $E > V_0$, the energies $E = \hbar^2 k^2 / 2m$ are forbidden, if the wave number k fulfills the condition

$$ka + \varepsilon\, b = n\,\pi \; ; \qquad n = 0, 1, 2, \ldots \; .$$

where

$$\varepsilon = \sqrt{\frac{2m}{\hbar^2}\,(E - V_0)} \; .$$

4.4 Harmonic Oscillator

We have already met the harmonic oscillator at several points in the framework of this *Ground Course in Theoretical Physics*, for the first time being in Sect. 2.3.6 of Vol.1. There we have characterized the harmonic oscillator as a self-oscillatory system, which obeys a typical differential equation:

$$m\,\ddot{q} + k\,q = 0 \; .$$

One can think thereby, for instance, of an elastic spring in the range of validity of Hooke's law,

$$F = -k\,q \qquad (k: \text{ spring constant}) ,$$

in which the restoring force F is proportional to the displacement q from the rest position. Hooke's law itself is of course an idealization and applicable only for small displacements. We have got to know, besides the spring or the pendulum, still several other realizations, which need not necessarily be of mechanical nature. One can think, for instance, of the electrical oscillator circuit (Sect. 2.3.6, Vol. 1).

In *Volume 2: Analytical Mechanics*, the harmonic oscillator was very often used, in order to demonstrate the new concepts, worked out there (Lagrange, Hamilton, Hamilton-Jacobi), as a rigorously tractable model system. So we found in the framework of the Hamilton Mechanics with Eq. (2.35) in Vol. 2, the following Hamilton function (Fig. 4.38):

$$H(q,p) = \frac{p^2}{2\,m} + \frac{1}{2}m\omega^2 q^2 ; \qquad \omega^2 = \frac{k}{m} . \tag{4.116}$$

The potential energy $V(q)$ is therefore everywhere continuous with $V \to \infty$ for $q \to \pm\infty$, corresponding to the situation, with which we had started in Sect. 4.1.3 our general and qualitative discussion of the energy-eigen value problem. We therefore already know now, without an explicit calculation, that the Hamilton operator of the linear harmonic oscillator, which has formally the same structure as the Hamilton function (4.116), if one interprets q and p as operators, will exhibit a

non-degenerate, discrete spectrum.

The harmonic oscillator possesses a remarkable wealth of important applications. One finds an outstanding example in the theory of the lattice vibrations in solids. By a suitable choice of coordinates (transformation to *normal coordinates*, see Sect. 2.2.1, Vol. 9), the vibrations of the lattice ions around their equilibrium positions can be simulated, under certain conditions, by a system of uncoupled harmonic oscillators. Their quantum-mechanical treatment leads to the important concept of the *phonon*.

We find further remarkable applications in quantum field theory. The electromagnetic field can be represented as a superposition of plane waves. It can therewith

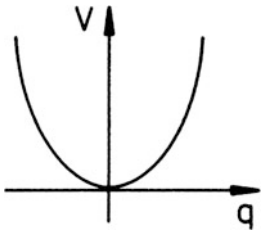

Fig. 4.38 Potential of the linear harmonic oscillator

be shown that the Hamilton operator of the quantized electromagnetic field can be understood as a superposition of harmonic oscillators. The quantization unit is the *photon*.

The decisive importance of the harmonic oscillator for Quantum Mechanics, though, may be seen in the fact that it is rigorously solvable. So it can serve to test and illustrate general concepts and formalisms.

Sometimes one also succeeds to transform the Hamilton operator of a physically, in principle, rather differently exposed problem, in an elegant manner, to that of the harmonic oscillator, so that its exact solution can be exploited. A prominent example of this is the motion of an electron in a magnetic field (see Exercise 4.4.17). The discreteness of the eigen-value spectrum of the harmonic oscillator, in this context, manifests itself in the fact that the electronic motion is *quantized* in the plane perpendicular to the magnetic field (*Landau levels*).

All these considerations, which could still be easily continued, justify an extensive investigation of the harmonic oscillator, which we now begin with.

4.4.1 Creation and Annihilation Operators

Starting point is the Hamilton operator of the harmonic oscillator,

$$H = \frac{p^2}{2\,m} + \frac{1}{2}\,m\,\omega^2 q^2 \;, \tag{4.117}$$

in which p and q are Hermitian operators, because they are the observables *momentum* and *position*, respectively, of a particle of mass m. A possible line of action, which we have always chosen in the preceding sections of this chapter, consists of solving, with the aid of H, the time-independent Schrödinger equation in the form of (4.5). That we will do later, but choose, at first, instead, a somewhat *more nonstandard way*. This starts with a tricky choice of operators a and a^+, which are non-Hermitian, but adjoint to each other, in order to transform the Hamilton operator (4.117) into an as simple as possible, and therefore mathematically easily tractable form. From reasons, which will later become clear, a^+ and a are called the *creation operator* and *annihilation operator*. They will play a central role, in particular, in the many-body physics (Vol. 9, keyword: *second quantization*). Since we want to express H by a and a^+, they must be functions of q and p. In this case, it suggests itself as the simplest ansatz:

$$a = c_1\,q + c_2\,p\;; \qquad c_{1,2} \in \mathbb{C}\;. \tag{4.118}$$

Because of the hermiticity of q and p, it must then be valid for the creation operator:

$$a^+ = c_1^*\,q + c_2^*\,p\;. \tag{4.119}$$

Since q and p are non-commutable operators, a and a^+ also do not commute. But our first demand on the coefficients $c_1,\ c_2$ shall be that the commutator of a and a^+ is as simple as possible, namely:

$$[a, a^+]_- = 1 \ . \tag{4.120}$$

With the known commutation relation (2.101) for position and momentum,

$$[q, p]_- = i\hbar \ ,$$

it follows by insertion of (4.118) and (4.119) into (4.120):

$$\begin{aligned} 1 &= [c_1 q + c_2 p,\ c_1^* q + c_2^* p]_- = \\ &= |c_1|^2\,[q, q]_- + |c_2|^2\,[p, p]_- + c_1 c_2^* [q, p]_- + c_2 c_1^* [p, q]_- = \\ &= i\hbar\big(c_1 c_2^* - c_2 c_1^*\big) \ . \end{aligned}$$

That yields the first condition for the coefficients:

$$\text{Im}\ c_1\, c_2^* = -\frac{1}{2\hbar} \ . \tag{4.121}$$

By reversing (4.118) and (4.119) we can express q and p by a and a^+:

$$q = i\hbar\big(c_2^*\, a - c_2\, a^+\big) \ ; \quad p = -i\hbar\big(c_1^*\, a - c_1\, a^+\big) \ . \tag{4.122}$$

This we insert into the Hamilton operator (4.117):

$$\begin{aligned} H = &-\frac{\hbar^2}{2m}\big[c_1^{*2}\, a^2 + c_1^2\, a^{+2} - |c_1|^2\,(2\, a^+ a + 1)\big] - \\ &-\frac{\hbar^2\, m\, \omega^2}{2}\big[c_2^{*2}\, a^2 + c_2^2\, a^{+2} - |c_2|^2\,(2\, a^+ a + 1)\big] \ . \end{aligned}$$

Here we have used (4.120). It turns out to be convenient to make the terms in a^2 and a^{+2} vanish. That is achieved by the following second demand on the coefficients:

$$\frac{1}{m}\, c_1^2 + m\, \omega^2\, c_2^2 = 0 \ . \tag{4.123}$$

This equation suggests to choose one of the coefficients to be purely real and the other purely imaginary. Then (4.121) and (4.123) are solved by

$$c_1 = \sqrt{\frac{m\,\omega}{2\,\hbar}} \ ; \quad c_2 = \frac{i}{\sqrt{2\,\hbar\, m\, \omega}} \ . \tag{4.124}$$

That yields eventually the following explicit transformation formulae:

$$a = \frac{1}{\sqrt{2\,\hbar}} \left(\sqrt{m\,\omega}\, q + i \frac{p}{\sqrt{m\,\omega}} \right) , \tag{4.125}$$

$$a^+ = \frac{1}{\sqrt{2\,\hbar}} \left(\sqrt{m\,\omega}\, q - i \frac{p}{\sqrt{m\,\omega}} \right) , \tag{4.126}$$

$$q = \sqrt{\frac{\hbar}{2\,m\,\omega}}\, (a + a^+) , \tag{4.127}$$

$$p = -i \sqrt{\frac{\hbar\, m\,\omega}{2}}\, (a - a^+) . \tag{4.128}$$

The Hamilton operator now takes indeed a very simple form:

$$H = \hbar\,\omega \left(a^+\, a + \frac{1}{2} \right) . \tag{4.129}$$

By our operator transformation, the solution of the time-independent Schrödinger equation for the harmonic oscillator is reduced to the eigen-value problem of a new operator, which is called the

occupation number operator

$$\widehat{n} = a^+\, a . \tag{4.130}$$

We therefore want to now investigate this operator in some detail.

4.4.2 *Eigen-Value Problem of the Occupation Number Operator*

The occupation number operator $\widehat{n}$ is obviously Hermitian (3.59); its eigen-values are therefore real. We write

$$\widehat{n}|n\rangle = n|n\rangle \; ; \quad n \in \mathbb{R} \tag{4.131}$$

and assume the eigen states $|n\rangle$ to be normalized. Let us now gather step by step further information about eigen-values and eigen-states.

1. Assertion: *The eigen-values n are non-negative!*
The proof is quickly done:

$$n = \langle n|\widehat{n}|n\rangle = \langle n|a^+ a|n\rangle = \| \, a|n\rangle \, \|^2 \geq 0 . \tag{4.132}$$

To the right there is the square of the norm of the state $a|n\rangle$. According to (3.18) this is zero if $a|n\rangle$ is the zero vector, and otherwise is of course positive.

2. Assertion: *Together with* $|n\rangle$*, also* $a|n\rangle$ *and* $a^+|n\rangle$ *are eigen-states with the eigen-values* $n-1$ *and* $n+1$*, respectively!*

For the proof, we need the commutators $[\widehat{n}, a]_-$ and $[\widehat{n}, a^+]_-$. With the relation, proven as Exercise 3.2.13,

$$[A\,B, C]_- = A[B, C]_- + [A, C]_- B\ , \tag{4.133}$$

where the sequence of the operators A, B, and C is strictly to be respected, we find because of (4.120):

$$[\widehat{n}, a]_- = [a^+, a]_- a + a^+ [a, a]_- = -a\ , \tag{4.134}$$

$$[\widehat{n}, a^+]_- = [a^+, a^+]_- a + a^+ [a, a^+]_- = a^+\ . \tag{4.135}$$

Therewith, we inspect now:

$$\widehat{n}(a^+|n\rangle) = ([\widehat{n}, a^+]_- + a^+\widehat{n})|n\rangle = (a^+ + n\,a^+)|n\rangle = (n+1)(a^+|n\rangle)\ . \tag{4.136}$$

Thus indeed, $a^+|n\rangle$ is eigen-state of the operator $\widehat{n}$ with the eigen-value $n+1$. Completely analogously, we also show that $a|n\rangle$ is eigen-state, but now with the eigen-value $n-1$:

$$\widehat{n}(a|n\rangle) = ([\widehat{n}, a]_- + a\,\widehat{n})|n\rangle = (-a + n\,a)|n\rangle = (n-1)(a|n\rangle)\ . \tag{4.137}$$

3. Assertion: *The eigen-values of* $\widehat{n}$ *are non-degenerate!*

Since $\widehat{n}$ agrees, except for a non-essential numerical factor, with H, this assertion follows, as already mentioned in the introduction of this Sect. 4.4, because of the special form of the potential of the harmonic oscillator, which allows for bound states only. We can, however, prove the statement explicitly also. If the eigen-values n were at least partially degenerate, then, in the sense of Sect. 3.3.3, $\widehat{n}$ would not yet represent a *complete (maximal) set of operators*. There would have to exist, therefore, another observable F, which commutes with $\widehat{n}$,

$$[\widehat{n}, F]_- = 0\ ,$$

and that, too, without itself being a function of $\widehat{n}$ only. Since, as proven, with $|n\rangle$ also $a|n\rangle$ and $a^+|n\rangle$ are eigen-states, F should be interpretable as a function of a and a^+. This means, according to Sect. 3.2.7:

$$F = F(a, a^+) = \sum_{n,\,m} c_{nm}\, a^{+n}\, a^m\ .$$

By the use of the commutator relation (4.120), the operators a and a^+ can always be arranged in the manner given above. For our further considerations we still need

the following commutator relations,

$$[\widehat{n}, a^m]_- = -m\, a^m \; ; \quad [\widehat{n}, a^{+m}]_- = m\, a^{+m} \qquad m \in \mathbb{N} \; , \tag{4.138}$$

which we prove as generalizations of (4.134) and (4.135) in Exercise 4.4.1. We get therewith:

$$0 = [\widehat{n}, F]_- = \sum_{n,\,m} c_{nm} ([\widehat{n}, a^{+n}]_- \, a^m + a^{+n} [\widehat{n}, a^m]_-) = \sum_{n,\,m} c_{nm} (n - m)\, a^{+n}\, a^m \; .$$

Since the individual summands are surely linearly independent, each of them has to vanish, which is possible only with

$$c_{nm} = c_n \, \delta_{nm} \; .$$

Therewith, contrary to the assumption, F is after all only a function of $\widehat{n}$. The occupation number operator $\widehat{n}$ represents therefore by itself already a *'complete set of operators'*. Its eigen-values are thus non-degenerate!

Because of this fact, we can conclude from (4.136) and (4.137) to

$$a^+ |n\rangle = d_{n+1} |n+1\rangle \; , \quad a|n\rangle = \overline{d}_{n-1} |n-1\rangle \; ,$$

where the coefficients can be easily calculated:

$$\begin{aligned} |d_{n+1}|^2 &= |d_{n+1}|^2 \langle n+1|n+1\rangle = \langle n| a\, a^+ |n\rangle = \\ &= \langle n| (\widehat{n} + 1) |n\rangle = n + 1 \; , \\ |\overline{d}_{n-1}|^2 &= |\overline{d}_{n-1}|^2 \langle n-1|n-1\rangle = \langle n| a^+ a |n\rangle = n \; . \end{aligned}$$

Since the arbitrary phase is not of interest, we can assume d and $\overline{d}$ to be real numbers:

$$a^+ |n\rangle = \sqrt{n+1} |n+1\rangle \; , \tag{4.139}$$

$$a|n\rangle = \sqrt{n} |n-1\rangle \; . \tag{4.140}$$

The states $a^+|n\rangle$ and $a|n\rangle$ are of course not normalized to one.

4. Assertion: *The smallest eigen-value of $\widehat{n}$ is $n_{\min} = 0$!*

Because of (4.132) and (4.140), there must exist a minimal n with

$$a|n_{\min}\rangle = 0 \; .$$

From that, it follows immediately:

$$0 = \langle n_{\min}| a^+ a |n_{\min}\rangle = n_{\min} \; . \tag{4.141}$$

The number zero is thus the smallest eigen-value of the occupation-number operator. We write

$$|n_{\min}\rangle = |0\rangle$$

and denote $|0\rangle$ as the *vacuum state*, which must not be mistaken for the zero vector $|0\rangle$ (3.11). Contrary to the zero vector, it is normalized to one:

$$\langle 0|0\rangle = 1 \; . \tag{4.142}$$

5. Assertion: *The eigen-value spectrum of $\widehat{n}$ does not have an upper bound!*

If there were a maximal n, then, because of (4.139), we must have $a^+|n_{\max}\rangle = 0$. But that would mean:

$$0 = \langle n_{\max}|a\,a^+|n_{\max}\rangle = \langle n_{\max}|(\widehat{n}+1)|n_{\max}\rangle = n_{\max} + 1 \; .$$

In contradiction to (4.132), $n_{\max}$ then has to be negative.

We come to the important conclusion that the eigen-states $|n\rangle$, created from $|0\rangle$ by successive application of a^+, can possess as eigen-values only non-negative integers. One easily finds with (4.139) the recursion formula:

$$|n\rangle = \frac{1}{\sqrt{n!}}\,(a^+)^n|0\rangle \; . \tag{4.143}$$

With $|0\rangle$ all $|n\rangle$ are normalized to one. As eigen-states of a Hermitian operator, they are also orthogonal (explicit proof as Exercise 4.4.2):

$$\langle n|m\rangle = \delta_{nm} \; . \tag{4.144}$$

It remains to check whether by (4.143) really all thinkable eigen-states are included.

6. Assertion: *Eigen-states $|n\rangle$ with non-integer n do not exist!*

Let $|\psi\rangle$ be an eigen-state of $\widehat{n}$ with

$$\widehat{n}|\psi\rangle = (m+x)|\psi\rangle \; ; \quad m \in \mathbb{N} \; , \; 0 < x < 1 \; .$$

Then at first, according to the presumption, $|\psi\rangle$ has a finite norm. It can be shown by the use of the commutator relation (4.138) that the state, which results from $|\psi\rangle$ by an $\overline{m}$-fold application of a, should have the eigen-value $m + x - \overline{m}$:

$$\widehat{n}\left(a^{\overline{m}}|\psi\rangle\right) = \left(-\overline{m}\,a^{\overline{m}} + a^{\overline{m}}\,\widehat{n}\right)|\psi\rangle = (-\overline{m} + m + x)\,\left(a^{\overline{m}}|\psi\rangle\right) \; .$$

This means that the norm of the state $a^{\overline{m}+1}|\psi\rangle$,

$$\left\langle a^{\overline{m}+1}\psi \middle| a^{\overline{m}+1}\psi \right\rangle = \left\langle a^{\overline{m}}\psi \middle| a^{+}a \middle| a^{\overline{m}}\psi \right\rangle = (-\overline{m}+m+x)\left\langle a^{\overline{m}}\psi \middle| a^{\overline{m}}\psi \right\rangle ,$$

does exist exactly when the norm of $a^{\overline{m}}|\psi\rangle$ exists, because the pre-factor $(-\overline{m}+m+x)$ can never become zero. We can therefore conclude inductively that for arbitrary $\overline{m} \in \mathbb{N}$ the norm of the state $a^{\overline{m}}|\psi\rangle$ is finite. But for $\overline{m} \geq m+1$ that would mean that there will exist normalizable eigen-states of the occupation-number operator with negative eigen-values. The contradiction to (4.132) is resolved by the fact that the initial assumption, that there exists an eigen-state $|\psi\rangle$ of $\widehat{n}$ with non-integer eigen-value is wrong. All eigen-states are already included in (4.143).

4.4.3 *Spectrum of the Harmonic Oscillator*

According to (4.129), the eigen-states of the Hamilton operator H of the harmonic oscillator are identical with those of the occupation-number operator. The eigen-value equation can therefore be written as follows:

$$H|n\rangle = E_n|n\rangle , \tag{4.145}$$

$$E_n = \hbar\,\omega\left(n+\frac{1}{2}\right) ; \quad n = 0, 1, 2, \ldots . \tag{4.146}$$

The spectrum of the linear harmonic oscillator is therefore discrete and non-degenerate with th energy values, lying equidistantly with a separation of $\hbar\,\omega$. For frequencies of *daily life* $\hbar\,\omega$ is of course only a very tiny energy, so that the energy quantization is not at all conspicuous for classical realizations (spring, pendulum, ...). Classically, the oscillator takes its lowest energy in the state of rest at $(E = 0,\ p = 0,\ q = q_0)$. Quantum-mechanically, however, the lowest energy is a finite energy, the so-called

zero-point energy

$$E_0 = \frac{1}{2}\,\hbar\,\omega . \tag{4.147}$$

The quantization of an oscillatory system has been *guessed and postulated* by M. Planck, in an ingenious manner, long before the development of Quantum Mechanics (see 'Planck's hypothesis', Sect. 1.2.3, (1.24)), by which he could explain the classically not understandable heat radiation. In his ansatz, however, the zero-point energy was still missing.

One can understand, illustratively, the result (4.146), as if the *oscillation* of the oscillator in the state $|n\rangle$ is composed by n oscillation-quanta (*vibrons*), where each of the quanta brings along the energy $\hbar\,\omega$. In this sense, the Hamilton operator H describes a system of indistinguishable *vibrons* of the same energy $\hbar\,\omega$, where the number n of which can change. The eigen-state $|n\rangle$ of H is then uniquely characterized by the number of oscillation quanta present. That makes the nomenclature *occupation-number operator* for $\widehat{n}$ understandable. The operator $\widehat{n}$ *'asks'*, how many *vibrons occupy* the oscillator state $|n\rangle$. The relations (4.139) and (4.140) then explain reasonably also the terms *creation operator* and *annihilation operator*. The action of $a^+(a)$ on the state $|n\rangle$ *creates (annihilates)* one *vibron*.

In the eigen-state $|n\rangle$, the energy of the *oscillating* particle is a sharply defined quantity. On the other hand, position and momentum are undetermined. One knows only their expectation values, which can be calculated rather easily with (4.127) and (4.128):

$$\langle n|q|n\rangle = \sqrt{\frac{\hbar}{2\,m\,\omega}}(\langle n|a|n\rangle + \langle n|a^+|n\rangle) = 0\,, \tag{4.148}$$

$$\langle n|p|n\rangle = -i\sqrt{\frac{1}{2}\hbar\,m\,\omega}\,(\langle n|a|n\rangle - \langle n|a^+|n\rangle) = 0\,. \tag{4.149}$$

Both the expectation values vanish because of (4.139), (4.140) and (4.144). The mean square deviations around these expectation values are still interesting:

$$\begin{aligned}(\Delta q)_n^2 = \langle n|q^2|n\rangle &= \frac{\hbar}{2\,m\,\omega}\langle n|(a^2 + a\,a^+ + a^+a + a^{+2})|n\rangle = \\ &= \frac{\hbar}{2\,m\,\omega}\langle n|(2\,\widehat{n} + 1)|n\rangle = \frac{\hbar}{m\,\omega}\left(n + \frac{1}{2}\right)\,, \\ (\Delta p)_n^2 = -\frac{1}{2}\hbar\,m\,\omega\langle n| - (2\widehat{n} + 1)|n\rangle &= \hbar\,m\,\omega\left(n + \frac{1}{2}\right)\,.\end{aligned}$$

This yields the uncertainty relation:

$$(\Delta q)_n\,(\Delta p)_n = \hbar\left(n + \frac{1}{2}\right)\,. \tag{4.150}$$

The uncertainty product is minimal for the ground state, but even for this it is not equal to zero. This is because of the appearance of the zero-point energy (4.147), which conveys the impression that the oscillator is not *at rest* even in the ground state. Being at rest indeed would have contradicted the uncertainty principle. The oscillator in the ground state executes something like a *zero-point vibration*. We recall that we have already concluded in Exercise 1.1.1, inversely, namely from the Heisenberg uncertainty relation (1.5) on the ground-state energy (4.147) of the harmonic oscillator. The existence of the zero-point uncertainty for the harmonic

oscillator documents impressively the objectivity of such uncertainties, which are not to be ascribed to any *'perturbations'* of the measuring apparatus, as it could be misleadingly assumed.

The harmonic oscillator has, amongst other things, its classical analog in the periodic swinging of the pendulum. Up to now, however, we still miss any indication to a corresponding time-periodicity of the quantum-mechanical oscillator. According to the considerations in Sect. 3.5.1 the correspondence between Classical Mechanics and Quantum Mechanics is mediated, in particular, by the Heisenberg picture. Let us therefore calculate the time-dependencies of the creation and annihilation operators, in this picture, where we suppress the index H for the identification of the Heisenberg representation, because there is no confusion to be feared. According to (3.191), the following equations of motion are to be solved:

$$i\hbar\frac{d}{dt}a(t) = [a,H]_-(t) = \hbar\,\omega[a,\widehat{n}]_-(t) \overset{(4.134)}{=} \hbar\,\omega\,a(t)\ ,$$
$$i\hbar\frac{d}{dt}a^+(t) = \hbar\,\omega[a^+,\widehat{n}](t) \overset{(4.135)}{=} -\hbar\,\omega\,a^+(t)\ .$$

These differential equations are easily integrated with $a^+(0) = a^+$ and $a(0) = a$ to give:

$$a(t) = a\,e^{-i\omega t}\ ; \quad a^+(t) = a^+\,e^{i\omega t}\ . \tag{4.151}$$

These time-dependencies transfer, according to (4.127) and (4.128), to the position and momentum operators:

$$q(t) = \sqrt{\frac{\hbar}{2\,m\,\omega}}\,(a\,e^{-i\omega t} + a^+\,e^{i\omega t})\ ,$$
$$p(t) = -i\sqrt{\frac{1}{2}\hbar\,m\,\omega}\,(a\,e^{-i\omega t} - a^+\,e^{i\omega t})\ .$$

In order to eliminate a and a^+ in these expressions, if one further applies (4.125) and (4.126), one obtains:

$$q(t) = q\cos\omega t + \frac{p}{m\,\omega}\sin\omega t\ , \tag{4.152}$$
$$p(t) = -m\,\omega\,q\sin\omega\,t + p\cos\omega\,t\ . \tag{4.153}$$

By these relations we can indeed recognize the time-periodicities, expected for a harmonic oscillator. In particular, the expectation values $\langle q\rangle_t$ and $\langle p\rangle_t$ fulfill the classical equations of oscillation and therewith the Ehrenfest's theorem (3.211).

4.4.4 Position Representation

By the transformation of the Hamilton operator in Sect. 4.4.1, we could find the eigen-values of the harmonic oscillator, $E_n = \hbar\,\omega(n + 1/2)$, without being forced to derive the corresponding wave functions. Also the expectation values of the observables q, p, q^2, p^2 in the energy-eigen states could easily be calculated. This way of solution, traced back to Dirac, proves to be distinctly more convenient than the direct evaluation of the time-independent Schroödinger equation, which, nevertheless, will be worked out in Sect. 4.4.5, mainly in order to get to know a special and powerful method of solution.

For certain purposes it is surely useful to explicitly know the space-dependent wave functions of the harmonic oscillator

$$\varphi_n(q) \equiv \langle q|n\rangle \; . \tag{4.154}$$

With the results, already at hand, the wave function can relatively easily be derived. At first, a scale transformation onto dimensionless quantities appears to be recommendable:

$$x = \sqrt{\frac{m\,\omega}{\hbar}}\,q \; . \tag{4.155}$$

This substitution also means:

$$dx = \sqrt{\frac{m\,\omega}{\hbar}}\,dq \; ; \quad \frac{d}{dq} = \sqrt{\frac{m\,\omega}{\hbar}}\,\frac{d}{dx} \; .$$

Therewith, the creation and annihilation operators a and a^+ read, according to (4.125) and (4.126), when we use the momentum operator in its position-representation (3.253) $p = (\hbar/i)\,(d/dq)$:

$$a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \; ; \quad a^+ = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right) \; . \tag{4.156}$$

One should bear in mind that the two operators are still adjoint operators! For the ground state wave function $\varphi_0(x)$ (wave function of the vacuum state $|0\rangle$) we must, because of $a|0\rangle = 0$, also have

$$\langle x|a|0\rangle = 0 \; ,$$

which leads to the following differential Eq. (3.252):

$$\left(x + \frac{d}{dx}\right)\varphi_0(x) = 0 \; . \tag{4.157}$$

This equation has the solution

$$\varphi_0(x) = c_0 \exp\left(-\frac{x^2}{2}\right) ,$$

where the constant c_0 is fixed by the normalization condition:

$$1 \stackrel{!}{=} \int_{-\infty}^{+\infty} dq |\varphi_0(q)|^2 = \sqrt{\frac{\hbar}{m\omega}} |c_0|^2 \int_{-\infty}^{+\infty} dx\, e^{-x^2} .$$

The integral on the right-hand side yields $\sqrt{\pi}$ (see the solution to Exercise 2.2.1). The phase of the complex number c_0 does not play any role here. Therefore we can assume c_0 to be real. Therewith, we have as the full solution of the ground state wave function of the harmonic oscillator:

$$\varphi_0(x) = \left(\frac{m\,\omega}{\hbar\pi}\right)^{1/4} \exp\left(-\frac{x^2}{2}\right) . \tag{4.158}$$

We gain the other eigen-functions, because of (4.143), simply by a repeated application of the creation operator a^+ on $\varphi_0(x)$:

$$\varphi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x|(a^+)^n|0\rangle = \frac{1}{\sqrt{2^n\, n!}} \left(x - \frac{d}{dx}\right)^n \varphi_0(x) .$$

That can be written as follows:

$$\varphi_n(x) = \left(\frac{m\,\omega}{\hbar\pi}\right)^{\frac{1}{4}} (n!\, 2^n)^{-\frac{1}{2}} \exp\left(-\frac{x^2}{2}\right) H_n(x) ; \quad n = 0, 1, 2, \ldots , \tag{4.159}$$

$$H_n(x) = \exp\left(\frac{x^2}{2}\right) \left(x - \frac{d}{dx}\right)^n \exp\left(-\frac{x^2}{2}\right) . \tag{4.160}$$

Hermite polynomials

It is evident that the Hermite polynomials are polynomials of n-th degree, which for all real x are real-valued. One directly realizes the symmetry character:

$$H_n(-x) = (-1)^n H_n(x) \iff \varphi_n(-x) = (-1)^n \varphi_n(x) . \tag{4.161}$$

The eigen-functions of the harmonic oscillator thus have each a well-defined parity what, however, is not surprising because

$$V(q) = V(-q) \stackrel{(4.25)}{\iff} [H, \Pi]_- = 0 . \tag{4.162}$$

Equation (4.160) is actually not the standard-representation of the Hermite polynomials. As Exercise 4.4.5 we verify the following equivalent and more convenient expression:

$$H_n(x) = (-1)^n \, e^{x^2} \, \frac{d^n}{dx^n} \, e^{-x^2} \; . \tag{4.163}$$

The orthonormality properties of the eigen-functions of the Hermitian operator H,

$$\int\limits_{-\infty}^{+\infty} dq \, \varphi_n(q) \, \varphi_m(q) = \delta_{nm} \; , \tag{4.164}$$

transfer directly to the Hermite polynomials:

$$\int\limits_{-\infty}^{+\infty} dx \, e^{-x^2} \, H_n(x) \, H_m(x) = \sqrt{\pi} \, 2^n \, n! \, \delta_{nm} \; . \tag{4.165}$$

Further useful relations result more or less directly from (4.139) and (4.140):

$$a^+ \, \varphi_n = \frac{1}{\sqrt{2}} \left(x - \frac{d}{dx} \right) \varphi_n = \sqrt{n+1} \, \varphi_{n+1} \; , \tag{4.166}$$

$$a \, \varphi_n = \frac{1}{\sqrt{2}} \left(x + \frac{d}{dx} \right) \varphi_n = \sqrt{n} \, \varphi_{n-1} \; . \tag{4.167}$$

The addition of these two equations leads to:

$$\sqrt{2} \, x \, \varphi_n(x) = \sqrt{n+1} \, \varphi_{n+1}(x) + \sqrt{n} \, \varphi_{n-1}(x) \; .$$

If one further inserts (4.159), one gets with

$$2 \, x \, H_n(x) = H_{n+1}(x) + 2 \, n \, H_{n-1}(x) \tag{4.168}$$

a formula by which the Hermite polynomials can be recursively calculated in quite a simple manner. So one gets, for instance, the following explicit expressions, if one takes at first H_0 and H_1 according to (4.163):

$$\begin{aligned} H_0(x) &= 1 \; , \\ H_1(x) &= 2x \; , \\ H_2(x) &= (2x)^2 - 2 \; , \\ H_3(x) &= (2x)^3 - 6(2x) \; , \end{aligned}$$

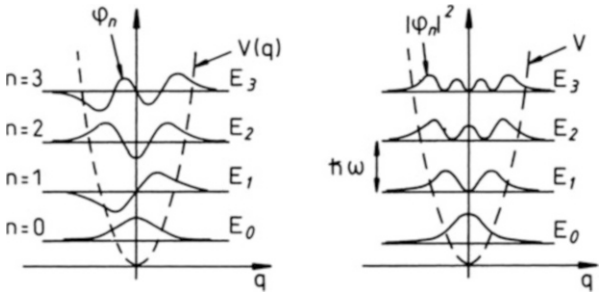

Fig. 4.39 Eigen-functions (*left*) and position-probability densities (*right*) of the linear harmonic oscillator as functions of the position q. E_n are the equidistant eigen-energies

$$
\begin{aligned}
H_4(x) &= (2x)^4 - 12(2x)^2 + 12 \,, \\
H_5(x) &= (2x)^5 - 20(2x)^3 + 60(2x) \,, \\
H_6(x) &= (2x)^6 - 30(2x)^4 + 180(2x)^2 - 120 \\
&\vdots
\end{aligned}
$$

The so determined eigen-functions $\varphi_n(x)$ (4.159) have, according to the law of nodes (Sect. 4.1.3), n zeros (Fig. 4.39, left part). In the *classically allowed region* they exhibit an oscillatory behavior, while, outside this region, they drop exponentially down to zero for $q \to \pm\infty$. $|\varphi_n(q)|^2$ represents the probability density of finding the oscillator with the energy E_n at the position q. Except for the ground state, these functions all show relatively distinct maxima near the classical turning points (Fig. 4.39, the right part).

If we eventually use once more (4.167),

$$
\frac{d}{dx}\,\varphi_n(x) = \sqrt{2n}\,\varphi_{n-1}(x) - x\,\varphi_n(x) \,,
$$

and insert (4.159), then it follows:

$$
\frac{d}{dx}\,H_n(x) = 2\,n\,H_{n-1}(x) \,. \tag{4.169}
$$

This relation can be rewritten with (4.168):

$$
\begin{aligned}
\frac{d^2}{dx^2}\,H_n(x) &= 2\,n\,\frac{d}{dx}\,H_{n-1}(x) = 2\,H_n(x) + 2\,x\,\frac{d}{dx}\,H_n(x) - \frac{d}{dx}\,H_{n+1}(x) = \\
&= 2\,H_n(x) + 2\,x\,\frac{d}{dx}\,H_n(x) - 2\,(n+1)\,H_n(x) \,.
\end{aligned}
$$

The result is a linear, homogeneous differential equation of second order for the Hermite polynomial $H_n(x)$:

$$\left(\frac{d^2}{dx^2} - 2x\frac{d}{dx} + 2n\right) H_n(x) = 0 \,. \tag{4.170}$$

4.4.5 *Sommerfeld's Polynomial Method*

In contrast to the procedures applied in the preceding sections of this fourth chapter, we have chosen so far for the solution of the eigen-value problem of the quantum-mechanical linear harmonic oscillator a rather *unorthodox* way with the introduction of the creation and the annihilation operators. The problem is completely solved in this way. We even succeeded to obtain the more familiar position representation from the abstract $(a,\, a^+)$-representation. Therewith, this section can in principle be closed. Of course, we could have also taken the *conventional* way by solving the time-independent Schrödinger Eq. (4.5). It is clear that the results would have been the same. Although no new findings about the physics of the harmonic oscillator are to be expected, we want to sketch, nevertheless, briefly the *direct* approach, in order to use the opportunity to broaden our *repertoire of solution techniques* by a variant, which is, as we will see, applicable also to other problems.

Hence, we choose now as the starting point the time-independent Schrödinger equation in the form of (4.5):

$$\frac{d^2}{dq^2}\varphi(q) + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 q^2\right)\varphi(q) = 0 \,. \tag{4.171}$$

At first, it is recommendable to transform the variables, as we already did in (4.155), to make all quantities involved dimensionless:

$$\frac{d^2}{dx^2}\varphi(x) + (\eta - x^2)\,\varphi(x) = 0 \,, \tag{4.172}$$

$$\eta = \frac{2E}{\hbar\omega} \,; \quad x = \sqrt{\frac{m\omega}{\hbar}}\, q \,.$$

(In the meantime we got accustomed to the mathematically *somewhat sloppy* peculiarity, to denote functions, even after variable transformations, by the same letter! In physics, it is *'normal'* and misinterpretations are hardly to be feared.) We have to make an important additional demand on the solution: $\varphi(x)$ must be square integrable! That is guaranteed surely only if $\varphi(x)$ approaches zero sufficiently rapidly for $x \to \pm\infty$. We now exploit this aspect in order to arrive at a suitable ansatz for the solution of the differential Eq. (4.172). The constant η in the bracket is certainly unimportant in the limit $x \to \pm\infty$. *Asymptotically*, (4.172) therefore

takes the following form:

$$\frac{d^2}{dx^2}\,\overline{\varphi}(x) - x^2\overline{\varphi}(x) = 0\ .$$

This equation is approximately solved by

$$\overline{\varphi}_{\pm}(x) \sim \exp\left(\pm\frac{1}{2}x^2\right)\ ,$$

because:

$$\frac{d^2}{dx^2}\overline{\varphi}_{\pm}(x) = (x^2 \pm 1)\exp\left(\pm\frac{1}{2}x^2\right) \underset{x^2\gg 1}{\longrightarrow} x^2\exp\left(\pm\frac{1}{2}x^2\right)\ .$$

$\overline{\varphi}_{+}(x)$ is, however, for our purposes an unusable solution because it diverges for $x \to \pm\infty$. But therewith we now already know the correct asymptotic behavior of the function $\varphi(x)$, which solves (4.172). That proposes the following ansatz:

$$\varphi(x) = v(x)\exp\left(-\frac{1}{2}x^2\right)\ . \tag{4.173}$$

When we insert this into (4.172), we obtain a differential equation for the still unknown function $v(x)$:

$$\left[\frac{d^2}{dx^2} - 2\,x\,\frac{d}{dx} + (\eta - 1)\right] v(x) = 0\ . \tag{4.174}$$

It appears as if we had not yet made substantial progress so far. Equation (4.174) is a linear differential equation of second order with non-constant coefficients. Since these coefficients are about powers of the variable x, a power-series ansatz appears to be promising, as one knows from the general theory of differential equations:

$$v(x) = \sum_{\nu} \alpha_\nu\, x^\nu\ .$$

Because of (4.162), $[H,\,\Pi]_- = 0$, our solution $\varphi(x)$ must have a well-defined parity. According to (4.173), the latter is determined by $v(x)$. We therefore presume, already at this stage, that the power-series ansatz has exclusively even indexes ν and exclusively odd indexes ν, respectively:

$$v_+(x) = \sum_{\nu}^{0,2,4,\ldots} \alpha_\nu\, x^\nu\ ; \quad v_-(x) = \sum_{\nu}^{1,3,5,\ldots} \alpha_\nu\, x^\nu\ . \tag{4.175}$$

With

$$x\frac{d}{dx}\,v_{\pm}(x) = \sum_{\nu} \nu\,\alpha_\nu\,x^\nu\ ,$$

$$\frac{d^2}{dx^2}\,v_{\pm}(x) = \sum_{\nu} \nu(\nu-1)\,\alpha_\nu\,x^{\nu-2} = \sum_{\mu} (\mu+2)\,(\mu+1)\,\alpha_{\mu+2}\,x^\mu$$

we then get after insertion of (4.175) into (4.174):

$$\sum_{\mu} \left[\alpha_{\mu+2}\,(\mu+2)\,(\mu+1) + \alpha_\mu(\eta-1-2\,\mu)\right] x^\mu = 0\ .$$

Because of the variable x, this equation can be fulfilled only if already each summand separately vanishes. That leads to a recursion formula,

$$\alpha_{\mu+2} = \frac{2\,\mu+1-\eta}{(\mu+2)\,(\mu+1)}\,\alpha_\mu\ , \tag{4.176}$$

which allows for the determination of all the coefficients with even indexes, if α_0 is given, and all the coefficients with odd indexes, if α_1 is given. If any $\alpha_{\overline{\mu}} = 0$, then all the following coefficients with higher indexes will also vanish. The series in (4.175) then terminates!

But let us assume, at first, that the series does not terminate, i.e., all coefficients α_ν are thus unequal zero. Then we should first assure ourselves that the power series $v(x)$ in our ansatz (4.173) does not, in fact, destroy the correct asymptotic behavior, which is ensured by the exponential function. For $x \to \pm\infty$, of course, the higher powers of x will dominate, whose coefficients can be estimated, according to (4.176), as follows:

$$\frac{\alpha_{\mu+2}}{\alpha_\mu} \approx \frac{2}{\mu} \quad \text{for large}\ \ \mu\ .$$

If we compare this for even indexes with

$$\exp(x^2) = \sum_{\mu=0}^{\infty} \frac{x^{2\mu}}{\mu!} = \sum_{\nu}^{0,2,4,\ldots} \beta_\nu\,x^\nu\ ,$$

$$\beta_\nu = \frac{1}{\left(\frac{\nu}{2}\right)!}\ ; \quad \frac{\beta_{\nu+2}}{\beta_\nu} = \frac{1}{\frac{\nu}{2}+1} \approx \frac{2}{\nu} \quad \text{for large}\ \nu,$$

and for odd indexes with

$$x\exp(x^2) = \sum_{\mu=0}^{\infty} \frac{x^{2\mu+1}}{\mu!} = \sum_{\nu}^{1,3,5,\ldots} \gamma_\nu\, x^\nu \ ,$$

$$\gamma_\nu = \frac{1}{\left(\frac{\nu-1}{2}\right)!} \ ; \quad \frac{\gamma_{\nu+2}}{\gamma_\nu} = \frac{2}{\nu+1} \approx \frac{2}{\nu} \quad \text{for large } \nu$$

then we recognize that our *fear* is confirmed that, in the case of a non-terminating series, $v_+(x)$ would asymptotically behave like $\exp(x^2)$ and $v_-(x)$ like $x\exp(x^2)$. In both the cases, $\varphi(x)$ in (4.173) would thus not be normalizable. The series (4.175) being not terminated is therefore physically unacceptable!

But how can we achieve the truncation of the series? According to (4.176), we have to obviously put very special conditions on the constant η. A *physically correct* solution always comes out, when, for any finite

$$\mu = n \ ; \qquad n = 0, 1, 2, \ldots \ ,$$

we have:

$$\eta = 2\,n + 1 \ . \tag{4.177}$$

If we remember the definition of η in (4.172), then we have herewith reproduced the meanwhile well-known energy condition (4.146)

$$E_n = \hbar\,\omega\left(n + \frac{1}{2}\right) \ ; \quad n = 0, 1, 2, \ldots \ . \tag{4.178}$$

The eigen-functions of the linear harmonic oscillator are therewith fixed. They are to be determined successively by the recursion formula (4.176) via (4.173) and (4.175). Let us demonstrate this for the first three eigen-functions ($n = 0, 1, 2$):

$$\begin{aligned}
n = 0 \implies & \quad \alpha_0 \neq 0 \ , \ \alpha_2 = \alpha_4 = \ldots = 0 \ , \\
& \quad v_+(x) \equiv \alpha_0 \ , \\
& \quad \varphi_0(x) = \alpha_0 \ \exp\left(-\frac{x^2}{2}\right) , \\
n = 1 \implies & \quad \alpha_1 \neq 0 \ , \ \alpha_3 = \alpha_5 = \ldots = 0 \ , \\
& \quad v_-(x) = \alpha_1\, x \ , \\
& \quad \varphi_1(x) = \alpha_1\, x \ \exp\left(-\frac{x^2}{2}\right) \ ,
\end{aligned}$$

$$n = 2 \implies \alpha_0 \neq 0\,, \quad \frac{\alpha_2}{\alpha_0} \overset{(4.176)}{=} -2,\ \alpha_4 = \alpha_6 = \ldots = 0\,,$$
$$v_+(x) = \alpha_0\,(1 - 2\,x^2)\,,$$
$$\varphi_2(x) = \frac{1}{2}\,\alpha_0\,\left(2 - (2\,x)^2\right)\,\exp\left(-\frac{x^2}{2}\right)\,.$$

In these relations, α_0 and α_1 follow from the normalization condition for $\varphi(x)$. But the functions φ_0, φ_1 and φ_2 are then indeed identical with the eigenfunctions (4.159) for $n = 0, 1, 2$. This can be shown, in the same manner, for any arbitrary n.

The *polynomial method*, developed in this section, is ascribed to A. Sommerfeld (1868–1951). It is always promising, when, for the coefficients of a power-series ansatz, as in (4.175), a bipartite recursion formula as that in (4.176) can be found.

4.4.6 Higher-Dimensional Harmonic Oscillator

In this chapter we have dealt so far exclusively with one-dimensional potential problems. But let us, at the end of this chapter, briefly refer to the three-dimensional oscillator. This does not pose, compared to the linear oscillator, any novel problems and can therefore be treated relatively quickly.

We think of the motion of a particle of the mass m in the potential

$$V(\mathbf{q}) = \frac{1}{2}\,m \sum_{i=1}^{3} \omega_i^2\,q_i^2\,. \tag{4.179}$$

Let q_1, q_2, q_3 be the three Cartesian components of the vector $\mathbf{q}$. The Hamilton operator,

$$H = \frac{\mathbf{p}^2}{2\,m} + V(\mathbf{q}) \equiv \sum_{i=1}^{3} H_i\,, \tag{4.180}$$

is then additively composed of three partial operators, where each of them describes a linear oscillator:

$$H_i = \frac{p_i^2}{2\,m} + \frac{1}{2}\,m\,\omega_i^2\,q_i^2\,; \quad i = 1, 2, 3\,. \tag{4.181}$$

For the solution of the eigen-value equation

$$H\,\psi(\mathbf{q}) = E\,\psi(\mathbf{q})$$

the so-called separation ansatz is always recommended:

$$\psi(\mathbf{q}) = f_1(q_1) f_2(q_2) f_3(q_3) \ . \tag{4.182}$$

If we insert this ansatz into the eigen-value equation and then divide it by $\psi(\mathbf{q})$,

$$\frac{1}{f_1(q_1)} H_1 f_1(q_1) + \frac{1}{f_2(q_2)} H_2 f_2(q_2) + \frac{1}{f_3(q_3)} H_3 f_3(q_3) = E \ ,$$

the equation decomposes into three additive parts, each of which depends only on one single variable. The equation can thus be fulfilled only if each term by itself is already constant. The original three-dimensional problem has thus been *separated* into three independent, linear oscillator problems,

$$\begin{aligned} H_1 f_1(q_1) &= \varepsilon_1 f_1(q_1) \ , \\ H_2 f_2(q_2) &= \varepsilon_2 f_2(q_2) \ , \\ H_3 f_3(q_3) &= (E - \varepsilon_1 - \varepsilon_2) f_3(q_3) \ , \end{aligned}$$

the solutions of which we already know. The eigen-functions correspond to those of (4.159):

$$\begin{aligned} f_{i n_i}(q_i) = \sqrt{\frac{m\,\omega_i}{\hbar\,\pi}}\, (2^{n_i}\, n_i!)^{-\frac{1}{2}}\, \exp\left(-\frac{m\,\omega_i}{2\hbar}\, q_i^2\right) \cdot \\ \cdot\ H_{n_i}\left(\sqrt{\frac{m\,\omega_i}{\hbar}}\, q_i\right) \ ; \qquad i = 1, 2, 3 \ . \end{aligned} \tag{4.183}$$

We can not assume any more, however, that the energy-eigen values,

$$E_{n_1 n_2 n_3} = \sum_{i=1}^{3} \hbar\,\omega_i \left(n_i + \frac{1}{2}\right) \ , \tag{4.184}$$

which now carry three indexes, are non-degenerate. That holds generally, according to Sect. 4.1, actually only for one-dimensional systems. It is quite possible that different eigen-functions exist to the same eigen-value

$$\psi_{n_1 n_2 n_3}(\mathbf{q}) = f_{1 n_1}(q_1) f_{2 n_2}(q_2) f_{3 n_3}(q_3) \ . \tag{4.185}$$

This can be demonstrated especially simply by the isotropic three-dimensional oscillator ($\omega_1 = \omega_2 = \omega_3 \equiv \omega$). Its eigen-values depend only on one quantum number N:

$$E_N = \hbar\,\omega \left(N + \frac{3}{2}\right) \ ; \quad N = n_1 + n_2 + n_3 \ . \tag{4.186}$$

A given N can be realized by different combinations n_1, n_2, n_3. So, for given N and n_1 the number n_2 can take the values $0, 1, \ldots, N-n_1$, where n_3 is then, however, fixed. These are then $N - n_1 + 1$ possibilities. Altogether it follows therewith:

$$\textit{degree of degeneracy}\,(E_N) = \sum_{n_1=0}^{N} (N - n_1 + 1) = \frac{1}{2}\,(N+1)\,(N+2)\,. \qquad (4.187)$$

4.4.7 Exercises

Exercise 4.4.1 $\widehat{n} = a^+ a$ is the occupation-number operator, and a^+ and a are the creation and the annihilation operators. Verify the following commutation relations:

1. $[a^m,\, a^+]_- = m\, a^{m-1}$,
2. $[a,\, a^{+m}]_- = m\,(a^+)^{m-1}$,
3. $[\widehat{n},\, a^m]_- = -m\, a^m$,
4. $[\widehat{n},\, a^{+m}]_- = m\, a^{+m}$.

Exercise 4.4.2 Prove explicitly the orthonormality of the eigen-states $|n\rangle$ (4.143) of the occupation-number operator.

Exercise 4.4.3 For the expectation values of the kinetic energy T and the potential energy V in the energy-eigen states of the harmonic oscillator, verify the quantum-mechanical virial theorem (Exercise 3.5.4):

$$\langle n|T|n\rangle = \langle n|V|n\rangle\,.$$

Exercise 4.4.4 The Hamilton operator of the linear harmonic oscillator in the occupation-number representation (4.129) reads:

$$H = \hbar\omega\left(\widehat{n} + \frac{1}{2}\right)\;;\quad \widehat{n} = a^+ a\,.$$

The relations between creation and annihilation operators on the one hand, and position and momentum operator on the other hand are given by the Eqs. (4.125) and (4.126).

1. Express a and a^+ by the variable

$$y = \frac{p}{\sqrt{\hbar m\omega}}$$

('y representation') in the momentum representation!

2. Except for a normalization constant, calculate the ground-state wave function $\varphi_0(y)$ of the linear harmonic oscillator in the momentum representation and the y representation, respectively!
3. Express the energy-eigen function $\varphi_n(y) = \langle y|n\rangle$ by the Hermite polynomial $H_n(y)$ (4.160)!
4. Derive a recursion formula among $\varphi_{n-1}(y)$, $\varphi_n(y)$ and $\varphi_{n+1}(y)$!

Exercise 4.4.5 1. Prove the general operator relation:

$$\frac{1}{f(x)}\,\frac{d}{dx}f(x) = \frac{d}{dx} + \frac{f'(x)}{f(x)}\ .$$

2. Show that

$$\frac{1}{f(x)}\,\frac{d^n}{dx^n}f(x) = \left(\frac{1}{f(x)}\,\frac{d}{dx}f(x)\right)^n\ .$$

3. Prove with 1. and 2. the equivalence of the representations (4.160) and (4.163) of the Hermite polynomials.

Exercise 4.4.6 Show that

$$\varphi(x) = \alpha\,(2\,x^2 - 1)\,\exp\left(-\frac{x^2}{2}\right)\ ;\quad x = q\sqrt{\frac{m\,\omega}{\hbar}}$$

is an eigen-function of the linear harmonic oscillator and calculate the corresponding energy-eigen value.

Exercise 4.4.7 A particle of mass m moves in the oscillator potential $V(q) = \frac{1}{2}m\,\omega^2 q^2$. Determine the probability that the particle, in its ground state, is outside the classically allowed region.

Exercise 4.4.8 By the linear harmonic oscillation of an atom of mass $m = 4.85 \cdot 10^{-23}$ g within a molecule, a photon of the energy $2\,\varepsilon = 7.2\,\text{eV}$ is emitted. This is interpreted as the transition from the lowest excited state of the harmonic oscillator to the ground state.

1. How large is the amplitude A of the oscillation of the atom according to Classical Mechanics? Find also the numerical value!
2. How large is the probability for the situation that the atom, which performs the harmonic oscillation, is displaced from its equilibrium position by a distance of more than A?

Numerical values: $\hbar = 1.055 \cdot 10^{-34}\,\text{J s}$;$1\,\text{eV} = 1.6019 \cdot 10^{-19}\,\text{J}$.

Exercise 4.4.9 The Hermite polynomials have the integral representation

$$H_n(x) = \frac{1}{\sqrt{\pi}}\, 2^n \int_{-\infty}^{+\infty} dy (x + i\,y)^n\, e^{-y^2}\ ; \qquad n = 0, 1, 2, \ldots\ :$$

1. By the use of this formula calculate H_0, H_1 and H_2.
2. By insertion of the integral formula show that the Hermite polynomials possess the following generating function

$$\exp(-t^2 + 2\,t\,x) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\, H_n(x)\ .$$

Exercise 4.4.10 For the eigen-solutions of the harmonic oscillator one finds:

$$\varphi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} (n!\, 2^n)^{-(1/2)}\, e^{-(x^2/2)} H_n(x)\ .$$

Show that the Hermite polynomials $H_n(x)$ possess the following explicit representation:

$$H_n(x) = \sum_{\nu=0}^{\langle n/2\rangle} \frac{(-1)^\nu \cdot n!}{\nu!(n-2\nu)!} (2x)^{n-2\nu}\ .$$

Thereby, $\langle n/2\rangle$ is the largest integer smaller than or equal to $n/2$.

Exercise 4.4.11 A particle of the mass m moves in the potential:

$$V(q) = \begin{cases} \infty & \text{for } q < 0\ , \\ \frac{1}{2}\, m\, \omega^2 q^2 & \text{for } q > 0\ . \end{cases}$$

Determine the eigen-values and the eigen-functions of the Hamilton operator

$$H = \frac{p^2}{2\,m} + V(q)\ .$$

Exercise 4.4.12 By using the eigen-functions of the harmonic oscillator in the position representation, calculate the matrix elements of the operators

1. q and q^2,
2. p and p^2.

For that, we use appropriately, the recursion formulae (4.168) and (4.169).

Exercise 4.4.13 Calculate the matrix representations of the position and the momentum operator in the basis of the eigen-states of the occupation-number operator. By the corresponding matrix multiplication verify the commutation relation:

$$[q, p]_- = i\hbar \ .$$

Exercise 4.4.14 A particle with the charge $\hat{q}$ and the mass m performs a one-dimensional motion in the harmonic oscillator potential and is, furthermore, subject to the influence of a constant electric field, which acts parallel to the direction of its motion. Formulate the Hamilton operator and determine its eigen-value spectrum and its eigen-functions.

Exercise 4.4.15 The Hamilton operator H of a charged harmonic oscillator (charge $\hat{q}$, mass m) in a constant electric field E is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 - \hat{q} E q \ ,$$

and the unitary translation operator (3.249) by:

$$T(y_0) = \exp\left(-\frac{i}{\hbar} y_0 p\right) \ ; \quad y_0 = -\frac{\hat{q} E}{m\omega^2} \in \mathbb{R} \ .$$

1. Calculate the commutator

$$[q, T]_- \ .$$

2. Transform the Hamilton operator

$$\overline{H} = T H T^+$$

and compare the result with Exercise 4.4.14.

Exercise 4.4.16 Prove that in the Hilbert space of the square integrable wave functions $\psi(q)$ of one variable q, the operator, defined by

$$\Pi(\hat{q}, \hat{p}) = \exp\left[i\pi\left(\frac{\hat{p}^2}{2\alpha} + \frac{\alpha}{2\hbar^2}\hat{q}^2 - \frac{1}{2}\right)\right] \ ,$$

represents the parity operator. $\hat{q}$ and $\hat{p}$ are thereby position and momentum operators, and α is an arbitrary positive-real constant with the dimension (momentum)^2.

Exercise 4.4.17 An electron with the charge $\hat{q} = -e$ moves in a homogeneous magnetic field $\mathbf{B} = B\,\mathbf{e}_z$ ($\mathbf{e}_z$: unit vector in z-direction).

1. Find the classical Hamilton function!
2. Choose the vector potential $\mathbf{A}(\mathbf{r}) \equiv (0, A_y(x), 0)$ such that the Coulomb gauge ($\mathrm{div}\mathbf{A} = 0$) is fulfilled.
3. Show that the eigen-value problem of the Hamilton **operator**,

$$H\,\psi = E\,\psi \ ,$$

reduces with the ansatz

$$\psi(\mathbf{r}) = \psi(x, y, z) = e^{i\,k_z\,z}\,e^{i\,k_y\,y}\,\varphi(x)$$

to that of the linear harmonic oscillator.
4. Determine the eigen-energies and the eigen-functions.

Exercise 4.4.18 A charged particle (mass m, charge $\hat{q} = -e$) moves in a homogeneous magnetic field $\mathbf{B} = B\,\mathbf{e}_z$ and in addition is subject to a harmonic potential $V(z) = \frac{1}{2}\,m\,\omega^2 z^2$.

1. Write down the Hamilton operator. Choose the vector potential so that the Coulomb gauge $\mathrm{div}\mathbf{A} = 0$ is realized.
   Ansatz: $A(\mathbf{r}) = (0, A_y(x), 0)$.
2. Choose a suitable separation ansatz for the eigen-function $\psi(\mathbf{r}) = \psi(x, y, z)$ of the Hamilton operator H.
3. Find explicitly the eigen-values and the eigen-functions!

Exercise 4.4.19 A particle of the mass m moves in the oscillator potential

$$V(q) = \frac{1}{2}\,m\,\omega^2 q^2 \ .$$

At the time $t = 0$ it is described by the Gaussian wave packet

$$\psi(q, 0) = \Big(\frac{m\,\omega}{\hbar\,\pi}\Big)^{1/4} \exp\Big[-\frac{m\,\omega}{2\,\hbar}\,(q - \overline{q})^2\Big] \ .$$

1. Expand $\psi(q, 0)$ in eigen-functions $\varphi_n(q)$ of the linear harmonic oscillator:

$$\psi(q, 0) = \sum_n \alpha_n\,\varphi_n(q) \ .$$

For the calculation of the coefficients α_n the formula

$$\int_{-\infty}^{+\infty} dx\,e^{-(x-x_0)^2}\,H_n(x) = \sqrt{\pi}\,(2\,x_0)^n$$

is useful.

2. Calculate the full time-dependence of the wave function $\psi(q,t)$. It is advisable to use thereby the representation of the generating function of the Hermite polynomials from part 2. of Exercise 4.4.9.
3. Determine the density of the position probability $|\psi(q,t)|^2$ and demonstrate therewith that the wave packet, contrary to the *free* particle (Sect. 2.2.3), does **not** have its width increasing.
4. Calculate the expectation value $\langle q\rangle_t$ and the mean square deviation Δq_t.
5. With an energy measurement on the particle at the time $t > 0$, what is the probability to get just the eigen-value

$$E_n = \hbar\,\omega\left(n+\frac{1}{2}\right)\,?$$

Exercise 4.4.20 A particle of the mass m moves in the oscillator potential

$$V(q) = \frac{1}{2}\,m\,\omega^2 q^2\ .$$

Let it be in a mixed state, characterized by the (not normalized) density matrix

$$\rho = \exp\left(-\frac{H}{k_B\,T}\right)$$

(k_B: Boltzmann constant, T: temperature).

1. How large is the expectation value $\langle H\rangle$ of the energy?
2. What is the probability that an energy measurement yields the value $E_n = \hbar\,\omega\left(n+\frac{1}{2}\right)$?

Exercise 4.4.21 Prove the formula used in Exercise 4.4.19 for the Hermite polynomials $H_n(x)$:

$$\int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2}\,H_n(x) = \sqrt{\pi}\,(2x_0)^n\ .$$

4.5 Self-Examination Questions

To Section 4.1

1. When is it recommendable to use a separation ansatz for the wave function $\psi(q,t)$?
2. When does $\psi(q,t)$ represent a stationary state?

3. Which conditions must be fulfilled by $\varphi(q)$ and $\varphi'(q)$? Give reasons for these requirements!
4. How is the *classically allowed region* defined? What can be said, very generally, about the behavior of the wave function in this region?
5. What are the *classical turning points*?
6. How does the wave function behave in the *classically forbidden region*?
7. What do we understand by the Wronski determinant?
8. What can be said about the Wronski determinant $W(\varphi_1, \varphi_2; q)$, when the functions $\varphi_1(q)$ and $\varphi_2(q)$ belong to the same eigen-value E?
9. What is a *bound state*?
10. Formulate the law of nodes and give reasons for it!
11. Under which conditions does H possess a discrete eigen-value spectrum?
12. How does the parity operator Π act on a wave function $\varphi(q)$?
13. What is to be understood by even (odd) parity?
14. When does the Hamilton operator commute with the parity operator?

To Section 4.2

1. Sketch the most important steps necessary for finding the bound states in the potential wall!
2. Which transcendental conditional equations fix the discrete energy spectrum of the potential wall?
3. Does there exist, independently of the height of the potential wall, always a symmetric and always an antisymmetric bound state?
4. Which quantities determine the number of discrete states in the potential wall? Is this number always finite for finite height and width of the wall?
5. How are the transmission and reflection coefficients T and R defined? Which kind of physical information is conveyed by them?
6. How do T and R behave qualitatively as functions of energy E?
7. At which energies (*resonances*) does the potential wall become *totally transparent* ($T = 1,\ R = 0$)?
8. How can we understand, illustratively, the *resonances*?

To Section 4.3

1. How does the density of the position-probability $|\varphi(q)|^2$ look like for a particle, which hits a potential step $V(q) = V_0\,\Theta(q)$ with the momentum $\hbar\, k_0/m$? Distinguish the cases $E > V_0$ and $E < V_0$!
2. How do the reflection and transmission coefficients (T and R) change, when the particle travels with the same energy $E > V_0$, but instead of coming from $q = -\infty$, now comes in the opposite direction, from $q = +\infty$ to $q = -\infty$?

3. Which conservation law is responsable for the relation $T + R = 1$?
4. How can one explain a finite reflection coefficient R at the potential step for the particle of energy $E > V_0$?
5. How do T and R behave at the potential step for $E < V_0$, $E \overset{>}{\to} V_0$ and $E \gg V_0$?
6. What can be said, in the case of an infinitely high potential step ($V_0 \to \infty$), about the wave function $\varphi(q)$ in the classically forbidden region ($q > 0$)?
7. Do you know from Classical Electrodynamics a situation which is analog to the quantum-mechanical tunneling?
8. Illustrate the tunnel effect by the example of the rectangular potential wall!
9. Do you know important consequences of the tunnel effect?
10. Which quantities predominantly determine the tunnel-probability through the rectangular potential wall?
11. How does the q-dependence of $|\varphi(q)|^2$, qualitatively, look like for the potential wall?
12. By which *trick* can the tunnel-probability through a realistic continuous potential hill be expressed, at least approximately, by the results for the simpler rectangular potential wall?
13. According to which formula can the tunnel-probability be calculated for a continuous potential hill?
14. How can α-radioactivity be qualitatively explained?
15. What is the relation between the lifetime of an α-radioactive nucleus and the energy of the emitted α-particle?
16. Which situation is described by the Kronig-Penney model?
17. What is to be taken into consideration concerning the wave function and its first derivative, if the potential energy $V(q)$ has the shape of a δ-function?
18. Comment on the Bloch theorem by the use of the Kronig-Penney- model!
19. What is the reason for the appearance of energy bands and energy gaps in solids?
20. In the Kronig-Penney model, how do the position and the width of the energy bands depend on the interaction strength D and the lattice distance a?
21. How many discrete energy levels build up an energy band? Do there exist energy levels, whose energetic position is independent of the potential strength D?
22. How can one introduce a *band index n*?
23. What is understood by a *band structure*?

To Section 4.4

1. Which is the Hamilton operator of the linear harmonic oscillator?
2. Why must this operator possess a discrete, non-degenerate energy spectrum?
3. Are creation and annihilation operator, a and a^+, commutable? If not, which commutation relation do they have to fulfill?

4. What is the relation between the position q, the momentum p of the harmonic oscillator and a, and a^+?
5. How can the Hamilton operator of the harmonic oscillator be expressed by the occupation number operator $\widehat{n} = a^+ a$?
6. Why does $\widehat{n} = a^+ a$ have only real eigen-values?
7. What can be said about the eigen-values of $\widehat{n}$?
8. How does one prove that together with $|n\rangle$ also $a|n\rangle$ and $a^+|n\rangle$ are eigen-states of $\widehat{n}$? To which eigen-values do they belong?
9. Which is the smallest eigen-value of $\widehat{n}$?
10. How is the eigen-state $|n\rangle$ connected to the *vacuum state* $|0\rangle$?
11. What does one understand by the zero-point energy of the harmonic oscillator?
12. How can one understand, in an illustrative manner, the terms *occupation number*, *creation* and *annihilation* operators?
13. Find the expectation values of position and momentum of the harmonic oscillator in the eigen-state $|n\rangle$!
14. How does the uncertainty product $\Delta p\, \Delta q$ read for the oscillator being in the state $|n\rangle$?
15. Which simple differential equation must be fulfilled by the wave function $\varphi_0(x)$ of the ground state?
16. How can one find, by the use of the wave function $\varphi_0(x)$ of the ground state, the other eigen-functions, $\varphi_n(x)$, $n \geq 1$, of the linear harmonic oscillator?
17. What do we know about the parity of the eigen-functions $\varphi_n(x)$?
18. How does $\varphi_n(x)$ behave, qualitatively, in the *classically allowed (forbidden) region*?
19. Sketch the idea of *Sommerfeld's polynomial method*. Which property of the wave function plays the decisive role with respect to the choice of the ansatz of solution for the time-independent Schrödinger equation?
20. By which ansatz of solution can the problem of the three-dimensional harmonic oscillator be traced back to that of the linear oscillator?
21. What can be said about the degree of degeneracy of the eigen-values of the isotropic three-dimensional oscillator?

Appendix A
Solutions of the Exercises

Section 1.1.1

Solution 1.1.1 Hamilton function of the harmonic oscillator:

$$H = \frac{p^2}{2\,m} + \frac{1}{2}\,m\,\omega^2 q^2 = E\ .$$

We must have:

$$E \geq \frac{(\Delta p)^2}{2\,m} + \frac{1}{2}\,m\,\omega^2 (\Delta q)^2\ .$$

Uncertainty relation:

$$(\Delta p)^2\,(\Delta q)^2 \geq \frac{1}{4}\,\hbar^2\ .$$

It follows therewith:

$$E \geq \frac{(\Delta p)^2}{2\,m} + \frac{1}{8}\,\hbar^2\,m\,\omega^2\,\frac{1}{(\Delta p)^2}\ .$$

From

$$\frac{dE}{d(\Delta p)^2} \stackrel{!}{=} 0 = \frac{1}{2\,m} - \frac{1}{8}\,\hbar^2\,m\,\omega^2 \frac{1}{(\Delta p)^4}$$

so that we get:

$$(\Delta p)_0^2 = \frac{1}{2}\,m\,\omega\,\hbar\ .$$

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Insertion into the inequality for E:

$$E \geq \frac{1}{4}\hbar\omega + \frac{1}{4}\hbar\omega = \frac{1}{2}\hbar\,\omega\ .$$

Solution 1.1.2 Hamilton function:

$$H = T + V = \frac{p^2}{2\,m} - \frac{e^2}{4\pi\,\varepsilon_0 r} \stackrel{!}{=} E\ .$$

Lower bound for the orbit radius, fixed by the uncertainty relation:

$$a \geq \Delta r\ ; \quad p \geq \Delta p\ .$$

We can thus estimate:

$$a\,p \geq \frac{\hbar}{2} \iff p \geq \frac{\hbar}{2\,a}\ .$$

Corresponding energy:

$$E(a) = \frac{\hbar^2}{8\,m\,a^2} - \frac{e^2}{4\pi\,\varepsilon_0 a}\ .$$

Minimum of energy:

$$\left.\frac{dE}{da}\right|_{a_0} = -\frac{\hbar^2}{4\,m\,a_0^3} + \frac{e^2}{4\pi\,\varepsilon_0 a_0^2} \stackrel{!}{=} 0$$

$$\Longrightarrow\ a_0 = \frac{1}{4}\,\frac{4\pi\,\varepsilon_0\,\hbar^2}{m\,e^2}\ .$$

The later quantum-mechanical calculation will yield the Bohr radius as the lower limit of the orbit radius:

$$a_\mathrm{B} = 4\,a_0\ .$$

A minimum energy (*ground state energy*) then corresponds to the smallest radius.

Solution 1.1.3

$$T = \frac{\mathbf{p}^2}{2\,m} = \frac{1}{2\,m}(p_x^2 + p_y^2 + p_z^2)\ .$$

Uncertainty relation:

$$(\Delta p_x)^2 \gtrsim \frac{\hbar^2}{4(\Delta x)^2}\,; \quad (\Delta p_y)^2 \gtrsim \frac{\hbar^2}{4(\Delta y)^2}\,; \quad (\Delta p_z)^2 \gtrsim \frac{\hbar^2}{4(\Delta z)^2}\,,$$
$$\Delta x \approx \Delta y \approx \Delta z \approx 2R$$
$$\Longrightarrow\ T \gtrsim \frac{3}{32\,m}\,\frac{\hbar^2}{R^2}\,.$$

Numerical values:

$$T \gtrsim \frac{3}{32 \cdot 1.7\,10^{-27}}\,\frac{(1.055)^2 \cdot 10^{-68}}{10^{-30}}\,\frac{\mathrm{J^2\,s^2}}{\mathrm{kg\,m^2}} \approx$$
$$\approx 0.614 \cdot 10^{-12}\,J = 0.614 \cdot 6.242 \cdot 10^{6}\mathrm{eV} \implies T \gtrsim 3.831\,\mathrm{MeV}\,.$$

Solution 1.1.4

$$V(x) = V_0 \left(\frac{x}{a}\right)^{2n} \quad \text{with } V_0 > 0,\ n \in \mathbb{N}$$

Position uncertainty:

$$b = |\Delta x|$$

Uncertainty relation:

$$|\Delta p| \geq \frac{\hbar}{2b}$$

Hamilton function:

$$H = \frac{p^2}{2m} + V(x) \stackrel{!}{=} E$$
$$E \geq E(b) = \frac{\hbar^2}{8mb^2} + V_0 \left(\frac{b}{a}\right)^{2n}$$

b is chosen such that $E(b)$ becomes minimal $\curvearrowright$

$$0 \stackrel{!}{=} \frac{dE}{db} = -\frac{\hbar^2}{4mb_0^3} + 2nV_0\frac{b_0^{2n-1}}{a^{2n}} \tag{A.1}$$
$$\curvearrowright\ V_0 \left(\frac{b_0}{a}\right)^{2n} = \frac{\hbar^2}{8mn} \cdot \frac{1}{b_0^2}$$
$$\curvearrowright\ E_0 = E(b_0) = \frac{\hbar^2}{8mb_0^2}\left(1 + \frac{1}{n}\right) = \frac{\hbar^2}{8mnb_0^2}(n+1)$$

From Eq. (A.1) it follows also

$$\left(\frac{1}{b_0^2}\right)^{n+1} = \frac{8mnV_0}{\hbar^2 a^{2n}}$$

$$\frac{1}{b_0^2} = V_0^{\frac{1}{n+1}} \left(\frac{8mn}{\hbar^2}\right)^{\frac{1}{n+1}} \cdot \left(\frac{1}{a^2}\right)^{\frac{n}{n+1}}$$

$$= V_0 \cdot \frac{8mn}{\hbar^2} \cdot \left(V_0 \frac{8mn}{\hbar^2}\right)^{-\frac{n}{n+1}} \cdot \left(\frac{1}{a^2}\right)^{\frac{n}{n+1}}$$

Inserting into E_0 $\curvearrowright$

$$E_0 = V_0(n+1)\left(\frac{\hbar^2}{8mnV_0a^2}\right)^{\frac{n}{n+1}}$$

Special case $n = 1$*:*

$$V(x) = V_0 \frac{x^2}{a^2} \;\rightarrow\; \text{harmonic oscillator}$$

$$\frac{V_0}{a^2} = \frac{1}{2}m\omega^2 \;\curvearrowright\; \omega = \frac{1}{a}\sqrt{\frac{2V_0}{m}}$$

$$E_0 = 2V_0 \cdot \frac{\hbar}{a}\frac{1}{\sqrt{8mV_0}} = \frac{\hbar}{a}\sqrt{\frac{V_0}{2m}}$$

$$= \frac{1}{2}\frac{\hbar}{a}\sqrt{\frac{2V_0}{m}}$$

$$= \frac{1}{2}\hbar\omega$$

That is the exact ground-state energy of the harmonic oscillator.

Special case $n \to \infty$*:*

$$V(x) = \begin{cases} 0, & \text{for } -a < x < +a \\ \infty, & \text{otherwise} \end{cases}$$

$\rightarrow$ square-well potential

$$E_0 \to V_0 n \left(\frac{\hbar^2}{8mnV_0a^2}\right)^1 \;\curvearrowright\; E_0 = \frac{\hbar^2}{8ma^2}$$

For comparison, the exact ground-state energy of the square-well potential:

$$E_0 = \frac{\hbar^2 \pi^2}{2ma^2} \,.$$

Section 1.2.4

Solution 1.2.1 It is to be calculated:

$$w = \int_0^\infty w_\nu \, d\nu = \frac{8\pi}{c^3} \int_0^\infty \frac{h\,\nu^3}{\exp(\beta\, h\,\nu) - 1} \, d\nu \,.$$

Substitution:

$$x = \beta\, h\,\nu \implies \nu^3 \, d\nu = \frac{1}{(\beta\, h)^4} \, x^3 \, dx \,.$$

Intermediate result:

$$w = \frac{8\pi}{c^3\, h^3\, \beta^4} \int_0^\infty dx \, \frac{x^3}{e^x - 1} \,,$$

$$\int_0^\infty dx \, \frac{x^3}{e^x - 1} = \int_0^\infty dx\, x^3\, e^{-x} \sum_{n=0}^\infty (e^{-x})^n = \sum_{n=1}^\infty \int_0^\infty dx\, x^3\, e^{-nx} =$$

$$= \sum_{n=1}^\infty \frac{\Gamma(4)}{n^4} = 3! \sum_{n=1}^\infty \frac{1}{n^4} = 3! \, \frac{\pi^4}{90} \,.$$

The Stefan-Boltzmann law holds,

$$w = \alpha\, T^4 \,,$$

with the constant

$$\alpha = \frac{8}{15} \pi^5 \, \frac{k_B^4}{c^3\, h^3} = 7.5648 \cdot 10^{-16} \, \frac{\mathrm{J}}{\mathrm{m}^3\, \mathrm{K}^4} \,.$$

Solution 1.2.2 We have the transformation formula:

$$w_\lambda = w_{\nu(\lambda)} \left| \frac{d\nu}{d\lambda} \right| = \frac{c}{\lambda^2} \, w_{\nu(\lambda)} \,.$$

Therewith one easily calculates:

Wien:

$$w_\nu^w = \nu^3\, g\left(\frac{\nu}{T}\right) = \nu^3\, a\, e^{-b\frac{\nu}{T}}$$

$$\Longrightarrow\ w_{\nu(\lambda)}^w = a\,\frac{c^3}{\lambda^3}\, e^{-b\frac{c}{\lambda T}}$$

$$\Longrightarrow\ w_\lambda^w = a\,\frac{c^4}{\lambda^5}\, e^{-b\frac{c}{\lambda T}}\ .$$

Planck:

$$w_\nu^P = \frac{8\pi}{c^3}\,\nu^3\,\frac{h}{\exp(\beta\, h\,\nu) - 1}$$

$$\Longrightarrow\ w_\lambda^P = \frac{8\pi}{\lambda^5}\,\frac{h\,c}{\exp\left(\frac{h\,c}{\lambda\, k_B\, T}\right) - 1}\ .$$

For $\beta\, h\, c \gg \lambda$ we get approximately:

$$w_\lambda^P \approx 8\pi\,\frac{h\,c}{\lambda^5}\, e^{-\frac{h}{k_B}\frac{c}{\lambda T}}\ .$$

This corresponds to the Wien formula, if

$$a = \frac{8\pi\, h}{c^3}\ ;\quad b = \frac{h}{k_B}\ .$$

In contrast, the other limit $\beta\, h\, c \ll \lambda$ yields:

$$w_\lambda^P \approx 8\pi\, k_B\,\frac{T}{\lambda^4}\ .$$

That is exactly the Rayleigh formula!

Section 1.3.4

Solution 1.3.1 Number of particles in the volume element d^3r at $\mathbf{r}$ of the position space and d^3v at $\mathbf{v}$ of the velocity space:

$$dN(\mathbf{r},\mathbf{v}) = f(\mathbf{r},\mathbf{v})\, d^3r\, d^3v\ .$$

Spatial density:

$$n(\mathbf{r}) = \int f(\mathbf{r}, \mathbf{v})\, d^3v \ .$$

Homogeneous gas at thermal equilibrium:

$$n(\mathbf{r}) = n = \frac{N}{V} \ ,$$
$$f(\mathbf{r}, \mathbf{v}) \equiv f(\mathbf{v}) \equiv f(v) \ .$$

All particles of velocity $\mathbf{v}$, whose perpendicular distance from the wall is not larger than

$$\Delta x = v_x \, \Delta t$$

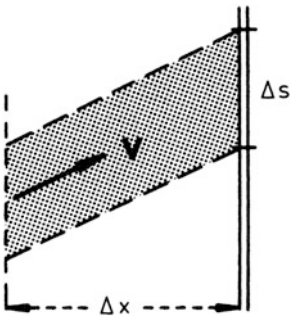
reach the wall in the time Δt. The area element ΔS is reached in the time Δt by

$$dN(\mathbf{v},\ \Delta S) = f(v)\, \Delta S\, v_x\, \Delta t\, d^3v$$

particles. These are the particles which are with suitable velocity in the cylinder sketched in Fig. A.1 Each particle transfers the momentum $2mv_x$ (= momentum change of the particle) onto the ideally reflecting wall.

$$\text{pressure} \ = \frac{\text{momentum transferred to the wall}}{\text{area} \cdot \text{time}}$$
$$\Longrightarrow \ dp(\mathbf{v}) = \frac{2m\, v_x\, dN\,(\mathbf{v}, \Delta S)}{\Delta S\, \Delta t} = 2m\, v_x^2 f(v)\, d^3v \ .$$

Fig. A.1



This means for the total pressure:

$$p = 2m \iint_{-\infty}^{+\infty} dv_y\, dv_z \int_0^{\infty} dv_x\, v_x^2 f(v)\, dv_x =$$

$$= m \int d^3v\, f(v)\, v_x^2 = \frac{1}{3} m \int d^3v\, f(v)\, \mathbf{v}^2 \quad \text{(isotropy)} .$$

Average square of the velocity:

$$\langle \mathbf{v}^2 \rangle = \frac{1}{n} \int d^3v\ \mathbf{v}^2 f(v) .$$

From that it finally follows:

$$p = \frac{1}{3} n\, m \langle \mathbf{v}^2 \rangle$$

Solution 1.3.2

1.

$$1 \stackrel{!}{=} f_0 \iint d^{3N}r\, d^{3N}v\, e^{-\beta H}$$

$$\Longrightarrow \quad f(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{v}_1, \ldots, \mathbf{v}_N) = \frac{e^{-\beta H}}{\iint d^{3N}r\, d^{3N}v\, e^{-\beta H}} .$$

This means for the velocity distribution:

$$w(\mathbf{v}_1, \ldots, \mathbf{v}_N) = \frac{e^{-\beta T}}{\int d^{3N}v\, e^{-\beta T}} ,$$

$$\int d^{3N}v\, e^{-\beta T} = \left(\int_{-\infty}^{+\infty} dv\, e^{-\beta \frac{m}{2} v^2} \right)^{3N} =$$

$$= \left(\frac{2}{m\beta} \right)^{\frac{3N}{2}} \left(\int_{-\infty}^{+\infty} dy\, e^{-y^2} \right)^{3N} = \left(\frac{2\pi}{m\beta} \right)^{\frac{3N}{2}} .$$

It follows:

$$w(\mathbf{v}_1, \dots \mathbf{v}_N) = \prod_{i=1}^{N} w_i(\mathbf{v}_i),$$

$$w_i(\mathbf{v}_i) = \left(\frac{m}{2\pi\, k_B T}\right)^{\frac{3}{2}} e^{-\frac{m v_i^2}{2k_B T}} .$$

2.

$$U = \langle H \rangle = \langle T \rangle = \int \dots \int d^{3N} r\, d^{3N} v \left(\frac{1}{2}\sum_{i=1}^{N} m\, v_i^2\right) f(\mathbf{r}_1 \dots \mathbf{r}_N, \mathbf{v}_1 \dots \mathbf{v}_N) =$$

$$= \int d^{3N} v \left(\frac{m}{2}\sum_{i=1}^{N} v_i^2\right) \prod_{j=1}^{N} w_j(\mathbf{v}_j) .$$

Since

$$\int d^3 v_i\, w_i\,(\mathbf{v}_i) = 1 ,$$

so that what remains to be calculated:

$$\begin{aligned} U &= N\frac{m}{2}\int d^3 v\, v^2 \left(\frac{m\beta}{2\pi}\right)^{3/2} e^{-\beta\frac{1}{2}m v^2} = \\ &= N\frac{m}{2}\left(\frac{m\beta}{2\pi}\right)^{3/2} 4\pi \int_0^{\infty} dv\, v^4\, e^{-\frac{\beta m}{2}v^2} = \\ &= N\frac{m}{2}\frac{4\pi}{\pi^{3/2}}\frac{2}{m\beta}\int_0^{\infty} dy\, y^4\, e^{-y^2} = N k_B T \frac{4}{\sqrt{\pi}}\frac{3}{8}\sqrt{\pi} \end{aligned}$$

$$\Longrightarrow\ U = \tfrac{3}{2} N k_B T$$

Solution 1.3.3 Equilibrium:

$$E = \frac{U}{d} = -\frac{m^* g}{q}$$

$$\Longrightarrow\ U = +\frac{2.4 \cdot 10^{-16}\,\mathrm{kg} \cdot 9.81\,\frac{\mathrm{J}}{\mathrm{m\,kg}} \cdot 1.5 \cdot 10^{-2}\,\mathrm{m}}{3 \cdot 1.6021 \cdot 10^{-19}\,\mathrm{A\,s}} = +73.5\,\mathrm{V} .$$

Solution 1.3.4 Fall velocity:

$$v_0 = \frac{\frac{4\pi}{3} r^3(\rho - \rho_\mathrm{L})g}{6\pi r\eta} = \frac{2}{9}\frac{r^2(\rho - \rho_\mathrm{L})\, g}{\eta}$$

$$\Longrightarrow \quad v_0 = \frac{2}{9}(0.39)^2\,\frac{0.98 - 0.001288}{183.2}\cdot 9.81\,\frac{\mathrm{cm}}{\mathrm{s}}\,,$$

$$v_0 \approx 0.002\,\frac{\mathrm{cm}}{\mathrm{s}}\,.$$

Solution 1.3.5 According to (1.46) it is to be calculated:

$$q = -n\,e = -\frac{18\pi(\eta\, v_0)^{3/2}}{E\sqrt{2(\rho - \rho_\mathrm{L})g}}\,.$$

With

$$1\,\mathrm{J} = 1\,\mathrm{V\,A\,s} = 10^7\,\frac{\mathrm{g\,cm^2}}{\mathrm{s^2}}$$

then:

$$n = \frac{1.6\cdot 18\pi(1.832\cdot 0.0029)^{3/2}\cdot 10^3}{1.602\cdot\sqrt{2(0.98 - 0.001288)\cdot 9.81}} \approx 5\,.$$

Radius:

$$r = \sqrt{\frac{9}{2}\,\frac{\eta\, v_0}{(\rho - \rho_\mathrm{L})g}} = \sqrt{\frac{9}{2}\,\frac{1.832\cdot 0.29}{9.81(0.98 - 0.001288)}}\cdot 10^{-4}\,\mathrm{cm}$$

$$\Longrightarrow \quad r \approx 0.5\,10^{-4}\,\mathrm{cm}\,.$$

Mass:

$$m^* = \frac{4\pi}{3}\,r^3(\rho - \rho_\mathrm{L}) \approx 0.51\cdot 10^{-12}\,\mathrm{g}\,.$$

Solution 1.3.6 The concept of the *classical electron radius* is based on the idea that the total rest mass of the electron is brought about by the electrostatic field of a sphere of the radius r_e, on the surface of which the elementary charge $-e$ is homogeneously distributed: According to ((2.48), Vol. 3), the energy reads:

$$W = \frac{\varepsilon_0}{2}\int d^3r|\mathbf{E}|^2 = \frac{\varepsilon_0}{2}\,\frac{e^2}{(4\pi\varepsilon_0)^2}\,4\pi\int_r^\infty dr\,\frac{r^2}{r^4} = \frac{1}{2}\,\frac{e^2}{4\pi\varepsilon_0\, r}\,.$$

The field is zero inside the sphere. One requires:

$$W \stackrel{!}{=} m_\mathrm{e}\, c^2 \implies r = \frac{1}{2}\, \frac{e^2}{(4\pi\varepsilon_0)\, m_\mathrm{e}\, c^2}\ .$$

If we had assumed that the charge $(-e)$ is distributed over the full sphere ((2.50), Vol. 3), then we would have found

$$r' = \frac{3}{5}\, \frac{e^2}{(4\pi\varepsilon_0)\, m_\mathrm{e}\, c^2}\ .$$

The two expressions differ only by the pre-factor. Furthermore, since both are based on not really justifiable hypotheses, it does not make very much sense to take the pre-factor too seriously. One therefore defines as *classical electron radius*:

$$r_\mathrm{e} = \frac{e^2}{(4\pi\varepsilon_0)\, m_\mathrm{e}\, c^2}\ .$$

Solution 1.3.7 L: Length of the capacitor.

1. Deflection by the electric field in the capacitor according to (1.49):

$$\Delta y \approx \frac{L\left(\frac{L}{2}+d\right)}{v^2}\, \left(\frac{q}{m}\right) E\ ,$$

v: particle velocity in z-direction.
Deflection by the magnetic field:

$$\frac{\Delta x}{\Delta z} = \frac{v_x}{v} \curvearrowright \Delta x \approx \left(\frac{L}{2}+d\right)\, \frac{v_x}{v}\ .$$

The magnetic field forces the charged particle onto a circular trajectory in the xz-plane. We assume, though, that the field is so weak that within the dimension L of the capacitor only a small part of the arc of the circular trajectory is performed. Then it holds, to a good approximation, for the Lorentz force:

$$\mathbf{F}_\mathrm{L} = q(\mathbf{v}\times\mathbf{B}) \approx -q\, B\, v\, \mathbf{e}_x = m\, \mathbf{a}\ ,$$

$$v_x = a_x\, t\ ,$$

$$t = \frac{L}{v}\ :\ \text{residence time within the region of the capacitor,}$$

$$v_x = -\frac{q}{m}\, B\, L\ .$$

This means:

$$\Delta x \approx -\left(\frac{L}{2}+d\right)\left(\frac{q}{m}\right) B\,\frac{L}{v}\,.$$

We eliminate v from the relations for Δx and Δy:

$$\begin{aligned} v^2 &= \frac{\left(\frac{L}{2}+d\right)^2}{(\Delta x)^2}\left(\frac{q}{m}\,B\,L\right)^2 \\ \Longrightarrow\quad \Delta y &= \alpha(\Delta x)^2\,, \\ \alpha &\approx \frac{1}{L\,d}\,\frac{E}{B^2}\left(\frac{m}{q}\right) \qquad (d \gg L)\,. \end{aligned}$$

2. High energy particles have a large v and therewith only small deviations $\Delta x,\ \Delta y$. Therefore they impinge on the screen closely to the apex of the parabola.
3. Relativistic mass increase of the energy-rich particles changes $\frac{m}{q}$ and therewith α. The curve on the screen becomes sharper closely to the apex than the parabola!

Solution 1.3.8 One recognizes with Fig. 1.18 for the particle positions for $t \to -\infty$ and $t \to +\infty$:

$$\begin{aligned} \boldsymbol{r}(-\infty) &= \big(-S_\alpha, p, 0\big)_{S_\alpha \to +\infty} \\ \boldsymbol{r}(+\infty) &= \big(S_\alpha\cos\varphi - p\sin\varphi, S_\alpha\sin\varphi + p\cos\varphi, 0\big)_{S_\alpha\to+\infty}\,. \end{aligned}$$

For the velocities it must hold (elastic scattering, motion in a fixed plane):

$$\begin{aligned} \dot{\mathbf{r}}(-\infty) &= \big(v_\infty, 0, 0\big) \\ \dot{\mathbf{r}}(+\infty) &= \big(v_\infty\cos\varphi, v_\infty\sin\varphi, 0\big)\,. \end{aligned}$$

Because of the central field, the angular momentum $\mathbf{L}$ represents a constant of motion. Therefore, we can calculate it, e.g., for $t \to -\infty$:

$$\mathbf{L} = m_\alpha\big(\mathbf{r}(-\infty)\times\dot{\mathbf{r}}(-\infty)\big) = -m_\alpha p\, v_\infty\,(0,0,1)\,.$$

One should check that the same result arises for $t \to +\infty$. For the Lenz vector we need:

$$\begin{aligned} \big(\dot{\mathbf{r}}\times\mathbf{L}\big)_{t\to-\infty} &= (v_\infty,0,0)\times(0,0,-m_\alpha p\, v_\infty) = m_\alpha p\, v_\infty^2(0,1,0) \\ V(r)\mathbf{r}(-\infty) &= \frac{\alpha}{r}(-S_\alpha, p, 0) \\ \big(\dot{\mathbf{r}}\times\mathbf{L}\big)_{t\to+\infty} &= (v_\infty\cos\varphi, v_\infty\sin\varphi, 0)\times(0,0,-m_\alpha p\, v_\infty) \end{aligned}$$

$$= (-m_\alpha p\, v_\infty^2 \sin\varphi, +m_\alpha p\, v_\infty^2 \cos\varphi, 0)$$
$$V(r)\mathbf{r}(+\infty) = \frac{\alpha}{r}(S_\alpha \cos\varphi - p\sin\varphi, S_\alpha \sin\varphi + p\cos\varphi, 0)\ .$$

When one now still exploits

$$S_\alpha \to \infty \quad \curvearrowright \quad \frac{S_\alpha}{r} = \frac{S_\alpha}{\sqrt{S_\alpha^2 + p^2}} \to +1\ ; \quad \frac{p}{r} \to 0\ ,$$

then one gets for the Lenz vectors:

$$\mathbf{A}(-\infty) = \big(-\alpha, m_\alpha p\, v_\infty^2, 0\big)$$
$$\mathbf{A}(+\infty) = \big(-m_\alpha p\, v_\infty^2 \sin\varphi + \alpha\cos\varphi, m_\alpha p\, v_\infty^2 \cos\varphi + \alpha\sin\varphi, 0\big)\ .$$

Since the Lenz vector is an integral of motion, it is to require

$$\mathbf{A}(-\infty) \stackrel{!}{=} \mathbf{A}(+\infty)\ .$$

This reads component by component:

$$-\alpha \stackrel{!}{=} -m_\alpha p\, v_\infty^2 \sin\varphi + \alpha\cos\varphi \tag{A.2}$$
$$m_\alpha p\, v_\infty^2 \stackrel{!}{=} m_\alpha p\, v_\infty^2 \cos\varphi + \alpha\sin\varphi\ . \tag{A.3}$$

Equation (A.2) leads to:

$$(1+\cos\varphi)\frac{1}{\sin\varphi} \equiv \cot\frac{\varphi}{2} = \frac{m_\alpha p\, v_\infty^2}{\alpha}\ .$$

When we further exploit the relation between α and b, which follows from (1.62),

$$\alpha = \frac{1}{2}\, b\, m_\alpha v_\infty^2\ ,$$

then we get the Rutherford scattering formula (1.65):

$$\cot\frac{\varphi}{2} = \frac{2p}{b}$$

With

$$\frac{\sin\varphi}{1-\cos\varphi} \equiv \cot\frac{\varphi}{2}$$

this formula follows of course also from Eq. (A.3).

Section 1.4.5

Solution 1.4.1 At first, the beams of rays of the single slits interfere as in Sect. 1.4.2 (see (1.70), (1.71)).

Principal maximum ($n = 0$: no path difference for the wave trains which propagate parallel to the axis of incidence):

$$\sin\alpha = 0 \,.$$

Maxima (*first order*):

$$\sin\alpha_n^{(1)} = (2n+1)\,\frac{\lambda}{2d}\,; \qquad n = 1, 2, \ldots \,.$$

Minima (*first order*):

$$\sin\alpha_n^{(1)} = n\frac{\lambda}{d}\,; \qquad n = 1, 2, \ldots \,.$$

In addition, there is still the interference of the beams of rays from the two different slits (Fig. A.2). Extinctions, for instance, sets in when the optical path difference between corresponding beams from slit 1 and slit 2 just amounts to $\lambda/2$. In general, we find:

Maxima (*second order*):

$$\sin\alpha_n^{(2)} = n\,\frac{\lambda}{a}\,; \qquad n = 1, 2, \ldots \,.$$

Minima (*second order*):

$$\sin\alpha_n^{(2)} = (2n+1)\,\frac{\lambda}{2a}\,; \qquad n = 0, 1, \ldots \,.$$

The principal maximum exhibits for $a = 2d$ four dark stripes, corresponding to the minima of second class for $n = 0$ and $n = 1$.

Fig. A.2

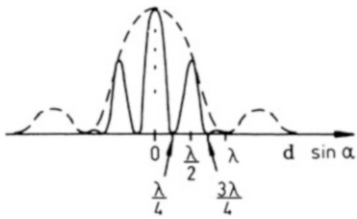
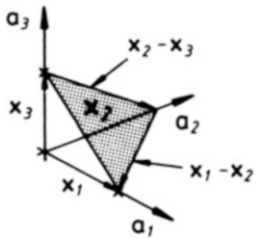


Fig. A.3



Solution 1.4.2 The (p_1, p_2, p_3)-plane has in the direct lattice the following intersection points with the axes:

$$\mathbf{x}_i = \frac{\alpha}{p_i}\,\mathbf{a}_i\,; \qquad i = 1, 2, 3\,.$$

Each vector **in** the plane can be written as (Fig. A.3):

$$\mathbf{r(p)} = \gamma_1(\mathbf{x}_1 - \mathbf{x}_2) + \gamma_2(\mathbf{x}_2 - \mathbf{x}_3)\,.$$

One then easily shows with (1.82):

$$\mathbf{K^p} \cdot \mathbf{r(p)} = 0\,.$$

Since $\mathbf{r(p)}$ could be chosen arbitrarily, the assertion is therewith proven.

Solution 1.4.3 We have shown in Exercise 1.4.2 that

$$\boldsymbol{\kappa} = \frac{\mathbf{K^p}}{|\mathbf{K^p}|}$$

is the normal-unit vector of the (p_1, p_2, p_3)-plane. A certain (p_1, p_2, p_3)-plane of the distance Δ from the origin of coordinates is then defined by such lattice vectors $\mathbf{R^n}$, for which:

$$\Delta = \boldsymbol{\kappa} \cdot \mathbf{R^n} = \frac{2\pi}{|\mathbf{K^p}|}\,(p_1 n_1 + p_2 n_2 + p_3 n_3) = \frac{2\pi}{|\mathbf{K^p}|}\,N\,; \quad N \in \mathbb{Z}\,.$$

p_1, p_2, p_3 are relatively prime integers. Therewith, N as well as the n_i run through **all** integers. The distance between neighboring planes is therefore

$$d = \Delta_{N+1} - \Delta_N\,,$$

which corresponds to the assertion (1.84).

Solution 1.4.4 For the primitive translations of the reciprocal lattice we have, very generally:

$$b_i^2 = \frac{4\pi^2}{a_i^2}\,\frac{a_1^2 a_2^2 a_3^2}{V_z^2}\,\sin^2\alpha_i\ ;$$
$$\alpha_i = \sphericalangle(\mathbf{a}_j, \mathbf{a}_k) \qquad (i,j,k) = (1,2,3) \text{ and cyclic.}$$

The interplanar spacing amounts to:

$$d(p_1,p_2,p_3) = \frac{V_z}{a_1 a_2 a_3}\left\{\frac{p_1^2}{a_1^2}\sin^2\alpha_1 + \frac{p_2^2}{a_2^2}\sin^2\alpha_2 + \frac{p_3^2}{a_3^2}\sin^2\alpha_3\right\}^{-\frac{1}{2}}.$$

These expressions simplify for orthorhombic lattices ($\alpha_i = \pi/2;\ i = 1,2,3$). The Bragg law (1.86) then reads:

$$\sin^2\vartheta = \frac{n^2\lambda^2}{4}\left(\frac{p_1^2}{a_1^2} + \frac{p_2^2}{a_2^2} + \frac{p_3^2}{a_3^2}\right).$$

For cubic lattices, we can use eventually as further simplification $a_1 = a_2 = a_3 = a$.

Solution 1.4.5

$$\nu_\mathrm{g} = \frac{c}{\lambda_\mathrm{g}} = \left(3\cdot 10^8 \frac{\mathrm{m}}{\mathrm{s}}\right)(6400\cdot 10^{-10}\mathrm{m})^{-1} = 4.69\cdot 10^{14}\,\mathrm{s}^{-1}\ ,$$
$$W = h\,\nu_\mathrm{g} = 6.624\cdot 10^{-34}\,\mathrm{J\,s}\cdot 4.69\cdot 10^{14}\,\mathrm{s}^{-1} = 3.11\cdot 10^{-19}\,\mathrm{J} = 1.94\,\mathrm{eV}\ .$$

Solution 1.4.6

$$\vartheta = \frac{\pi}{2} \implies \Delta\lambda = \lambda_\mathrm{c} \implies \frac{\Delta\lambda}{\lambda_0} = \frac{\lambda_\mathrm{c}}{\lambda_0} = \frac{0.024263\,\text{Å}}{\lambda_0}\ .$$

1.

$$\frac{\Delta\lambda}{\lambda_0} = 6.06575\cdot 10^{-6} = 0.6\cdot 10^{-3}\,\%\ ;$$

2.

$$\frac{\Delta\lambda}{\lambda_0} = 0.0485 = 4.85\,\%\ ,$$

3.

$$\frac{\Delta\lambda}{\lambda_0} = 1.2132 = 121.32\,\%\ .$$

Recoil energy of the electron:

$$\frac{\Delta T}{h\nu_0} = \frac{h\Delta\nu}{h\nu_0} = 1 - \frac{\nu}{\nu_0} = 1 - \frac{\lambda_0}{\lambda} = \frac{\Delta\lambda}{\lambda_0 + \Delta\lambda} = \frac{\frac{\Delta\lambda}{\lambda_0}}{1 + \frac{\Delta\lambda}{\lambda_0}}$$

$$\Longrightarrow \quad 1)\ \frac{\Delta T}{h\nu_0} = 0.0000061\ ; \quad 2)\ \frac{\Delta T}{h\nu_0} = 0.04626\ ; \quad 3)\ \frac{\Delta T}{h\nu_0} = 0.54817\ .$$

Normally the *recoil electrons* can easily be distinguished from the *photoelectrons*, which, by absorption of a photon, always receive an energy of the order of magnitude of $h\nu_0$.

Solution 1.4.7 Intensity of the incident radiation

$$I = 0.01\,\frac{\mathrm{W}}{\mathrm{m}^2}$$

'area of the atom': $A = 0.01\,\mathrm{nm}^2 = 1 \cdot 10^{-20}\,\mathrm{m}^2$

(a) Work P = energy per time
Intensity I = work per area = $\frac{P}{A}$

$$\curvearrowright \quad P = I \cdot A = 0.01 \cdot 10^{-20}\,\mathrm{W} = 10^{-22}\,\mathrm{W}$$

as the energy which impinges per second onto the *'area of the atom'*.

(b) Work function $W_W = 2\,\mathrm{eV}$

$$1\,\mathrm{W} = 1\,\frac{\mathrm{J}}{\mathrm{s}}$$

$$1\,\mathrm{eV} = 1.602 \cdot 10^{-19}\,\mathrm{J}$$

$$10^{-22}\,\frac{\mathrm{J}}{\mathrm{s}} = 6.25 \cdot 10^{-4}\,\frac{\mathrm{eV}}{\mathrm{s}}$$

The energy $6.25 \cdot 10^{-4}\,\mathrm{eV}$ impinges per second. In order to gather 2 eV, a time of

$$\Delta t = \frac{2\,\mathrm{eV}}{6.25 \cdot 10^{-4}\,\frac{\mathrm{eV}}{\mathrm{s}}} = 3200\,\mathrm{s} = 53.3\,\mathrm{min}$$

would be necessary. This is the classically to be expected *time delay* until the release of the photoelectron. However, that is **not** observed in the experiment!

Solution 1.4.8 Compton effect:

$$\Delta\lambda = \lambda_c(1-\cos\vartheta)\,; \qquad \lambda_c = \frac{h}{mc}: \quad \text{'Compton wave length'}$$

$h = 6.624 \cdot 10^{-34}\,\mathrm{J\,s}$
$m = 9.11 \cdot 10^{-31}\,\mathrm{kg}$
$c = 2.997 \cdot 10^{10}\,\frac{\mathrm{cm}}{\mathrm{s}}$

$$\curvearrowright \quad \lambda_c = 2.426 \cdot 10^{-2}\,\mathring{\mathrm{A}}$$

1.

$$\vartheta = \frac{\pi}{2} \quad \curvearrowright \quad \Delta\lambda = \lambda_c$$
$$\Delta\lambda = 2.426 \cdot 10^{-2}\,\mathring{\mathrm{A}}$$

2. Energy conservation law:

$$h\nu_0 + mc^2 = h\nu + \sqrt{c^2p_r^2 + m^2c^4}$$

Transferred kinetic energy:

$$\begin{aligned}\Delta T &= \sqrt{c^2p_r^2 + m^2c^4} - mc^2\\ &= h(\nu_0 - \nu)\\ &= hc\left(\frac{1}{\lambda} - \frac{1}{\lambda+\Delta\lambda}\right)\\ &= \frac{hc\Delta\lambda}{\lambda(\lambda+\Delta\lambda)}\end{aligned}$$

$\lambda = 1\,\mathring{\mathrm{A}} = 10^{-10}\,\mathrm{m}\,; \quad \Delta\lambda = 2.426 \cdot 10^{-12}\,\mathrm{m}$

$$\curvearrowright \quad \Delta T = \frac{6.624 \cdot 10^{-34}\,\mathrm{J\,s} \cdot 2.997 \cdot 10^{8}\,\frac{\mathrm{m}}{\mathrm{s}} \cdot 2.426 \cdot 10^{-12}\,\mathrm{m}}{10^{-10}\,\mathrm{m} \cdot (1+0.02426) \cdot 10^{-10}\,\mathrm{m}}$$
$$= 4.72 \cdot 10^{-17}\,\mathrm{J} = 295\,\mathrm{eV}$$

3. Initial photon energy:

$$h\nu_0 = \frac{hc}{\lambda} = \frac{6.624 \cdot 10^{-34}\,\mathrm{J\,s} \cdot 2.997 \cdot 10^{8}\,\frac{\mathrm{m}}{\mathrm{s}}}{10^{-10}\,\mathrm{m}} = 1.985 \cdot 10^{-15}\,\mathrm{J}$$

Relative loss:

$$\frac{h(\nu_0 - \nu)}{h\nu_0} = 2.38 \cdot 10^{-2}$$

Section 1.5.4

Solution 1.5.1 Classically:

$$E = \frac{1}{2} J \omega^2 = 2\pi^2 J \nu^2 \implies \nu = \frac{1}{\pi} \frac{1}{\sqrt{2J}} \sqrt{E} \,.$$

Principle of correspondence:

$$\int \frac{dE}{\nu} = \pi\sqrt{2J} \int \frac{dE}{\sqrt{E}} = 2\pi\sqrt{2J}\,\sqrt{E} \stackrel{!}{=} h(n+\alpha) \quad \text{(see (1.129))}$$

$$\implies E_n = \frac{1}{2J} \hbar^2 (n+\alpha)^2 \,.$$

The energy levels of the rigid rotator move apart quadratically with increasing principal quantum number. The experimental rotation spectra of molecules suggest $\alpha = 0$.

Solution 1.5.2 The classical eigen-frequency of the harmonic oscillator,

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}} = \frac{\omega_0}{2\pi} \quad (k\text{: spring constant}) \,,$$

is independent of E. The quantum condition (1.129) therefore yields immediately:

$$E_n = \hbar\omega_0 \,(n+\alpha) \,; \quad n = 0, 1, 2, \ldots \,.$$

The experiment (*molecular vibrations*) in this case leads to $\alpha = (1/2)$.

Solution 1.5.3 Coulomb force:

$$\frac{e^2}{4\pi\varepsilon_0 r^2} \,.$$

Centrifugal force:

$$mr\omega^2 = mr\dot{\varphi}^2 \,.$$

Quantum condition:

$$\int p\,dq = \int mvr\,d\varphi = \int \underbrace{mr^2\dot{\varphi}}_{=L_z=\text{const}}\,d\varphi = 2\pi mr^2\dot{\varphi} \stackrel{!}{=} h\,n$$

$$\Longrightarrow\quad \dot{\varphi} = \frac{\hbar}{mr^2}\,n\ .$$

Equilibrium:

$$\frac{e^2}{4\pi\varepsilon_0 r^2} \stackrel{!}{=} mr\dot{\varphi}^2 = mr\frac{\hbar^2}{m^2r^4}\,n^2$$

$$\Longrightarrow \text{ Bohr radii: } \quad r_n = \frac{\hbar^2(4\pi\varepsilon_0)}{me^2}\,n^2\ .$$

Radius of the first Bohr orbit:

$$r_1 = a_\mathrm{B} = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529\,\text{Å}\ .$$

Rotational frequency:

$$\dot{\varphi}_n = \omega_n = \frac{\hbar}{mr_n^2}\,n\ ,$$

$$\omega_n = \frac{me^4}{(4\pi\varepsilon_0)^2\,\hbar^3}\,\frac{1}{n^3}\ ,$$

in particular:

$$\omega_1 = 4.06\cdot 10^{16}\,\frac{1}{\mathrm{s}}\ .$$

Section 2.1.4

Solution 2.1.1

1. According to (2.20): $\lambda(e^-) \approx 12.25$ Å.
2. For this energy it must be relativistically calculated:

$$\text{((2.63), Vol. 4):}\quad E = \sqrt{c^2p^2 + m_\mathrm{e}^2\,c^4}$$

$$\Longrightarrow\quad c^2p^2 = E^2 - \left(m_\mathrm{e}\,c^2\right)^2\ ,$$

$$m_e c^2 = 0.5110\,\text{MeV} \qquad \text{(see (1.58))}$$
$$\Longrightarrow\ E^2 \gg \left(m_e c^2\right)^2 \ \Longrightarrow\ p \approx \frac{E}{c}\,.$$

De Broglie-wave length: $\lambda = h\,c/E$

$$\Longrightarrow\ \lambda \approx \frac{12.4}{E[\text{keV}]} \qquad \text{(see (2.22))}\,,$$
$$\lambda \approx 1.24 \cdot 10^{-4}\,\text{Å} = 12.4\,\text{fm}$$
$$(1\ \text{Fermi} = 1\,\text{fm} = 10^{-15}\,\text{m})\,.$$

3.

$$k_B \approx 0.862 \cdot 10^{-4}\,\frac{\text{eV}}{\text{K}}$$
$$\Longrightarrow\ k_B T \approx 0.0259\,\text{eV} \qquad \text{at}\quad T = 300\,\text{K}$$
$$\Longrightarrow\ \lambda(n) \approx \frac{0.28}{\sqrt{0.0259}}\,\text{Å} \approx 1.741\,\text{Å}\,.$$

Solution 2.1.2 m_e: rest mass of the electron.

Kinetic energy:

$$E = mc^2 - m_e c^2 = m_e c^2 \left(\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right)$$

$$\Longrightarrow\ 1 - \frac{v^2}{c^2} = \left(\frac{m_e c^2}{E + m_e c^2} \right)^2$$
$$\Longrightarrow\ v = c\,\frac{\sqrt{E^2 + 2E\,m_e c^2}}{E + m_e c^2}\,.$$

De Broglie-wave length:

$$\lambda = \frac{h}{p} = \frac{h}{m_e v}\sqrt{1 - \frac{v^2}{c^2}} = \frac{h}{v}\,\frac{c^2}{E + m_e c^2} = \frac{h\,c}{\sqrt{E^2 + 2E\,m_e c^2}}$$
$$\Longrightarrow\ \lambda = \frac{h}{\sqrt{2m_e E}}\,\frac{1}{\sqrt{1 + \frac{E}{2m_e c^2}}}\,.$$

This means with $2m_e c^2 = 1.022 \cdot 10^6\,\text{eV}$:

$$\lambda \approx \frac{12.25}{\sqrt{E[\text{eV}]}} \frac{1}{\sqrt{1 + 0.978 \cdot 10^{-6} \cdot E[\text{eV}]}} .$$

Solution 2.1.3 Bragg law:

$$2d \sin\vartheta = n\lambda ; \qquad n = 1, 2, \ldots .$$

Thermal neutrons (see Exercise 2.1.1, part 3.):

$$\begin{aligned} \lambda &= 1.741\,\text{Å} \\ \Longrightarrow \quad \sin\vartheta &= n \cdot 0.249 . \end{aligned}$$

Deflection angle:

$$\begin{aligned} n = 1: &\quad \vartheta = 14.4^\circ , \\ n = 2: &\quad \vartheta = 29.8^\circ , \\ n = 3: &\quad \vartheta = 48.3^\circ , \\ n = 4: &\quad \vartheta = 84.2^\circ . \end{aligned}$$

Section 2.2.7

Solution 2.2.1

1. The total probability of finding is given by

$$\int d^3r |\psi(\mathbf{r}, t)|^2 ,$$

where the integral is extended over the entire space:

$$\int d^3r |\psi(\mathbf{r}, t)|^2 = \frac{1}{(\pi\, b^2(t))^{3/2}} \int d^3r\, e^{-\frac{(\mathbf{r}-\mathbf{v}_0 t)^2}{b^2(t)}} = \frac{1}{\pi^{3/2}} \int d^3r'\, e^{-\mathbf{r}'^2} .$$

Trick of integration:

$$\left(\int_{-\infty}^{+\infty} dx\, e^{-x^2}\right)^2 = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy\, e^{-(x^2+y^2)} = \int_0^{2\pi} d\varphi \int_0^{\infty} r\, dr\, e^{-r^2} =$$

$$= 2\pi \left(-\frac{1}{2}\, e^{-r^2}\right)\Big|_0^{\infty} = \pi \ .$$

This means:

$$\int_{-\infty}^{+\infty} dx\, e^{-x^2} = \sqrt{\pi}\ ; \quad \int d^3r\, e^{-r^2} = \pi^{3/2} \ .$$

It is shown therewith that the probability of finding is normalized to one:

$$\int d^3r |\psi(\mathbf{r}, t)|^2 = 1 \ .$$

2. The most probable position $\mathbf{r}^*$ is given by the maximum of $|\psi(\mathbf{r}, t)|^2$:

$$\mathbf{r}^* = \mathbf{v}_0\, t \ .$$

Solution 2.2.2

1.

$$1 \stackrel{!}{=} \int_{-\infty}^{+\infty} dz |\psi(z, 0)|^2 = A^2 \int_{-\infty}^{+\infty} dz\, e^{-\frac{z^2}{b^2}} = A^2 \sqrt{\pi\, b^2}$$

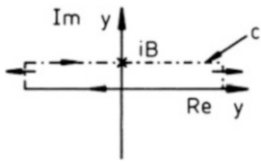
$$\Longrightarrow\ A = \left(\pi\, b^2\right)^{-\frac{1}{4}} \ .$$

2. Fourier inversion (Sect. 4.3.6, Vol. 3):

$$\widehat{\psi}(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dz\, \psi(z, 0)\, e^{-ikz} =$$

$$= \frac{A}{2\pi} \int_{-\infty}^{+\infty} dz\, \exp\left\{-\frac{z^2}{2b^2} - i(k - k_0)z\right\} \ .$$

Fig. A.4



Substitution:

$$y = \frac{z}{\sqrt{2}\,b} + i(k-k_0)\frac{b}{\sqrt{2}}$$

$$\Longrightarrow\ \widehat{\psi}(k) = \frac{A}{2\pi}\, e^{-B^2}\, b\sqrt{2} \int\limits_{-\infty+iB}^{+\infty+iB} dy\, e^{-y^2}\ ,$$

$$B = (k-k_0)\,\frac{b}{\sqrt{2}}\ .$$

Complex integration (Sect. 4.4.5, Vol. 3):

In the region enclosed by the path C (Fig. A.4) e^{-y^2} is holomorphic everywhere. Then it follows according to the residue theorem ((4.4.2.), Vol. 3):

$$\oint\limits_{C} dy\, e^{-y^2} = 0 = \int\limits_{-\infty+iB}^{+\infty+iB} dy\, e^{-y^2} + \int\limits_{+\infty}^{-\infty} dy\, e^{-y^2} = \int\limits_{-\infty+iB}^{+\infty+iB} dy\, e^{-y^2} - \sqrt{\pi}\ .$$

Hence we have:

$$\widehat{\psi}(k) = \frac{A\,b}{\sqrt{2\pi}} \exp\left(-\frac{b^2}{2}(k-k_0)^2\right)\ .$$

3. The maximum of

$$|\widehat{\psi}(k)|^2 = \frac{b^2A^2}{2\pi}\, e^{-b^2(k-k_0)^2}$$

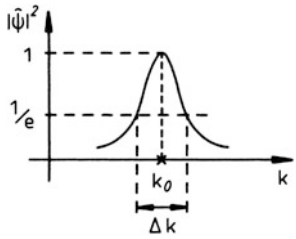
is obviously at $k = k_0$. For the width we have (Fig. A.5):

$$\Delta k = \frac{2}{b}\ .$$

4.

$$\psi(z,t) = \frac{b\,A}{\sqrt{2\pi}} \int\limits_{-\infty}^{+\infty} dk\ e^{-\frac{b^2}{2}(k-k_0)^2}\, e^{ikz}\, e^{-i\frac{\hbar k^2}{2m}t}\ .$$

Fig. A.5



With the abbreviations

$$C(t) = \sqrt{\frac{1}{2}b^2 + i\frac{\hbar}{2m}t}\,,$$

$$D(z,t) = \frac{k_0 b^2 + i\,z}{2C(t)}$$

it remains to be calculated:

$$\psi(z,t) = \frac{b\,A}{\sqrt{2\pi}}\,\exp\left(D^2 - \frac{1}{2}b^2k_0^2\right)\int_{-\infty}^{+\infty} dk\,\exp\left[-(k\,C - D)^2\right]\,.$$

With the substitution

$$y = k\,C - D \qquad (C, D:\ \text{complex})$$

and a complex integration similar to that in part 2., -one has to choose a suitable path C-, it follows:

$$\psi(z,t) = \frac{b\,A}{\sqrt{2}\,C(t)}\,\exp\left\{D^2(z,t) - \frac{1}{2}b^2k_0^2\right\}\,.$$

5.

$$|\psi(z,t)|^2 = \frac{b^2A^2}{2|C|^2}\,\exp\left[2\,\mathrm{Re}\,\left(D^2 - \frac{1}{2}b^2k_0^2\right)\right]\,,$$

$$b\,A^2 = \frac{1}{\sqrt{\pi}}\,,$$

$$|C|^2 = C\,C^* = \sqrt{\frac{1}{4}b^4 + \frac{1}{4}\left(\frac{\hbar}{m}t\right)^2} = \frac{b}{2}\Delta b(t)\,,$$

$$D^2 = \frac{1}{4}\,\frac{k_0^2 b^4 - z^2 + i\,2z\,k_0 b^2}{\frac{1}{2}b^2 + i\frac{\hbar}{2m}t}$$

$$\begin{aligned}
\Longrightarrow \quad \mathrm{Re}\, D^2 &= \frac{\frac{1}{2}b^2(k_0^2 b^4 - z^2) + 2z\,k_0 b^2 \frac{\hbar}{2m}t}{b^4 + \left(\frac{\hbar}{m}t\right)^2} = \\
&= \frac{1}{2(\Delta b(t))^2}\left(k_0^2 b^4 - z^2 + 2z\,k_0 \frac{\hbar}{m}t\right) \\
\Longrightarrow \quad 2\,\mathrm{Re}\left(D^2 - \frac{1}{2}b^2 k_0^2\right) &= \\
&= \frac{1}{(\Delta b(t))^2}\left[k_0^2 b^4 - z^2 + 2z\,k_0 \frac{\hbar}{m}t - b^4 k_0^2 - k_0^2\left(\frac{\hbar}{m}t\right)^2\right] = \\
&= \frac{-1}{(\Delta b(t))^2}\left(z - \frac{\hbar\,k_0}{m}t\right)^2 .
\end{aligned}$$

At the end, it follows therewith:

$$|\psi(z,t)|^2 = \frac{1}{\sqrt{\pi}\,\Delta b(t)} \exp\left\{-\frac{\left(z - \frac{\hbar\,k_0}{m}t\right)^2}{(\Delta b(t))^2}\right\}$$

The width of the wave packet $2\Delta b(t)$ thus changes as function of time!

Solution 2.2.3

1. Width of the wave packet:

$$\begin{aligned}
2\Delta b(t) &= \frac{2}{b}\sqrt{b^4 + \left(\frac{\hbar}{m}t\right)^2}\,, \\
2\Delta b(0) &= 2b\,, \\
\\
\Delta b(t_2) &\stackrel{!}{=} 2\Delta b(0) = 2b \\
\Longleftrightarrow \quad 4b^2 &= \frac{1}{b^2}\left[b^4 + \left(\frac{\hbar}{m}t_2\right)^2\right] \\
\Longleftrightarrow \quad 3b^4 &= \left(\frac{\hbar}{m}\right)^2 t_2^2 \\
\Longleftrightarrow \quad t_2 &= \sqrt{3}\,b^2\,\frac{m}{\hbar}\,.
\end{aligned}$$

2. Length of run:

$$S_2 = \frac{p}{m} t_2 = \sqrt{3}\, b^2 \frac{p}{\hbar} .$$

3.

$$\begin{aligned} \hbar &= 1.055 \cdot 10^{-34}\,\mathrm{J\,s} , \\ M_\mathrm{p} &= 1.673 \cdot 10^{-27}\,\mathrm{kg} \\ \Longrightarrow \quad \frac{p}{\hbar} &= \sqrt{\frac{2M_\mathrm{p}\,T}{\hbar^2}} = \left\{ \frac{2 \cdot 1.673 \cdot 10^{-27}\,\mathrm{kg} \cdot 10^6 \cdot 1.602 \cdot 10^{-19}\,\mathrm{J}}{(1.055)^2 \cdot 10^{-68}\mathrm{J}^2\,\mathrm{s}^2} \right\}^{1/2} = \\ &= 2.195 \cdot 10^{14}\,\mathrm{m}^{-1} = 2.195 \cdot 10^4\,\mathring{\mathrm{A}}^{-1} , \\ S_2 &= 3.802\,\mathring{\mathrm{A}} . \end{aligned}$$

Solution 2.2.4

1.

$$\begin{aligned} m_\mathrm{e} &= 9.1096 \cdot 10^{-31}\,\mathrm{kg} , \\ \frac{\hbar}{m_\mathrm{e}} &= 1.158 \cdot 10^{-4}\,\frac{\mathrm{m}^2}{\mathrm{s}} . \end{aligned}$$

Width after 1 s:

$$2\Delta b(1) = 4\sqrt{(0.5)^4 + 1.3410 \cdot 10^{32}}\,\mathring{\mathrm{A}} \approx 4.632 \cdot 10^6\,\mathrm{m} = 4632\,\mathrm{km} .$$

The diffluence of the wave packet thus takes place remarkably rapidly.

2.

$$\frac{p}{m_\mathrm{e}} = \sqrt{\frac{2E}{m_\mathrm{e}}} = \left(\frac{200 \cdot 1.602 \cdot 10^{-19}\,\mathrm{J}}{9.1096 \cdot 10^{-31}\,\mathrm{kg}} \right)^{1/2} = 5.931 \cdot 10^6\,\frac{\mathrm{m}}{\mathrm{s}} .$$

Flight time for 10 cm:

$$\begin{aligned} t_0 &= 1.686 \cdot 10^{-8}\,\mathrm{s} \\ \Longrightarrow \quad \frac{\hbar}{m_\mathrm{e}} t_0 &= 1.953 \cdot 10^8\,\mathring{\mathrm{A}}^2 . \end{aligned}$$

Width of the wave packet:

$$2\Delta b(t_0) \approx 7.810\,\mathrm{cm} .$$

3.

$$2\Delta b(1) = 4 \cdot 10^3 \sqrt{(0.5)^4 \cdot 10^{-12} + 1.341}\ \text{cm} \approx 46.321\ \text{m}\ .$$

The diffluence of the wave packet is even now still very rapid. But, because of

$$b^2 = 0.25 \cdot 10^{10} \mathring{\text{A}}^2 \gg \frac{\hbar}{m_\text{e}} t_0\ ,$$

the packet has after the flight distance of 10 cm practically still the same width as at the beginning.

Solution 2.2.5

1. Calculation of the normalization constant

$$|\psi|^2 = A^2 r^2 e^{-(r/a)} \sin^2\vartheta \quad \text{w. l. o. g.: } A \text{ real}$$

Normalization constant:

$$\begin{aligned}
1 &\stackrel{!}{=} \int d^3r\, |\psi(\mathbf{r},t)|^2 \\
&= 2\pi A^2 \int_0^\infty dr\, r^4 e^{-\frac{r}{a}} \underbrace{\int_{-1}^{+1} d\cos\vartheta\ \left(1-\cos^2\vartheta\right)}_{2-\frac{2}{3}=\frac{4}{3}} \\
&= \frac{8\pi}{3} A^2 a^5 \underbrace{\int_0^\infty dx\, x^4 e^{-x}}_{\Gamma(5)=4!=24} \\
&= 64\pi A^2 a^5 \\
\curvearrowright\ A &= \frac{1}{8\sqrt{\pi a^5}}
\end{aligned}$$

2. Probability-current density:

$$\begin{aligned}
\mathbf{j}(\mathbf{r},t) &= \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \\
&= \frac{\hbar}{m}\Im\left(\psi^*(\mathbf{r},t)\nabla\psi(\mathbf{r},t)\right)
\end{aligned}$$

Spherical coordinates:

$$\nabla \equiv \left(\frac{\partial}{\partial r}, \frac{1}{r}\frac{\partial}{\partial \vartheta}, \frac{1}{r\sin\vartheta}\frac{\partial}{\partial \varphi}\right)$$

$$\curvearrowright\ j_r = \frac{\hbar}{m}\mathrm{Im}\underbrace{\left(A^2\sin^2\vartheta\left(re^{-\frac{r}{2a}}\frac{\partial}{\partial r}re^{-\frac{r}{2a}}\right)\right)}_{\text{real}}$$

$$= 0$$

$$\text{analogously: } j_\vartheta = 0$$

$$j_\varphi(\mathbf{r},t) = \frac{\hbar}{m}A^2r^2\sin^2\vartheta e^{-\frac{r}{a}}\mathrm{Im}\left(e^{-i\varphi}\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}e^{i\varphi}\right)$$

$$= \frac{\hbar}{m}A^2r\sin\vartheta e^{-\frac{r}{a}}$$

3. Time-dependent Schrödinger equation:

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

$$\curvearrowright\ E = -\frac{\hbar^2}{8ma^2}$$

4. Schrödinger equation:

$$\widehat{H}\psi(\mathbf{r},t) = E\psi(\mathbf{r},t)$$

$$= \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r})\right)\psi(\mathbf{r},t)$$

Laplace operator in spherical coordinates:

$$\Delta = \Delta_r + \Delta_{\vartheta,\varphi}$$

$$\Delta_r = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}$$

$$\Delta_{\vartheta,\varphi} = \frac{1}{r^2\sin^2\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{\partial^2}{\partial\varphi^2}\right)$$

$$\frac{d}{dr}re^{-\frac{r}{2a}} = \left(1 - \frac{r}{2a}\right)e^{-\frac{r}{2a}}$$

$$\frac{d^2}{dr^2}re^{-\frac{r}{2a}} = \left(-\frac{1}{2a} - \frac{1}{2a} + \frac{r}{4a^2}\right)e^{-\frac{r}{2a}}$$

$$\curvearrowright \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right) re^{-\frac{r}{2a}} = \left(-\frac{1}{a}+\frac{r}{4a^2}+\frac{2}{r}-\frac{1}{a}\right) e^{-\frac{r}{2a}}$$

$$\curvearrowright \Delta_r \psi = \left(-\frac{2}{ra}+\frac{1}{4a^2}+\frac{2}{r^2}\right)\psi$$

$$\begin{aligned}\sin\vartheta \frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)\sin\vartheta &= \sin\vartheta\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\cos\vartheta\right)\\ &= \sin\vartheta\left(\cos^2\vartheta-\sin^2\vartheta\right)\\ &= \sin\vartheta\left(1-2\sin^2\vartheta\right)\end{aligned}$$

$$\begin{aligned}\curvearrowright \Delta_{\vartheta,\varphi}\psi &= \frac{1}{r\sin^2\vartheta}\left(1-2\sin^2\vartheta-1\right)\psi\\ &= -\frac{2}{r^2}\psi\end{aligned}$$

It remains:

$$\Delta\psi = \left(-\frac{2}{ra}+\frac{1}{4a^2}\right)\psi$$

It follows then from the Schrödinger equation:

$$V(\mathbf{r})\psi = \left(-\frac{\hbar^2}{8ma^2}-\frac{\hbar^2}{mra}+\frac{\hbar^2}{8ma^2}\right)\psi$$

$$\curvearrowright V(\mathbf{r}) = -\frac{k}{r}$$

Hydrogen, i.e., Kepler problem with $k = \dfrac{\hbar^2}{ma}$ and $a = \dfrac{4\pi\varepsilon_0\hbar^2}{me^2}$ Bohr radius

$$\curvearrowright k = \frac{e^2}{4\pi\varepsilon_0}$$

Solution 2.2.6

1. Normalization

$$\begin{aligned}1 &= A^2\int_0^\infty dx\, x^2 e^{-2\alpha x}\\ &= A^2\frac{1}{4}\frac{d^2}{d\alpha^2}\int_0^\infty dx\, e^{-2\alpha x}\end{aligned}$$

$$= A^2 \frac{1}{4} \frac{d^2}{d\alpha^2} \frac{1}{2\alpha}$$
$$= A^2 \frac{1}{4\alpha^3}$$
$$\curvearrowright \; A = 2\alpha^{\frac{3}{2}}$$

2. Fourier transformation:

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx \, e^{-\frac{i}{\hbar}px} \psi(x)$$
$$= \frac{A}{\sqrt{2\pi\hbar}} \int_{0}^{+\infty} dx \, e^{-\frac{i}{\hbar}px} x e^{-\alpha x}$$

It follows with $y = (\alpha + \frac{i}{\hbar}p)x$:

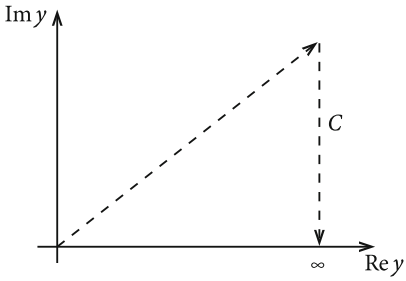
$$\curvearrowright \; \psi(p) = \frac{2\alpha^{\frac{3}{2}}}{\sqrt{2\pi\hbar}} \cdot \frac{1}{\left(\alpha + \frac{i}{\hbar}p\right)^2} \underbrace{\int_{0}^{\infty + i\infty} dy \, y e^{-y}}_{\text{complex integration}}$$

Since the integral $\oint_C dy \, y e^{-y} = 0$ (Fig. A.6) vanishes:

$$\int_{0}^{\infty + i\infty} dy \, y e^{-y} = -\int_{\infty}^{0} dy \, y e^{-y} = \int_{0}^{\infty} dy \, y e^{-y} = 1$$

$$\curvearrowright \; \psi(p) = \frac{2\alpha^{\frac{3}{2}}}{\sqrt{2\pi\hbar}} \frac{\left(\alpha^2 - \frac{p^2}{\hbar^2}\right) - i2\alpha\frac{p}{\hbar}}{\left(\alpha^2 - \frac{p^2}{\hbar^2}\right)^2 + 4\alpha^2\frac{p^2}{\hbar^2}}$$

Fig. A.6



$$\curvearrowright \quad |\psi(p)|^2 = \frac{4\alpha^3}{2\pi\hbar} \frac{\left(\alpha^2 - \frac{p^2}{\hbar^2}\right)^2 + 4\alpha^2 \frac{p^2}{\hbar^2}}{\left(\alpha^2 + \frac{p^2}{\hbar^2}\right)^4}$$

3. Probability:

$$\begin{aligned} \underbrace{|\psi(p)|^2}_{\text{probability density}} &= \frac{4\alpha^3}{2\pi\hbar} \cdot \frac{1}{\left(\alpha^2 + \frac{p^2}{\hbar^2}\right)^2} \\ &= \frac{1}{\pi} 2\alpha^3\hbar^3 \cdot \frac{1}{(\hbar^2\alpha^2 + p^2)^2} \\ \curvearrowright \quad W &= \int_{-\hbar\alpha}^{+\hbar\alpha} dp \, |\psi(p)|^2 \\ &= \frac{2}{\pi}\alpha^3\hbar^3 \int_{-\hbar\alpha}^{+\hbar\alpha} \frac{dp}{(\hbar^2\alpha^2 + p^2)^2} \end{aligned}$$

Standard integrals:

$$\int \frac{dx}{(x^2+\alpha^2)^2} = \frac{x}{2\alpha^2 (x^2+\alpha^2)} + \frac{1}{2\alpha^3} \arctan\frac{x}{\alpha} + C$$

$$\begin{aligned} \curvearrowright \quad W &= \frac{2}{\pi}\alpha^3\hbar^3 \left(\frac{p}{2\hbar^2\alpha^2 (p^2 + \hbar^2\alpha^2)} \Bigg|_{-\hbar\alpha}^{+\hbar\alpha} + \frac{1}{2\hbar^3\alpha^3} \arctan\frac{p}{\hbar\alpha} \Bigg|_{-\hbar\alpha}^{+\hbar\alpha} \right) \\ &= \frac{2}{\pi}\alpha^3\hbar^3 \left(\frac{2\hbar\alpha}{4\hbar^4\alpha^4} + \frac{1}{2\hbar^3\alpha^3} \left(\frac{\pi}{4} + \frac{\pi}{4} \right) \right) \\ W &= \frac{1}{\pi} + \frac{1}{2} = 0.818 \, . \end{aligned}$$

Solution 2.2.7

1. The position of the particle is not precisely fixed. In the case of the here assumed one-dimensional problem,

$$-\infty < z < +\infty$$

are the values of the particle position which come into question. Each *thinkable* value is multiplied with the probability of its realization:

$$\frac{z|\psi(z,t)|^2}{\int\limits_{-\infty}^{+\infty} dz|\psi(z,t)|^2} .$$

Subsequently, it is summed and integrated, respectively, over all the possibilities in order to get the average value. The denominator takes care for the usual convention that probabilities are normalized to one .

2.

$$\langle z\rangle_t = \frac{\int\limits_{-\infty}^{+\infty} dz\, z\, \exp\left[-\left(z-\frac{\hbar k_0}{m}t\right)^2 \Big/ (\Delta b(t))^2\right]}{\int\limits_{-\infty}^{+\infty} dz\, \exp\left[-\left(z-\frac{\hbar k_0}{m}t\right)^2 \Big/ (\Delta b(t))^2\right]} .$$

Substitution:

$$y \equiv \frac{1}{\Delta b(t)}\left(z-\frac{\hbar k_0}{m}t\right)$$

$$\Longrightarrow \langle z\rangle_t = \frac{\int\limits_{-\infty}^{+\infty} dy\left(\Delta b(t)y+\frac{\hbar k_0}{m}t\right) e^{-y^2}}{\int\limits_{-\infty}^{+\infty} dy\, e^{-y^2}} =$$

$$= \frac{-\frac{1}{2}\Delta b(t)\, e^{-y^2}\Big|_{-\infty}^{+\infty}}{\sqrt{\pi}} + \frac{\hbar k_0}{m}t .$$

The average value is therewith equal to the most probable value:

$$\langle z\rangle_t = \frac{\hbar k_0}{m}t .$$

3.

$$\left\langle (z-\langle z\rangle)^2\right\rangle = \frac{\int\limits_{-\infty}^{+\infty} dz\left(z-\frac{\hbar k_0}{m}t\right)^2 \exp\left[-\left(z-\frac{\hbar k_0}{m}t\right)^2 \Big/ (\Delta b(t))^2\right]}{\int\limits_{-\infty}^{+\infty} dz\, \exp\left[-\left(z-\frac{\hbar k_0}{m}t\right)^2 \Big/ (\Delta b(t))^2\right]} =$$

$$= (\Delta b(t))^2 \frac{\int_{-\infty}^{+\infty} dy\, y^2\, e^{-y^2}}{\int_{-\infty}^{+\infty} dy\, e^{-y^2}} =$$

$$= (\Delta b(t))^2 \frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} = \frac{1}{2}(\Delta b(t))^2$$

$$\Longrightarrow \quad \Delta z = \frac{1}{\sqrt{2}}\,\Delta b(t) = \frac{1}{\sqrt{2}}\,\frac{1}{b}\sqrt{b^4 + \left(\frac{\hbar}{m}t\right)^2}\,.$$

4. According to (2.27) we have:

$$j(z,0) = \frac{\hbar}{m}\,\mathrm{Im}\left(\psi^*(z,0)\,\frac{d}{dz}\,\psi(z,0)\right)\,,$$

$$\psi(z,0) = A\, e^{-\frac{z^2}{2b^2}}\, e^{ik_0 z}$$

$$\Longrightarrow \quad j(z,0) = \frac{\hbar}{m}|A|^2\,\mathrm{Im}\left(e^{-\frac{z^2}{2b^2}}\, e^{-ik_0 z}\left(-\frac{z}{b^2} + ik_0\right) e^{-\frac{z^2}{2b^2}}\, e^{ik_0 z}\right) =$$

$$= \frac{\hbar}{m}|A|^2\, e^{-\frac{z^2}{b^2}}\,\mathrm{Im}\left(-\frac{z}{b^2} + ik_0\right) = \frac{\hbar}{m}|A|^2\, e^{-\frac{z^2}{b^2}}\, k_0$$

$$\Longrightarrow \quad j(z,0) = \frac{\hbar\, k_0}{m}\,|\psi(z,0)|^2\,.$$

velocity · density

Solution 2.2.8 Fourier transform,

$$\psi(\mathbf{r},t) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\,\overline{\psi}(\mathbf{p},t)\,,$$

$$V(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\, V(\mathbf{p})\,.$$

to be inserted into the Schrödinger equation:

$$\frac{1}{(2\pi\hbar)^{3/2}}\int d^3\overline{p}\left(i\hbar\frac{\partial}{\partial t} - \frac{\overline{\mathbf{p}}^2}{2m}\right) e^{\frac{i}{\hbar}\overline{\mathbf{p}}\cdot\mathbf{r}}\,\overline{\psi}(\overline{\mathbf{p}},t) -$$

$$- \frac{1}{(2\pi\hbar)^3}\int d^3\overline{p}\int d^3p'\, e^{\frac{i}{\hbar}(\mathbf{p}'+\overline{\mathbf{p}})\cdot\mathbf{r}}\, V(\mathbf{p}')\,\overline{\psi}(\overline{\mathbf{p}},t) = 0\,.$$

Multiply this equation by $e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}$ and integrate over the whole space:

$$(2\pi\hbar)^{3/2}\int d^3\overline{p}\left(i\hbar\frac{\partial}{\partial t}-\frac{\overline{\mathbf{p}}^2}{2m}\right)\overline{\psi}(\overline{\mathbf{p}},t)\,\frac{1}{(2\pi\hbar)^3}\int d^3r\,e^{\frac{i}{\hbar}(\overline{\mathbf{p}}-\mathbf{p})\cdot\mathbf{r}}-$$

$$-\int d^3\overline{p}\int d^3p'\,V(\mathbf{p}')\,\overline{\psi}(\overline{\mathbf{p}},t)\,\frac{1}{(2\pi\hbar)^3}\int d^3r\,e^{\frac{i}{\hbar}(\mathbf{p}'+\overline{\mathbf{p}}-\mathbf{p})\cdot\mathbf{r}}=0\,.$$

Exploit the representation (2.74) of the δ-function:

$$\left(i\hbar\frac{\partial}{\partial t}-\frac{\mathbf{p}^2}{2m}\right)\overline{\psi}(\mathbf{p},t)-\frac{1}{(2\pi\hbar)^{3/2}}\int d^3p'\,V(\mathbf{p}')\,\overline{\psi}(\mathbf{p}-\mathbf{p}',t)=0\,.$$

The second term represents a convolution integral (see (4.188), Vol. 3).

Solution 2.2.9

1. $\mathbf{p}=\mathbf{p}'$:

$$\frac{1}{V}\int_V d^3r=1\,.$$

2. $\mathbf{p}\neq\mathbf{p}'$:

$$\frac{1}{V}\int_V d^3r\,e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}}= \qquad (2.76)$$

$$=\frac{1}{V}\int_0^{L_x}dx\int_0^{L_y}dy\int_0^{L_z}dz\,\exp\left(-\frac{i}{\hbar}2\pi\hbar\left\{\frac{n_x-n_x'}{L_x}x+\frac{n_y-n_y'}{L_y}y+\frac{n_z-n_z'}{L_z}z\right\}\right)\,,$$

$$(n_x,n_y,n_z)\neq(n_x',n_y',n_z')\,.$$

Let $n_x\neq n_x'$:

$$\int_0^{L_x}dx\,\exp\left(-i\,2\pi\left\{\frac{n_x-n_x'}{L_x}x\right\}\right)=$$

$$=i\,\frac{L_x}{2\pi(n_x-n_x')}\left(e^{-i2\pi(n_x-n_x')}-1\right)=0\,,$$

since $n_x-n_x'\in\mathbb{Z}$; $n_x\neq n_x'$.

Thus it follows:

$$\frac{1}{V}\int_V d^3r\, e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} = 0\ ,\ \text{if}\ \mathbf{p}\neq\mathbf{p}'\ .$$

Solution 2.2.10

1. Due to the discretization, caused by periodic boundary conditions, the *'grid volume'* in the momentum space (2.77)

$$\Delta^3 p = \frac{2\pi\hbar}{L_x}\frac{2\pi\hbar}{L_y}\frac{2\pi\hbar}{L_z} = \frac{(2\pi\hbar)^3}{V}$$

contains just one *allowed* value of the momentum. Therewith:

$$1 = \sum_{\mathbf{p}'}\delta_{\mathbf{p}\mathbf{p}'} = \sum_{\mathbf{p}'}\Delta^3 p\,\frac{V}{(2\pi\hbar)^3}\delta_{\mathbf{p}\mathbf{p}'}\ .$$

If we now go over to the infinitely large system ($V\to\infty$, *thermodynamic limit*), then the grid volume $\Delta^3 p$ will become a volume element d^3p, and the sum changes into a Riemannian integral. If one compares the so arising expression, then one gets immediately with

$$1 = \int d^3p'\,\delta(\mathbf{p}-\mathbf{p}')$$

the following assignment:

$$\delta(\mathbf{p}-\mathbf{p}') \to \lim_{V\to\infty}\frac{V}{(2\pi\hbar)^3}\delta_{\mathbf{p}\mathbf{p}'}\ .$$

2.

$$\int d^3r \exp\left(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)\psi(\mathbf{r},t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}'}c_{\mathbf{p}'}(t)\underbrace{\int d^3r \exp\left(-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}\right)}_{V\delta_{\mathbf{p}\mathbf{p}'}\ \text{(Exercise 2.2.9)}}$$

$$= \sqrt{V}\,c_{\mathbf{p}}(t)$$

$$\curvearrowright\quad c_{\mathbf{p}}(t) = \frac{1}{\sqrt{V}}\int d^3r \exp\left(-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)\psi(\mathbf{r},t)$$

$|c_{\mathbf{p}}(t)|^2$ is the probability that the particle possesses the *discrete* momentum $\mathbf{p}$ at the time t!

Solution 2.2.11 Time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_1}\Delta_1\psi - \frac{\hbar^2}{2m_2}\Delta_2\psi + V(\mathbf{r}_1,\mathbf{r}_2)\,\psi\ . \tag{A.4}$$

Δ_i is thereby the Laplace operator, which acts on the spatial coordinates of the i-th particle. Transition to the complex conjugate:

$$-i\hbar\frac{\partial\psi^\star}{\partial t} = -\frac{\hbar^2}{2m_1}\Delta_1\psi^\star - \frac{\hbar^2}{2m_2}\Delta_2\psi^\star + V(\mathbf{r}_1,\mathbf{r}_2)\,\psi^\star\ . \tag{A.5}$$

Multiply Eq. (A.4) by $\psi^\star$ and (A.5) by ψ and then subtract the one from the other:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi|^2 &= -\frac{\hbar^2}{2m_1}\psi^\star\Delta_1\psi - \frac{\hbar^2}{2m_2}\psi^\star\Delta_2\psi + \frac{\hbar^2}{2m_1}\psi\Delta_1\psi^\star + \frac{\hbar^2}{2m_2}\psi\Delta_2\psi^\star \\ &= -\frac{\hbar^2}{2m_1}(\nabla_1\cdot(\psi^\star\nabla_1\psi - \psi\nabla_1\psi^\star)) - \frac{\hbar^2}{2m_2}(\nabla_2\cdot(\psi^\star\nabla_2\psi - \psi\nabla_2\psi^\star))\ . \end{aligned}$$

With the particle-current density and the density of the position probability,

$$\mathbf{j}_{1,2}(\mathbf{r}_1,\mathbf{r}_2,t) = \frac{\hbar}{2m_{1,2}i}(\psi^\star\nabla_{1,2}\psi - \psi\nabla_{1,2}\psi^\star)\ ; \quad \rho(\mathbf{r}_1,\mathbf{r}_2,t) = |\psi(\mathbf{r}_1,\mathbf{r}_2,t)|^2\ ,$$

it eventually leads to the continuity equation:

$$\frac{\partial}{\partial t}\rho(\mathbf{r}_1,\mathbf{r}_2,t) + \nabla_1\cdot\mathbf{j}_1(\mathbf{r}_1,\mathbf{r}_2,t) + \nabla_2\cdot\mathbf{j}_2(\mathbf{r}_1,\mathbf{r}_2,t) = 0\ .$$

Solution 2.2.12 Because of $\frac{\partial}{\partial t}\mathbf{r} = 0$ it holds at first:

$$\langle\mathbf{p}\rangle_t = m\int d^3r\left(\frac{\partial\psi^*}{\partial t}\mathbf{r}\,\psi + \psi^*\mathbf{r}\frac{\partial\psi}{\partial t}\right)\ .$$

Schrödinger equation with real potential ($V^* = V$):

$$\begin{aligned} \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r})\right)\psi(\mathbf{r},t) &= i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t)\ , \\ \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r})\right)\psi^*(\mathbf{r},t) &= -i\hbar\frac{\partial}{\partial t}\psi^*(\mathbf{r},t)\ . \end{aligned}$$

Multiply from the left by $\psi^* x$ and ψx, respectively, and subtract the second from the first equation:

$$-\frac{\hbar^2}{2m}(\psi^* x\,\Delta\psi - \psi\,x\,\Delta\psi^*) = i\hbar\left(\psi^* x\frac{\partial}{\partial t}\psi + \psi\,x\frac{\partial}{\partial t}\psi^*\right)\ .$$

Insertion into the above equation for the x-component:

$$\begin{aligned}\langle p_x\rangle_t &= -\frac{\hbar}{2i}\int d^3r[\psi^* x\,\Delta\psi - \psi\, x\,\Delta\psi^*] = \\ &= -\frac{\hbar}{2i}\int d^3r\ \mathrm{div}\,[\psi^* x\,\nabla\psi - \psi\, x\,\nabla\psi^*] + \\ &\quad +\frac{\hbar}{2i}\int d^3r[(\nabla\psi^* x)\nabla\psi - (\nabla\psi\, x)\nabla\psi^*]\ .\end{aligned}$$

Gauss theorem ((1.53), Vol. 3) and square-integrability of the wave function:

$$\begin{aligned}&\int\limits_V d^3r\ \mathrm{div}\,[\psi^* x\,\nabla\psi - \psi\, x\,\nabla\psi^*] = \\ &= \int\limits_{S(V)} d\mathbf{f}\cdot[\psi^* x\,\nabla\psi - \psi\, x\,\nabla\psi^*] \underset{V\to\infty}{\longrightarrow} 0\ .\end{aligned}$$

Furthermore we have:

$$\nabla\psi^*\, x = (\nabla\psi^*)\, x + \psi^*\,\mathbf{e}_x\ ;\quad \nabla\psi\, x = (\nabla\psi)\, x + \psi\,\mathbf{e}_x\ .$$

It remains therewith:

$$\begin{aligned}\langle p_x\rangle_t &= \frac{\hbar}{2i}\int d^3r\,[\psi^*\ \mathbf{e}_x\cdot\nabla\psi - \psi\,\mathbf{e}_x\cdot\nabla\psi^*] = \\ &= -\frac{\hbar}{2i}\int d^3r\ \mathbf{e}_x\cdot\nabla(\psi\ \psi^*) + \frac{\hbar}{i}\int d^3r\,\psi^*\frac{\partial}{\partial x}\psi\ .\end{aligned}$$

Gauss theorem and square-integrability:

$$\int\limits_V d^3r\,\nabla(\psi\ \psi^*) = \int\limits_{S(V)} d\mathbf{f}|\psi|^2 \underset{V\to\infty}{\longrightarrow} 0\ .$$

It thus remains:

$$\langle p_x\rangle_t = \int d^3r\,\psi^*\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\ .$$

In an analogous manner one proves the assertions for the two other components:

$$\langle\mathbf{p}\rangle_t = \int d^3r\,\psi^*\frac{\hbar}{i}\nabla\psi\ ;\quad \nabla = \left(\frac{\partial}{\partial x},\,\frac{\partial}{\partial y},\,\frac{\partial}{\partial z}\right)\ .$$

Solution 2.2.13 (2.72) $\Longrightarrow$

$$\overline{\psi}^*(\mathbf{p},t) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} \underbrace{\psi^*(\mathbf{r},t)}_{=\psi(\mathbf{r},t)} = \overline{\psi}(-\mathbf{p},t)\ .$$

Expectation value of the momentum:

$$\langle\mathbf{p}\rangle_t = \int d^3p\, \overline{\psi}^*(\mathbf{p},t)\, \mathbf{p}\, \overline{\psi}(\mathbf{p},t) = \int d^3p\, \overline{\psi}(-\mathbf{p},t)\, \mathbf{p}\, \overline{\psi}(\mathbf{p},t) =$$

$$= \int d^3p'\, \overline{\psi}(\mathbf{p}',t)\, (-\mathbf{p}')\, \overline{\psi}(-\mathbf{p}',t) = -\int d^3p'\ \overline{\psi}(\mathbf{p}',t)\, \mathbf{p}'\, \overline{\psi}^*(\mathbf{p}',t) = -\langle\mathbf{p}\rangle_t = 0\ .$$

Solution 2.2.14

$$\psi^*(\mathbf{r},t) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int d^3p\, e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} \underbrace{\overline{\psi}^*(\mathbf{p},t)}_{\overline{\psi}(\mathbf{p},t)} = \psi(-\mathbf{r},t)$$

Expectation value of the position $\mathbf{r}$:

$$\begin{aligned}
\langle\mathbf{r}\rangle &= \int d^3r\, \psi^*(\mathbf{r},t)\, \mathbf{r}\, \psi(\mathbf{r},t) \\
&\overset{\mathbf{r}\to-\mathbf{r}}{=} \int d^3r\, \underbrace{\psi^*(-\mathbf{r},t)}_{\psi(\mathbf{r},t)}\, (-\mathbf{r})\, \underbrace{\psi(-\mathbf{r},t)}_{\psi^*(\mathbf{r},t)} \\
&= -\int d^3r\, \psi(\mathbf{r},t)\, \mathbf{r}\, \psi^*(\mathbf{r},t) \\
&= -\langle\mathbf{r}\rangle \\
\curvearrowright\quad \langle\mathbf{r}\rangle &= 0
\end{aligned}$$

Solution 2.2.15 One calculates conveniently:

$$\langle\mathbf{r}\rangle_t - \langle\mathbf{r}\rangle_t^\star = \int d^3p\, \overline{\psi}^\star(\mathbf{p},t) \left(-\frac{\hbar}{i}\nabla_p\right) \overline{\psi}(\mathbf{p},t) - \int d^3p\, \overline{\psi}(\mathbf{p},t) \left(+\frac{\hbar}{i}\nabla_p\right) \overline{\psi}^\star(\mathbf{p},t)$$

$$= -\frac{\hbar}{i} \int d^3p\, \nabla_p \left(\overline{\psi}^\star(\mathbf{p},t)\overline{\psi}(\mathbf{p},t)\right)$$

$$= -\frac{\hbar}{i} \int\limits_{S(V_p\to\infty)} df_p\, |\overline{\psi}(\mathbf{p},t)|^2 \quad \text{(Gauss theorem, (1.53) in Vol. 3)}$$

$$= 0 \qquad \text{(square-integrability)}$$

$S(V_p)$ is the surface of the volume V_p in the momentum space and df_p the corresponding surface element. $|\overline{\psi}|$ vanishes at infinity stronger than $1/p$. It is therefore:

$$\langle \mathbf{r} \rangle_t = \langle \mathbf{r} \rangle_t^\star$$

Section 2.3.4

Solution 2.3.1 We calculate:

$$\begin{aligned}\langle \mathbf{p} \rangle_t - \langle \mathbf{p} \rangle_t^* &= \int d^3r\, \psi^*(\mathbf{r},t)\, \frac{\hbar}{i}\, \nabla_r \psi(\mathbf{r},t) - \int d^3r\, \psi(\mathbf{r},t) \left(-\frac{\hbar}{i}\right) \nabla_r\, \psi^*(\mathbf{r},t) = \\ &= \frac{\hbar}{i} \int d^3r\, (\psi^*\, \nabla_r \psi + \psi\, \nabla_r \psi^*) = \frac{\hbar}{i} \int d^3r\, \nabla_r (\psi^*(\mathbf{r},t)\, \psi(\mathbf{r},t)) = \\ &= \frac{\hbar}{i} \int\limits_{S(V\to\infty)} d\mathbf{f}\, |\psi(\mathbf{r},t)|^2 = 0\ .\end{aligned}$$

In the step before the last we have used the Gauss theorem ((1.53), Vol. 3), and in the last step the square-integrability of the wave function $\psi(\mathbf{r},t)$. Hence it is:

$$\langle \mathbf{p} \rangle_t = \langle \mathbf{p} \rangle_t^*\ ,$$

$\langle \mathbf{p} \rangle_t$ is therewith real.

Solution 2.3.2

1. $\psi(\mathbf{r})$ real; spherical coordinates convenient.
   Volume element ((1.390), Vol. 1):

$$d^3r = r^2 dr \sin\vartheta\, d\vartheta\, d\varphi\ ,$$

$$\int d^3r |\psi(\mathbf{r})|^2 = \frac{1}{\pi\, a_\mathrm{B}^3} \int d^3r\, \exp\left(-\frac{2r}{a_\mathrm{B}}\right) = \frac{4}{a_\mathrm{B}^3} \int\limits_0^\infty dr\, r^2\, \exp\left(-\frac{2r}{a_\mathrm{B}}\right)\ .$$

   Substitution:

$$y = \frac{2r}{a_\mathrm{B}}$$

$$\Longrightarrow\ r^2\, dr = \frac{a_\mathrm{B}^3}{8}\, y^2\, dy\ .$$

Therewith it remains to be calculated:

$$\int d^3r|\psi(\mathbf{r})|^2 = \frac{1}{2}\int_0^\infty dy\, y^2\, e^{-y}\ .$$

Gamma function:

$$\Gamma(x) = \int_0^\infty dt\, t^{x-1}\, e^{-t}$$

a) $\Gamma(x+1) = x\,\Gamma(x)$,

b) $\Gamma(n+1) = n!$,

c) $\Gamma(1) = \Gamma(2) = 1$,

d) $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$.

The wave function is therefore already normalized:

$$\int d^3r|\psi(\mathbf{r})|^2 = \frac{1}{2}\Gamma(3) = \frac{1}{2}\,2! = 1\ .$$

2. $\langle\mathbf{r}\rangle = 0$, since

$$\langle\mathbf{r}\rangle = \frac{1}{\pi\, a_\mathrm{B}^3}\int d^3r\ \mathbf{r}\, e^{-\frac{2r}{a_\mathrm{B}}}\ ,$$

$$\mathbf{r} = r(\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)\ ,$$

$$\int_0^{2\pi}\cos\varphi\, d\varphi = \int_0^{2\pi}\sin\varphi\, d\varphi = \int_{-1}^{+1}\cos\vartheta\ d\cos\vartheta = 0\ ,$$

$$\langle\mathbf{r}^2\rangle = \frac{4}{a_\mathrm{B}^3}\int_0^\infty dr\, r^4\, \exp\left(-\frac{2r}{a_\mathrm{B}}\right) = \frac{4}{a_\mathrm{B}^3}\,\frac{a_\mathrm{B}^5}{32}\int_0^\infty dy\, y^4\, e^{-y} =$$

$$= \frac{1}{8}\,a_\mathrm{B}^2\,\Gamma(5) = \frac{1}{8}\,a_\mathrm{B}^2\,4! = 3\,a_\mathrm{B}^2\ .$$

$\Longrightarrow$ mean square deviation:

$$\Delta r = \sqrt{3}\,a_\mathrm{B}\ .$$

3.

$$\mathbf{p} \implies \frac{\hbar}{i}\,\nabla_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial x},\,\frac{\partial}{\partial y}\,,\,\frac{\partial}{\partial z}\right)\,.$$

One calculates:

$$\frac{\partial}{\partial x}\,e^{-\frac{r}{a_\mathrm{B}}} = -\frac{1}{a_\mathrm{B}}\,e^{-\frac{r}{a_\mathrm{B}}}\,\frac{\partial r}{\partial x}\,,$$

$$\frac{\partial r}{\partial x} = \frac{\partial}{\partial x}\,\sqrt{x^2+y^2+z^2} = \frac{x}{r}\,.$$

Thus:

$$\nabla_r\,e^{-\frac{r}{a_\mathrm{B}}} = -\frac{1}{a_\mathrm{B}}\,\frac{\mathbf{r}}{r}\,e^{-\frac{r}{a_\mathrm{B}}}\,.$$

From that it follows eventually:

$$\langle\mathbf{p}\rangle = \int d^3r\,\psi^*(\mathbf{r})\,\frac{\hbar}{i}\,\nabla_r\psi(\mathbf{r}) = -\frac{\hbar}{i}\,\frac{1}{\pi\,a_\mathrm{B}^4}\int d^3r\,\frac{\mathbf{r}}{r}\,e^{-\frac{2r}{a_\mathrm{B}}} = 0$$

(substitute $\mathbf{r}$ by $-\mathbf{r}$). Reasoning as for $\langle\mathbf{r}\rangle$ in part 2.!

$$\frac{\partial^2}{\partial x^2}\,e^{-\frac{r}{a_\mathrm{B}}} = \frac{\partial}{\partial x}\left(-\frac{1}{a_\mathrm{B}}\,e^{-\frac{r}{a_\mathrm{B}}}\,\frac{x}{r}\right) = e^{-\frac{r}{a_\mathrm{B}}}\left(\frac{1}{a_\mathrm{B}^2}\,\frac{x^2}{r^2} - \frac{1}{a_\mathrm{B}}\,\frac{1}{r} + \frac{1}{a_\mathrm{B}}\,\frac{x^2}{r^3}\right)$$

$$\implies \Delta e^{-\frac{r}{a_\mathrm{B}}} = \frac{1}{a_\mathrm{B}^2}\,e^{-\frac{r}{a_\mathrm{B}}}\left(1-\frac{2a_\mathrm{B}}{r}\right)\,.$$

We calculate therewith:

$$\langle\mathbf{p}^2\rangle = \int d^3r\,\psi^*(\mathbf{r})\,(-\hbar^2\Delta)\,\psi(\mathbf{r}) =$$

$$= -\hbar^2\,\frac{4}{a_\mathrm{B}^3}\int_0^\infty dr\,r^2\,\frac{1}{a_\mathrm{B}^2}\left(1-\frac{2a_\mathrm{B}}{r}\right)\,e^{-\frac{2r}{a_\mathrm{B}}} =$$

$$= \frac{-4\hbar^2}{a_\mathrm{B}^5}\int_0^\infty dr(r^2-2a_\mathrm{B}\,r)\,e^{-\frac{2r}{a_\mathrm{B}}} =$$

$$= -\frac{4\hbar^2}{a_\mathrm{B}^5}\left(\frac{a_\mathrm{B}^3}{8}\int_0^\infty dy\, y^2\, e^{-y} - 2a_\mathrm{B}\,\frac{a_\mathrm{B}^2}{4}\int_0^\infty dy\, y\, e^{-y}\right) =$$

$$= -\frac{\hbar^2}{a_\mathrm{B}^2}\left(\frac{1}{2}\Gamma(3) - 2\Gamma(2)\right) = \frac{\hbar^2}{a_\mathrm{B}^2}\,.$$

Mean square deviation:

$$\Delta p = \frac{\hbar}{a_\mathrm{B}}\,.$$

4.

$$\Delta r\,\Delta p = \sqrt{3}\,a_\mathrm{B}\,\frac{\hbar}{a_\mathrm{B}} = \sqrt{3}\,\hbar\,,$$

see uncertainty relation (1.5).

5. Current density:

$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2m\,i}\,\{\psi^*\nabla\psi - \psi\,\nabla\psi^*\} = \frac{\hbar}{2m\,i}\,\{\psi\,\nabla\psi - \psi\,\nabla\psi\} = 0\,,$$

since ψ is real!

Solution 2.3.3 Gradient in spherical coordinates ((1.394), Vol. 1):

$$\nabla \equiv \left(\frac{\partial}{\partial r},\ \frac{1}{r}\,\frac{\partial}{\partial\vartheta},\ \frac{1}{r\sin\vartheta}\,\frac{\partial}{\partial\varphi}\right)\,.$$

Current density:

$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2m\,i}\,(\psi^*(\mathbf{r})\,\nabla_r\psi(\mathbf{r}) - \psi(\mathbf{r})\,\nabla\psi^*(\mathbf{r})) = \frac{\hbar}{m}\,\mathrm{Im}\,(\psi^*(\mathbf{r})\,\nabla_r\psi(\mathbf{r}))\,.$$

r- and ϑ-parts are real:

$$j_r(\mathbf{r}) = j_\vartheta(\mathbf{r}) = 0\,.$$

We therefore have to calculate only the φ-part:

$$j_\varphi(\mathbf{r}) = \frac{\hbar}{m}\,\frac{r^2\exp\left(-\frac{r}{a_\mathrm{B}}\right)}{64\,\pi\,a_\mathrm{B}^5}\,\sin^2\vartheta\,\frac{1}{r\sin\vartheta}\,\mathrm{Im}\,\left(e^{-i\varphi}\,\frac{\partial}{\partial\varphi}\,e^{i\varphi}\right)$$

$$\Longrightarrow\quad j_\varphi(\mathbf{r}) = \frac{\hbar}{m}\,\frac{r\sin\vartheta}{64\,\pi\,a_\mathrm{B}^5}\,\exp\left(-\frac{r}{a_\mathrm{B}}\right)\,.$$

Solution 2.3.4

1. $\psi(x)$ arbitrary; $\quad n \geq 1$:

$$[p, x^n]_- \psi(x) = \left(\frac{\hbar}{i} \frac{d}{dx} x^n \psi(x) - x^n \frac{\hbar}{i} \frac{d}{dx} \psi(x) \right) = \frac{\hbar}{i} n x^{n-1} \psi(x)$$

$$\Longrightarrow \quad [p, x^n]_- = n \frac{\hbar}{i} x^{n-1} \, .$$

2. $\psi(x)$ arbitrary:

$$[x^{-1}, p]_- \psi(x) = \left(x^{-1} \frac{\hbar}{i} \frac{d}{dx} \psi(x) - \frac{\hbar}{i} \frac{d}{dx} x^{-1} \psi(x) \right) = \frac{\hbar}{i} x^{-2} \psi(x)$$

$$\Longrightarrow \quad [x^{-1}, p]_- = \frac{\hbar}{i} x^{-2} \, .$$

3. $\widehat{\psi}(p)$ arbitrary; $\quad n \geq 1$:

$$[p^n, x]_- \widehat{\psi}(p) = \left[p^n \left(-\frac{\hbar}{i} \frac{d}{dp} \right) \widehat{\psi}(p) + \frac{\hbar}{i} \frac{d}{dp} p^n \widehat{\psi}(p) \right] = \frac{\hbar}{i} n p^{n-1} \widehat{\psi}(p)$$

$$\Longrightarrow \quad [p^n, x]_- = n \frac{\hbar}{i} p^{n-1} \, .$$

Solution 2.3.5

1. Position representation:

$$\left[x^{-1}, xp\right]_- \psi(x) = \left(\frac{\hbar}{i} \frac{d}{dx} - x \frac{\hbar}{i} \frac{d}{dx} x^{-1} \right) \psi(x) = x^{-1} \frac{\hbar}{i} \psi(x)$$

$\psi(x)$ arbitrary $\curvearrowright$

$$\left[x^{-1}, xp\right]_- = \frac{\hbar}{i} x^{-1}$$

2. Angular momentum:

$$L_x = y p_z - z p_y \; ; \quad L_y = z p_x - x p_z \; ; \quad L_z = x p_y - y p_x$$

One shows at first: (A, B, C : operators)

$$[A, BC]_- = B \, [A, C]_- + [A, B]_- \, C$$
$$[AB, C]_- = A \, [B, C]_- + [A, C]_- \, B$$

Therewith:

$$\begin{aligned}\left[L_x, L_y\right]_- &= \left[\, yp_z - zp_y, zp_x - xp_z\right]_- \\ &= \left[yp_z, zp_x\right]_- - \left[yp_z, xp_z\right]_- - \left[zp_y, zp_x\right]_- + \left[zp_y, xp_z\right]_- \\ &= y\left[p_z, z\right]_- p_x - 0 - 0 + x\left[z, p_z\right]_- p_y \\ &= \frac{\hbar}{i}\left(yp_x - xp_y\right) \\ &= i\hbar L_z\end{aligned}$$

One should compare it with the classical Poisson bracket:

$$\left\{L_x, L_y\right\} = L_z$$

Analogously one shows:

$$\left[L_y, L_z\right]_- = i\hbar L_x \;;\;\; \left[L_z, L_x\right]_- = i\hbar L_y$$

3. Square of the angular momentum:

$$\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$\begin{aligned}\left[\mathbf{L}^2, L_z\right]_- &= \left[L_x^2 + L_y^2, L_z\right]_- \\ &= \left[L_x^2, L_z\right]_- + \left[L_y^2, L_z\right]_- \\ &= L_x\left[L_x, L_z\right]_- + \left[L_x, L_z\right]_- L_x + L_y\left[L_y, L_z\right]_- + \left[L_y, L_z\right]_- L_y \\ &= -i\hbar L_x L_y - i\hbar L_y L_x + i\hbar L_y L_x + i\hbar L_x L_y \\ &= 0\end{aligned}$$

Solution 2.3.6

1. $\psi(x)$ arbitrary:

$$\left[p_x, F(x)\right]_- \psi(x) = \left(\frac{\hbar}{i}\frac{d}{dx}F(x)\,\psi(x)\right) - F(x)\frac{\hbar}{i}\frac{d}{dx}\psi(x) = \left(\frac{\hbar}{i}\frac{d}{dx}F(x)\right)\psi(x)$$

$$\Longrightarrow \left[p_x, F(x)\right]_- = \frac{\hbar}{i}\frac{d}{dx}F(x)\;.$$

2. $\widehat{\psi}(p_x)$ arbitrary:

$$[G(p_x), x]_- \widehat{\psi}(p_x) = G(p_x) \left(-\frac{\hbar}{i} \frac{d}{dp_x} \widehat{\psi}(p_x)\right) + \frac{\hbar}{i} \frac{d}{dp_x} G(p_x) \widehat{\psi}(p_x) =$$

$$= \left(\frac{\hbar}{i} \frac{d}{dp_x} G(p_x)\right) \widehat{\psi}(p_x)$$

$$\Longrightarrow \quad [G(p_x), x]_- = \frac{\hbar}{i} \frac{d}{dp_x} G(p_x) \; .$$

Solution 2.3.7

1. Taylor expansion ((1.27), Vol. 3):

$$\psi(\mathbf{r} + \mathbf{a}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{a} \cdot \nabla_r)^n \psi(\mathbf{r}) = \exp(\mathbf{a} \cdot \nabla_r) \psi(\mathbf{r})$$

$$\Longrightarrow \quad T(\mathbf{a}) \equiv \exp(\mathbf{a} \cdot \nabla_r) = \exp\left(\frac{i}{\hbar} \mathbf{a} \cdot \mathbf{p}\right) \; .$$

2.

$$T(\mathbf{a})\, x\, T^{-1}(\mathbf{a}) =$$

$$= \exp\left(\frac{i}{\hbar}\, \mathbf{a} \cdot \mathbf{p}\right) x \exp\left(-\frac{i}{\hbar}\, \mathbf{a} \cdot \mathbf{p}\right) = \exp\left(\frac{i}{\hbar}\, a_x p_x\right) x \exp\left(-\frac{i}{\hbar}\, a_x p_x\right) =$$

$$= \exp\left(\frac{i}{\hbar}\, a_x p_x\right) \exp\left(-\frac{i}{\hbar}\, a_x p_x\right) x + \exp\left(\frac{i}{\hbar}\, a_x p_x\right) \left[x, \exp\left(-\frac{i}{\hbar}\, a_x p_x\right)\right]_- =$$

$$= x + \exp\left(\frac{i}{\hbar}\, a_x p_x\right) \left[-\frac{\hbar}{i} \frac{d}{dp_x} \exp\left(-\frac{i}{\hbar}\, a_x p_x\right)\right] = x + a_x \; .$$

Here part 2. of Exercise 2.3.6 is used. The other components are calculated completely analogously. Altogether we therewith have:

$$T(\mathbf{a}) \mathbf{r}\, T^{-1}(\mathbf{a}) = \mathbf{r} + \mathbf{a} \qquad \text{q.e.d.}$$

Solution 2.3.8 The Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r})\right) \psi(\mathbf{r}, t)$$

can be rewritten:

$$V(\mathbf{r}) \psi(\mathbf{r}, t) = \left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \Delta\right) \psi(\mathbf{r}, t) \; .$$

The first term on the right-hand side yields:

$$i\hbar\,\frac{\partial}{\partial t}\,\psi(\mathbf{r},t) = \frac{\hbar^2}{2mb^2}\,\psi(\mathbf{r},t) = \frac{\hbar\,\omega}{2}\,\psi(\mathbf{r},t)\ .$$

Laplace operator in spherical coordinates (2.112):

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

No angle-dependence:

$$\Delta_{\vartheta,\varphi}\,\psi(\mathbf{r},t) = 0\ .$$

Radial part:

$$\frac{\partial\psi}{\partial r} = -\frac{r}{b^2}\,\psi \implies \Delta\psi = \frac{1}{r^2}\,\frac{\partial}{\partial r}\left(-\frac{r^3}{b^2}\psi\right) = \left(-\frac{3}{b^2} + \frac{r^2}{b^4}\right)\psi$$
$$\implies \frac{\hbar^2}{2m}\,\Delta\psi(\mathbf{r},t) = \left(-\frac{3}{2}\,\hbar\,\omega + \frac{1}{2}\,m\omega^2 r^2\right)\psi(\mathbf{r},t)\ .$$

It thus remains:

$$V(\mathbf{r}) = -\hbar\,\omega + \frac{1}{2}\,m\omega^2 r^2\ .$$

This is just the oscillator potential, except for the constant $-\hbar\,\omega$.

Solution 2.3.9

$$H\psi(q) = E\psi(q)$$
$$\overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dq\; e^{-\frac{i}{\hbar}pq}\psi(q)$$
$$H = \frac{p^2}{2m} + V(q) \longrightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + V(q)$$
$$\curvearrowright \quad \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dq\; e^{-\frac{i}{\hbar}pq}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + V(q)\right)\psi(q)$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dq\; e^{-\frac{i}{\hbar}pq}E\psi(q) = E\overline{\psi}(p)\ .$$

It holds in detail:

$$\int_{-\infty}^{+\infty} dq\, e^{-\frac{i}{\hbar}pq} \frac{d^2}{dq^2}\psi(q) = e^{-\frac{i}{\hbar}pq} \underbrace{\frac{d}{dq}\psi(q)\Big|_{-\infty}^{+\infty}}_{=0} - \left(-\frac{i}{\hbar}p\right) \int_{-\infty}^{+\infty} dq\, e^{-\frac{i}{\hbar}pq} \frac{d}{dq}\psi(q)$$

$$= \frac{i}{\hbar}pe^{-\frac{i}{\hbar}pq} \underbrace{\psi(q)}_{=0}\Big|_{-\infty}^{+\infty} + \left(\frac{i}{\hbar}p\right)^2 \int_{-\infty}^{+\infty} dq\, e^{-\frac{i}{\hbar}}\psi(q)$$

Therewith:

$$\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dq\, e^{-\frac{i}{\hbar}pq} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}\psi(q)\right) = \frac{p^2}{2m}\overline{\psi}(p)$$

Fourier transform of the potential:

$$\overline{V}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dq\, V(q) e^{-\frac{i}{\hbar}pq}$$

Therewith we can rearrange:

$$\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dq\, e^{-\frac{i}{\hbar}pq} V(q)\psi(q)$$

$$= \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int_{-\infty}^{+\infty} dq\, e^{-\frac{i}{\hbar}pq} \iint_{-\infty}^{+\infty} dp'dp''\, e^{\frac{i}{\hbar}(p'+p'')q} \overline{V}(p')\overline{\psi}(p'')$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \iint_{-\infty}^{+\infty} dp'dp''\, \overline{V}(p')\overline{\psi}(p'')\delta(p'+p''-p)$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp''\, \overline{V}(p-p'')\overline{\psi}(p'')$$

Finally, the Schrödinger equation reads in momentum representation:

$$\frac{p^2}{2m}\overline{\psi}(p) + \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp'\, \overline{V}(p-p')\overline{\psi}(p') = E\overline{\psi}(p)$$

Solution 2.3.10 Free particle:

$$H_0 = \frac{\mathbf{p}^2}{2m}$$
$$\langle \mathbf{r} \rangle = \int d^3r \; \psi^*(\mathbf{r},t) \; \mathbf{r} \; \psi(\mathbf{r},t)$$

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = H_0 \psi(\mathbf{r},t)$$
$$-i\hbar \frac{\partial}{\partial t}\psi^*(\mathbf{r},t) = (H_0\psi(\mathbf{r},t))^* \qquad H_0: \text{ Hermitian}$$

$$\begin{aligned}
\frac{\partial}{\partial t}\langle \mathbf{r} \rangle &= \int d^3r \left(\left(\frac{\partial}{\partial t}\psi^*(\mathbf{r},t) \right) \mathbf{r} \; \psi(\mathbf{r},t) + \psi^*(\mathbf{r},t) \; \mathbf{r} \left(\frac{\partial}{\partial t}\psi(\mathbf{r},t) \right) \right) \\
&= \int d^3r \left(\left(-\frac{1}{i\hbar}(H_0\psi)^* \right) \mathbf{r} \; \psi + \psi^* \; \mathbf{r} \left(\frac{1}{i\hbar} H_0 \psi \right) \right) \\
&= \int d^3r \left(\frac{1}{i\hbar}\psi^*(\mathbf{r} \cdot H_0)\psi - \frac{1}{i\hbar}\psi^*(\underbrace{H_0^+}_{=H_0} \cdot \mathbf{r})\psi \right) \\
&= \frac{1}{i\hbar} \int d^3r \; \psi^*(\mathbf{r},t) \; [\mathbf{r}, H_0]_- \; \psi(\mathbf{r},t)
\end{aligned}$$

$$\begin{aligned}
[x, H_0]_- &= \left[x, \frac{\mathbf{p}^2}{2m} \right]_- \\
&= \left[x, \frac{p_x^2}{2m} \right]_- \\
&= \frac{1}{2m} \left(p_x \underbrace{[x, p_x]_-}_{i\hbar} + \underbrace{[x, p_x]_-}_{i\hbar} p_x \right) \\
&= i\hbar \frac{p_x}{m} \\
\curvearrowright \; [\mathbf{r}, H_0]_- &= \frac{i\hbar}{m}\mathbf{p}
\end{aligned}$$

$$\curvearrowright \quad \frac{\partial}{\partial t}\langle \mathbf{r}\rangle = \frac{1}{m}\int d^3r\ \psi^*(\mathbf{r},t)\ \mathbf{p}\ \psi(\mathbf{r},t)$$
$$= \frac{1}{m}\langle \mathbf{p}\rangle$$

Section 3.2.9

Solution 3.2.1

$$\| \alpha+\beta \|^2 + \| \alpha-\beta \|^2 = \langle \alpha+\beta|\alpha+\beta\rangle + \langle \alpha-\beta|\alpha-\beta\rangle =$$
$$= \langle\alpha|\alpha\rangle + \langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle + \langle\beta|\beta\rangle + \langle\alpha|\alpha\rangle - \langle\alpha|\beta\rangle - \langle\beta|\alpha\rangle + \langle\beta|\beta\rangle =$$
$$= 2\langle\alpha|\alpha\rangle + 2\langle\beta|\beta\rangle = 2\| \alpha \|^2 + 2\| \beta \|^2 \ .$$

Solution 3.2.2 Decompose $|\beta\rangle$ into a parallel and a perpendicular component with respect to $|\alpha\rangle$:

Parallel:

$$\frac{|\alpha\rangle\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle} = z|\alpha\rangle \ .$$

Perpendicular:

$$\left(|\beta\rangle - \frac{|\alpha\rangle\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\right) \equiv |\gamma\rangle \ .$$

One realizes:

$$\langle\alpha|\gamma\rangle = 0,$$
$$|\beta\rangle = z|\alpha\rangle + |\gamma\rangle \ .$$

We construct therewith:

$$\| \beta \|^2 = \| z\alpha+\gamma \|^2 = \langle z\alpha+\gamma|z\alpha+\gamma\rangle =$$
$$= |z|^2\langle\alpha|\alpha\rangle + \langle\gamma|\gamma\rangle + z^*\langle\alpha|\gamma\rangle + z\langle\gamma|\alpha\rangle =$$
$$= \frac{|\langle\alpha|\beta\rangle|^2}{\| \alpha \|^2} + \| \gamma \|^2 \geq \frac{|\langle\alpha|\beta\rangle|^2}{\| \alpha \|^2} \ .$$

$\Longrightarrow$ Schwarz's inequality:

$$|\langle\alpha|\beta\rangle| \leq \| \alpha \|\, \| \beta \| \ .$$

Solution 3.2.3

1. Assertion

$$\begin{aligned} & \big|\, \| \alpha \| - \| \beta \| \,\big| \leq \| \alpha + \beta \| \\ \Longleftrightarrow \quad & \| \alpha \|^2 - 2 \| \alpha \| \| \beta \| + \| \beta \|^2 \leq \| \alpha + \beta \|^2 \ . \end{aligned}$$

Proof:

$$\begin{aligned} \| \alpha + \beta \|^2 = \langle \alpha + \beta | \alpha + \beta \rangle = & \| \alpha \|^2 + \| \beta \|^2 + \langle \alpha | \beta \rangle + \langle \beta | \alpha \rangle = \\ = & \| \alpha \|^2 + \| \beta \|^2 + 2 \,\mathrm{Re}\, \langle \alpha | \beta \rangle \geq \| \alpha \|^2 + \| \beta \|^2 - 2 |\langle \alpha | \beta \rangle| \geq \\ \geq & \| \alpha \|^2 + \| \beta \|^2 - 2 \| \alpha \| \| \beta \| \qquad \text{q.e.d.} \end{aligned}$$

$\uparrow$ Schwarz's inequality

2. Assertion:

$$\begin{aligned} & \| \alpha + \beta \| \leq \| \alpha \| + \| \beta \| \\ \Longleftrightarrow \ & \| \alpha + \beta \|^2 \leq \| \alpha \|^2 + \| \beta \|^2 + 2 \| \alpha \| \| \beta \| \ . \end{aligned}$$

Proof:

$$\begin{aligned} \| \alpha + \beta \|^2 = & \| \alpha \|^2 + \| \beta \|^2 + 2 \,\mathrm{Re}\, \langle \alpha | \beta \rangle \leq \| \alpha \|^2 + \| \beta \|^2 + 2 |\langle \alpha | \beta \rangle| \\ \leq & \| \alpha \|^2 + \| \beta \|^2 + 2 \| \alpha \| \| \beta \| \qquad \text{q.e.d.} \end{aligned}$$

$\uparrow$ Schwarz's inequality

Solution 3.2.4 Proof by complete induction:

$\underline{j = 1}$

$$|d_1\rangle = \frac{|\psi_1\rangle}{\| \psi_1 \|} \implies \langle d_1 | d_1 \rangle = 1 \ .$$

$\underline{j = 2}$

$$\begin{aligned} |d_2\rangle &= \frac{|\psi_2\rangle - \langle d_1 | \psi_2 \rangle |d_1\rangle}{\| \ |\psi_2\rangle - \langle d_1 | \psi_2 \rangle d_1 \|} \ , \\ \langle d_1 | d_2 \rangle &\sim \langle d_1 | \psi_2 \rangle - \langle d_1 | \psi_2 \rangle \langle d_1 | d_1 \rangle = 0 \ . \end{aligned}$$

Normalization already clear!

$\underline{j \to j+1}$

$$|d_{j+1}\rangle = \frac{1}{\| \dots \|} \left\{ |\psi_{j+1}\rangle - \sum_{i=1}^{j} \langle d_i|\psi_j\rangle |d_i\rangle \right\} .$$

Let: $0 < n \leq j; \quad n \in \mathbb{N}$:

$$\langle d_n|d_{j+1}\rangle \sim \langle d_n|\psi_{j+1}\rangle - \sum_{i=1}^{j} \langle d_i|\psi_{j+1}\rangle \langle d_n|d_i\rangle$$

Induction hypothesis: $\langle d_n|d_i\rangle = \delta_{ni} \qquad \text{for} \quad i, n \leq j$

$$\Longrightarrow \quad \langle d_n|d_{j+1}\rangle \sim (\langle d_n|\psi_{j+1}\rangle - \langle d_n|\psi_{j+1}\rangle) = 0 .$$

Normalization already given by the ansatz!

Solution 3.2.5

1.

$$\langle \varphi_1|\varphi_1\rangle = a^2\langle v_1|v_1\rangle + b^2\langle v_2|v_2\rangle = a^2 \parallel v_1 \parallel^2 + b^2 \parallel v_2 \parallel^2 = \langle \varphi_2|\varphi_2\rangle ,$$
$$\langle \varphi_1|\varphi_2\rangle = a^2 \parallel v_1 \parallel^2 - b^2 \parallel v_2 \parallel^2 .$$

If one chooses

$$a = \frac{1}{\| v_1 \| \sqrt{2}} ; \qquad b = \frac{1}{\| v_2 \| \sqrt{2}} .$$

then:

$$\langle \varphi_1|\varphi_1\rangle = \langle \varphi_2|\varphi_2\rangle = 1 ; \qquad \langle \varphi_1|\varphi_2\rangle = 0 .$$

2. Norm:

$$\| \psi_1 \|^2 = \langle \psi_1|\psi_1\rangle = \frac{2}{\pi} \iint_a^{a+\pi} dp\, dp' \langle v_p|v_{p'}\rangle \cos p \cos p' =$$

$$= \frac{2}{\pi} \iint_a^{a+\pi} dp\, dp'\, \delta(p - p') \cos p \cos p' =$$

$$= \frac{2}{\pi} \int_a^{a+\pi} dp \cos^2 p = \frac{2}{\pi} \left[\frac{1}{2} \sin p \cos p + \frac{p}{2} \right]_a^{a+\pi} = 1 .$$

One finds analogously:

$$\| \psi_2 \|^2 = \langle \psi_2 | \psi_2 \rangle = 1 \ .$$

Scalar product:

$$\langle \psi_1 | \psi_2 \rangle = \frac{2}{\pi} \iint_a^{a+\pi} dp\, dp' \, \langle v_p | v_{p'} \rangle \cos p \sin p' =$$

$$= \frac{2}{\pi} \int_a^{a+\pi} dp \cos p \sin p = \frac{1}{\pi} \sin^2 p \Big|_a^{a+\pi} = 0 \ .$$

Solution 3.2.6

1. $\mathcal{H}$ is a complex linear vector space:

   a)

$$\sum_n |a_n + b_n|^2 \leq \sum_n \left(|a_n + b_n|^2 + |a_n - b_n|^2 \right) = 2 \sum_n \left(|a_n|^2 + |b_n|^2 \right) < \infty$$

   $\Longrightarrow$ when $\mathbf{a}$, $\mathbf{b} \in \mathcal{H}$, then also $\mathbf{a}+\mathbf{b}$. $\mathcal{H}$ is thus closed with respect to addition! That holds of course also for the multiplication by complex numbers!

   b) Requirements (3.9) to (3.14) are obviously fulfilled!

2. $\mathcal{H}$ is a unitary vector space:
   Because of

$$0 \leq \sum_n (|a_n| - |b_n|)^2$$

   we have

$$2 \sum_n |a_n| \, |b_n| \leq \sum_n \left(|a_n|^2 + |b_n|^2 \right) < \infty \ .$$

   For $\mathbf{a}$, $\mathbf{b} \in \mathcal{H}$ thus there exists the scalar product!

3. $\mathcal{H}$ is separable:
   Consider the column vectors

$$\mathbf{e}_n = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ \vdots \end{pmatrix} \leftarrow n\text{-th component},$$

   for which only the n-th component is equal to one, while all the others are zero. They build obviously a CON-basis:

$$\mathbf{e}_n \cdot \mathbf{e}_m = \delta_{nm} \ .$$

   Each vector $\mathbf{a}$ can be written as a linear combination of the $\mathbf{e}_n$!
4. $\mathcal{H}$ is complete:
   Cauchy sequence:

$$\left\| \mathbf{a}^{(n)} - \mathbf{a}^{(m)} \right\|^2 = \sum_\nu \left| a_\nu^{(n)} - a_\nu^{(m)} \right|^2 \ \to \ 0 \ .$$

   The summands are all non-negative, therefore each of them must already vanish:

$$\begin{aligned} & \left| a_\nu^{(n)} - a_\nu^{(m)} \right| \ \to \ 0 \qquad \forall \nu \\ \Longrightarrow \ & \left(a_\nu^{(n)} - a_\nu^{(m)} \right) \ \to \ 0 \qquad \forall \nu \ . \end{aligned}$$

   The complex numbers are complete. Therefore for each ν there exists a unique limit element α_ν with

$$\lim_{n \to \infty} a_\nu^{(n)} = \alpha_\nu \in \mathbb{C} \ .$$

   Hence, there is a limit vector $\boldsymbol{\alpha}$ with the components α_ν. We still have to show that $\boldsymbol{\alpha}$ belongs to $\mathcal{H}$. For this purpose we exploit once more the Cauchy sequence:

$$\sum_\nu \left| a_\nu^{(n)} - a_\nu^{(m)} \right|^2 < \varepsilon, \ \text{if } n, m > N(\varepsilon) \ .$$

Since the limit values exist, this holds in particular for $n \to \infty$:

$$\sum_{\nu} \left|\alpha_\nu - a_\nu^{(m)}\right|^2 < \varepsilon \ .$$

$\Longrightarrow$ the *new* vector $\left(\boldsymbol{\alpha} - \mathbf{a}^{(m)}\right)$ belongs to $\mathcal{H}$. Furthermore, $\mathbf{a}^{(m)} \in \mathcal{H}$. According to 1a) this is then also valid for the sum:

$$\left[(\boldsymbol{\alpha} - \mathbf{a}^{(m)}) + \mathbf{a}^{(m)}\right] = \boldsymbol{\alpha} \in \mathcal{H} \qquad \text{q.e.d.}$$

Solution 3.2.7 *A* Hermitian if

$$\langle\psi|\, A\, |\varphi\rangle = \langle\varphi|\, A\, |\psi\rangle^* \quad \forall\, |\varphi\rangle\,, |\psi\rangle \in \mathcal{H}$$

Now:

$$\begin{aligned}
\langle\psi|\, A\, |\varphi\rangle &= \langle\psi\ |\ A\ \varphi\rangle \\
&= \int_a^b dx\ \psi^*(x)\ (A\varphi)(x) \\
&= \int_a^b dx\ \psi^*(x)\varphi'(x) \\
&= \psi^*(x)\varphi(x)\Big|_a^b - \int_a^b dx\ \psi^{*\prime}(x)\varphi(x) \\
&= -\left\{\int_a^b dx\ \varphi^*(x)\psi'(x)\right\}^* \\
&= -\left\{\int_a^b dx\ \varphi^*(x)\ (A\psi)(x)\right\}^* \\
&= -\langle\varphi|\, A\, |\psi\rangle^* \\
&\stackrel{!}{=} \langle\varphi|\, A^\dagger\, |\psi\rangle^* \\
\curvearrowright \quad A^\dagger &= -A \ .
\end{aligned}$$

Solution 3.2.8

1.

$$\begin{aligned}\langle\gamma|(A+B)|\alpha\rangle &\overset{\text{Def.}}{=} \langle\alpha|(A+B)^+|\gamma\rangle^*\,,\\ \langle\gamma|(A+B)|\alpha\rangle &= \langle\gamma|A|\alpha\rangle + \langle\gamma|B|\alpha\rangle = \langle\alpha|A^+|\gamma\rangle^* + \langle\alpha|B^+|\gamma\rangle^* =\\ &= \langle\alpha|(A^+ + B^+)|\gamma\rangle^*\,.\end{aligned}$$

By comparison:

$$(A+B)^+ = A^+ + B^+\,.$$

2.

$$\begin{aligned}\langle\gamma|cA|\alpha\rangle &\overset{\text{Def.}}{=} \langle\alpha|(cA)^+|\gamma\rangle^*,\\ \langle\gamma|cA|\alpha\rangle &= c\langle\gamma|A|\alpha\rangle = c\langle\alpha|A^+|\gamma\rangle^* =\\ &= (c^*\langle\alpha|A^+|\gamma\rangle)^* = \langle\alpha|c^*A^+|\gamma\rangle^*\,.\end{aligned}$$

By comparison:

$$(cA)^+ = c^*A^+\,.$$

3.

$$\begin{aligned}\langle\gamma|(|\varphi\rangle\langle\psi|)|\alpha\rangle &\overset{\text{Def.}}{=} \langle\alpha|(|\varphi\rangle\langle\psi|)^+|\gamma\rangle^*,\\ \langle\gamma|(|\varphi\rangle\langle\psi|)|\alpha\rangle &= \langle\gamma|\varphi\rangle\langle\psi|\alpha\rangle = \langle\varphi|\gamma\rangle^*\langle\alpha|\psi\rangle^* =\\ &= (\langle\alpha|\psi\rangle\langle\varphi|\gamma\rangle)^* = \langle\alpha|(|\psi\rangle\langle\varphi|)|\gamma\rangle^*\,.\end{aligned}$$

By comparison:

$$(|\varphi\rangle\langle\psi|)^+ = |\psi\rangle\langle\varphi|\,.$$

4.

$$\begin{aligned}\langle\gamma|\mathbb{1}|\alpha\rangle &\overset{\text{Def.}}{=} \langle\alpha|\mathbb{1}^+|\gamma\rangle^*,\\ \langle\gamma|\mathbb{1}|\alpha\rangle &= \langle\gamma|\alpha\rangle = \langle\alpha|\gamma\rangle^* = \langle\alpha|\mathbb{1}|\gamma\rangle^*\,.\end{aligned}$$

By comparison:

$$\mathbb{1}^+ = \mathbb{1}\,.$$

Solution 3.2.9

1.

$$\begin{aligned} A = A^+ \,, \quad B = B^+ \\ (A\,B)^+ = B^+\,A^+ = B\,A \,, \\ (A\,B)^+ = A\,B \iff [A,B]_- = 0 \,. \end{aligned}$$

2a)

$$\begin{aligned} A = A^+ \,, \quad B = B^+ \\ \Longrightarrow \; [A,B]_-^+ = (A\,B)^+ - (B\,A)^+ = B^+A^+ - A^+B^+ \\ = B\,A - A\,B = -[A,B]_- \,. \end{aligned}$$

The commutator is *antihermitian*.

2b) Take

$$\begin{aligned} x = i\,\alpha [A,B]_- \,; \quad \alpha \in \mathbb{R} \\ \Longrightarrow \; x^+ = (i\,\alpha)^*\,[A,B]_-^+ = (-i\,\alpha)\,(-[A,B]_-) = x \,. \end{aligned}$$

Solution 3.2.10

1. For the adjoint operator we must have:

$$\varphi(x),\ \psi(x) \in L^2 :$$

$$\int\limits_{-\infty}^{+\infty} dx\,\varphi^\star(x)\,x\,\psi(x) \stackrel{!}{=} \int\limits_{-\infty}^{+\infty} dx\,\left((x^+\varphi(x)\right)^\star\,\psi(x) \,.$$

But we also have:

$$\int\limits_{-\infty}^{+\infty} dx\,\varphi^\star(x)\,x\,\psi(x) = \int\limits_{-\infty}^{+\infty} dx\,\left(x\varphi(x)\right)^\star\,\psi(x) \,.$$

The comparison yields, since φ and ψ are *arbitrary* elements from L^2:

$$x^+ = x \,.$$

2. The adjoint operator is defined by:

$$\varphi(x),\ \psi(x) \in L^2 :$$
$$\int_{-\infty}^{+\infty} dx\, \varphi^\star(x)\, \frac{d}{dx}\, \psi(x) \overset{!}{=} \int_{-\infty}^{+\infty} dx \left(\left(\frac{d}{dx} \right)^+ \varphi(x) \right)^\star \psi(x)\ .$$

On the other hand, we have:

$$\begin{aligned}\int_{-\infty}^{+\infty} dx\, \varphi^\star(x)\, \frac{d}{dx}\, \psi(x) &= \int_{-\infty}^{+\infty} dx\, \frac{d}{dx}\, (\varphi^\star(x)\, \psi(x)) - \\ &\quad - \int_{-\infty}^{+\infty} dx \left(\frac{d}{dx} \varphi^\star(x) \right) \psi(x) \\ &= \varphi^\star(x) \psi(x) \Big|_{-\infty}^{+\infty} - \\ &\quad - \int_{-\infty}^{+\infty} dx \left(\frac{d}{dx} \varphi(x) \right)^\star \psi(x)\ .\end{aligned}$$

The integrated part vanishes because φ and ψ are square integrable. The comparison yields then:

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

The differential operator is thus *antihermitian*!

3.

$$\left(\frac{\hbar}{i} \frac{d}{dx} \right)^+ \overset{(3.61)}{=} -\frac{\hbar}{i} \left(\frac{d}{dx} \right)^+ \overset{1.}{=} \frac{\hbar}{i} \frac{d}{dx}\ .$$

The component of the momentum operators $\hat{p}_x = \frac{\hbar}{i} \frac{d}{dx}$ is therewith Hermitian!

4. With (3.59) and the results from part 1. and part 2. it follows immediately:

$$\begin{aligned}\left(x p_y \right)^+ &= p_y^+ x^+ = p_y x = x p_y \quad \curvearrowright \text{ Hermitian} \\ \left(x p_x \right)^+ &= p_x^+ x^+ = p_x x = \left[p_x,\, x \right]_- + x p_x = \\ &= \frac{\hbar}{i} + x p_x \quad \curvearrowright \text{ non-Hermitian.}\end{aligned}$$

According to Exercise 3.2.9, the product of two Hermitian operators is also Hermitian if and only if the two operators commute!

5.

$$\left(-\hbar^2\frac{d^2}{dx^2}\right)^+ \overset{(3.59)}{=} \left(\frac{\hbar}{i}\frac{d}{dx}\right)^+\left(\frac{\hbar}{i}\frac{d}{dx}\right)^+ \overset{3.}{=} \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right) = -\hbar^2\frac{d^2}{dx^2}\ .$$

Real potential:

$$\varphi(x),\ \psi(x) \in L^2:$$
$$\int_{-\infty}^{+\infty} dx\,\varphi^\star(x)\,V(x)\,\psi(x) = \int_{-\infty}^{+\infty} dx\ (V(x)\varphi(x))^\star\,\psi(x)\ .$$

Therewith:

$$V^+(x) = V(x) \quad \curvearrowright \quad H^+ = H \quad \curvearrowright \text{ Hermitian.}$$

Solution 3.2.11

$$\begin{aligned} A|\alpha\rangle &= \alpha|\alpha\rangle\ ; \quad \alpha \text{ real} \\ \langle\alpha|[A,B]_-|\alpha\rangle &= \langle\alpha|A\,B|\alpha\rangle - \langle\alpha|B\,A|\alpha\rangle \\ &= \langle\alpha|B^+\,A^+|\alpha\rangle^* - \alpha\,\langle\alpha|B|\alpha\rangle \\ &= \langle\alpha|B^+\,A|\alpha\rangle^* - \alpha\,\langle\alpha|B|\alpha\rangle \\ &= \alpha\langle\alpha|B^+|\alpha\rangle^* - \alpha\langle\alpha|B|\alpha\rangle \\ &= \alpha\langle\alpha|B|\alpha\rangle - \alpha\langle\alpha|B|\alpha\rangle = 0\ . \end{aligned}$$

Solution 3.2.12 No! Take $B = \mathbb{1}$. Then certainly:

$$[A,\mathbb{1}]_- = 0\ ; \quad [\mathbb{1},C]_- = 0\ ,$$

although it must not necessarily be $[A,C]_- = 0$. Think of $A = x,\ C = p_x$!

Solution 3.2.13

1.

$$\begin{aligned} [A,B\,C]_- &= A\,B\,C - B\,C\,A = A\,B\,C - B\,A\,C + B\,A\,C - B\,C\,A \\ &= [A,B]_-\,C + B[A,C]_- \quad \text{q.e.d.} \end{aligned}$$

2.

$$\begin{aligned}[AB, C]_- &= A\,B\,C - C\,A\,B = A\,B\,C - A\,C\,B + A\,C\,B - C\,A\,B \\ &= A[B, C]_- + [A, C]_-\,B \quad \text{q.e.d.}\end{aligned}$$

3.

$$\begin{aligned}&A(B\,C - C\,B) - (B\,C - C\,B)\,A + \\ &+B(C\,A - A\,C) - (C\,A - A\,C)\,B + \\ &+C\,(A\,B - B\,A) - (A\,B - B\,A)\,C = 0\,.\end{aligned}$$

Solution 3.2.14 Complete induction:

The statements are obviously correct for $n = 1$. Let they be valid also for n. We check it for $(n + 1)$. For that we use the partial results 1. and 2. from Exercise 3.2.13:

1.

$$\left[A, B^{n+1}\right]_- = [A, B]\,B^n + B[A, B^n] = i\,\mathbb{1}\,B^n + B\,i\,n\,B^{n-1} = i\,(n+1)\,B^n \quad \text{q.e.d.}$$

2.

$$\left[A^{n+1}, B\right] = A^n[A, B] + [A^n, B]\,A = A^n\,i\,\mathbb{1} + i\,n\,A^{n-1}\,A = i\,(n+1)\,A^n \quad \text{q.e.d.}$$

Solution 3.2.15

1. Proof by complete induction:
   $\underline{n = 2:}$

$$[A, B_1 \cdot B_2]_- = B_1\,[A, B_2]_- + [A, B_1]_-\,B_2$$

   $\underline{n \to n + 1:}$
   Given: $C_n = B_1 \cdot B_2 \cdot \cdots \cdot B_n$

$$\begin{aligned}\curvearrowright \quad [A, C_{n+1}]_- &= [A, C_n \cdot B_{n+1}]_- \\ &= C_n\,[A, B_{n+1}]_- + [A, C_n]_-\,B_{n+1} \\ &= B_1 \cdot \cdots \cdot B_n\,[A, B_{n+1}]_- \\ &\quad + \sum_{m=1}^{n} B_1 \cdot \cdots \cdot B_{m-1}\,[A, B_m]_-\,B_{m+1} \cdot \cdots \cdot B_n B_{n+1} \\ &= \sum_{m=1}^{n+1} B_1 \cdot \cdots \cdot B_{m-1}\,[A, B_m]_-\,B_{m+1} \cdot \cdots \cdot B_{n+1} \quad \text{q. e. d.}\end{aligned}$$

2. Take in 1.: $B_1 = B_2 = \cdots = B_n = B$

$$[A, B^n]_- = \sum_{m=1}^{n} B^{m-1} [A, B]_- B^{n-m}$$

especially:

$$[A, B]_- = 0 \quad \curvearrowright \quad [A, B^n]_- = 0$$

3. $[A, B]_- = C \neq 0$
with part 2.:

$$[A, B^n]_- = \sum_{m=1}^{n} B^{m-1} C B^{n-m} \quad (*)$$

furthermore:

$$[C, B]_- = 0$$

means according to 2.:

$$[C, B^n]_- = 0$$

used in $(*)$:

$$\begin{aligned} [A, B^n]_- &= \sum_{m=1}^{n} C B^{m-1} B^{n-m} \\ &= \sum_{m=1}^{n} C B^{n-1} \\ &= n C B^{n-1} \\ &= n [A, B]_- B^{n-1} \end{aligned}$$

Solution 3.2.16 Baker-Hausdorff theorem

1.

$$e^{\lambda A} B e^{-\lambda A} = \sum_{n=0}^{\infty} \underbrace{\alpha_n}_{\text{operators}} \lambda^n \equiv f(\lambda)$$

$$\text{with} \quad A \neq A(\lambda) \text{ and } B \neq B(\lambda)$$

$$
\begin{aligned}
\curvearrowright \quad \frac{d}{d\lambda} f(\lambda) &= e^{\lambda A}(AB - BA)e^{-\lambda A} \\
&= e^{\lambda A}\,[A,B]_-\,e^{-\lambda A} \\
\curvearrowright \quad \frac{d^2}{d\lambda^2} f(\lambda) &= e^{\lambda A}\,(A\,[A,B]_- - [A,B]_-\,A)\,e^{-\lambda A} \\
&= e^{\lambda A}\,[A,[A,B]_-]_-\,e^{-\lambda A} \\
&\vdots \\
\frac{d^n}{d\lambda^n} f(\lambda) &= e^{\lambda A}\,\underbrace{\big[A,[A,\ldots[A,B]_-\ldots]_-\big]_-}_{n\text{-fold commutator}}\,e^{-\lambda A}
\end{aligned}
$$

Expand $f(\lambda)$ around $\lambda = 0$:

$$
\begin{aligned}
f(\lambda) &= f(0) + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} \left(\frac{d^n}{d\lambda^n} f(\lambda) \right)_{\lambda=0} \\
&= B + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} \underbrace{\big[A,[A,\ldots[A,B]_-\ldots]_-\big]_-}_{n\text{-fold commutator}}
\end{aligned}
$$

by comparison one gets:

$$
\begin{aligned}
\alpha_0 &= B \\
\alpha_n &= \big[A,[A,\ldots[A,B]_-\ldots]_-\big]_- \cdot \frac{1}{n!} \qquad n \geq 1
\end{aligned}
$$

2.

$$
\begin{aligned}
[A,[A,B]_-]_- &= 0 \\
\curvearrowright \quad \alpha_n &= 0 \ \text{ for } n \geq 2 \\
\alpha_0 &= B \\
\alpha_1 &= [A,B]_- \\
\curvearrowright \quad f(\lambda) &= e^{\lambda A} B e^{-\lambda A} = B + \lambda\,[A,B]_-
\end{aligned}
$$

3.

$$
\begin{aligned}
g(\lambda) &\equiv e^{\lambda A} e^{\lambda B} \\
\curvearrowright \quad \frac{d}{d\lambda} g(\lambda) &= e^{\lambda A}(A + B)\,\underbrace{e^{\lambda B}}_{e^{-\lambda A} g(\lambda)} \\
&= (A + f(\lambda))\,g(\lambda)
\end{aligned}
$$

with the result from 2.:

$$\frac{d}{d\lambda}g(\lambda) = (A + B + \lambda\,[A, B]_-)\,g(\lambda)$$

4. According to the presumption:

$$[(A + B), [A, B]_-]_- = 0$$

because of the commutability of $(A + B)$ and $[A, B]_-$, the coefficient $(A + B + \lambda[A, B]_-)$ in the differential equation from 3. behaves during the integration process like a simple c-number:

$$\begin{aligned}
&\frac{d}{d\lambda}g(\lambda) = (c_1 + \lambda c_2)\,g(\lambda)\\
\curvearrowright\ &g(\lambda) = \exp\left(c_1\lambda + \frac{1}{2}c_2\lambda^2\right)\\
\curvearrowright\ &g(1) = \exp\left(c_1 + \frac{1}{2}c_2\right)\\
\curvearrowright\ &e^A e^B = \exp\left(A + B + \frac{1}{2}[A, B]_-\right)
\end{aligned}$$

Solution 3.2.17

1. Let $\{|\varphi_\nu\rangle\}, \{|\psi_\nu\rangle\}$ be two different CON-bases of M. Expansion law:

$$\begin{aligned}
|\varphi_\nu\rangle &= \sum\!\!\!\!\!\!\int_\mu |\psi_\mu\rangle\langle\psi_\mu|\varphi_\nu\rangle\ ,\\
\langle\varphi_\nu| &= \sum\!\!\!\!\!\!\int_\mu \langle\psi_\mu|\langle\varphi_\nu|\psi_\mu\rangle
\end{aligned}$$

$$\begin{aligned}
\Longrightarrow\ P_M &= \sum\!\!\!\!\!\!\int_\nu |\varphi_\nu\rangle\langle\varphi_\nu| = \sum\!\!\!\!\!\!\int_\nu \sum\!\!\!\!\!\!\int_\mu \sum\!\!\!\!\!\!\int_{\mu'} |\psi_\mu\rangle\langle\psi_\mu|\varphi_\nu\rangle\langle\varphi_\nu|\psi_{\mu'}\rangle\langle\psi_{\mu'}| =\\
&= \sum\!\!\!\!\!\!\int_\mu \sum\!\!\!\!\!\!\int_{\mu'} |\psi_\mu\rangle\langle\psi_\mu| \underbrace{P_M|\psi_{\mu'}\rangle}_{=|\psi_{\mu'}\rangle,\ \text{since}\ |\psi_{\mu'}\rangle\in M} \langle\psi_{\mu'}| =\\
&= \sum\!\!\!\!\!\!\int_\mu \sum\!\!\!\!\!\!\int_{\mu'} |\psi_\mu\rangle\delta_{\mu\mu'}\langle\psi_{\mu'}| = \sum\!\!\!\!\!\!\int_\mu |\psi_\mu\rangle\langle\psi_\mu| \quad \text{q.e.d.}
\end{aligned}$$

2. $|\psi_{1,2}\rangle \in \mathcal{H}$.

$$\langle\psi_1|P_M|\psi_2\rangle \overset{\text{Def.}}{=} \langle\psi_2|P_M^+|\psi_1\rangle^* ,$$

$$\langle\psi_1|P_M|\psi_2\rangle = \langle\psi_1|\left(\sum_\nu |\varphi_\nu\rangle\langle\varphi_\nu|\right)|\psi_2\rangle = \sum_\nu \langle\psi_2|\varphi_\nu\rangle^*\langle\varphi_\nu|\psi_1\rangle^*$$

$$= \left[\langle\psi_2|\left(\sum_\nu |\varphi_\nu\rangle\langle\varphi_\nu|\right)|\psi_1\rangle\right]^* = \langle\psi_2|P_M|\psi_1\rangle^* .$$

$|\psi_1\rangle$, $|\psi_2\rangle$ **arbitrary** from $\mathcal{H}$. It follows therefore by comparison:

$$P_M^+ = P_M .$$

3.

$$P_M^2 = \sum_{\nu,\mu} |\varphi_\nu\rangle\langle \underbrace{\varphi_\nu|\varphi_\mu}_{\delta_{\nu\mu}}\rangle\langle\varphi_\mu| = \sum_\nu |\varphi_\nu\rangle\langle\varphi_\nu| = P_M .$$

4a)

$$(P_L P_M)^2 = P_L P_M P_L P_M = P_L (P_L P_M) P_M + P_L [P_M, P_L]_- P_M$$
$$= P_L P_M + P_L [P_M, P_L]_- P_M ,$$
$$(P_L P_M)^+ = P_M^+ P_L^+ = P_M P_L = P_L P_M + [P_M, P_L]_- .$$

$\Longrightarrow$ $P_L P_M$ Hermitian and idempotent, if $[P_M, P_L]_- = 0$.
$\Longrightarrow$ $P_L P_M$ projects onto the intersection $M \cap L$!

4b)

$$(P_L + P_M)^+ = P_L^+ + P_M^+ = P_L + P_M, \text{ thus Hermitian,}$$
$$(P_L + P_M)^2 = P_L^2 + P_M^2 + P_L P_M + P_M P_L \overset{!}{=} P_L + P_M,$$
$$\text{if } P_L P_M = P_M P_L = 0 .$$

Holds exactly when $M \cap L = \emptyset$. $(P_L + P_M)$ projects onto $M \cup L$.

4c)

$$(P_L - P_M)^+ = P_L - P_M, \text{ thus Hermitian,}$$
$$(P_L - P_M)^2 = P_L^2 + P_M^2 - P_L P_M - P_M P_L$$

$$= P_L + P_M - (P_L P_M + P_M P_L)$$
$$\stackrel{!}{=} P_L - P_M, \text{ if } P_L P_M + P_M P_L = 2 P_M \ .$$

This is fulfilled if $L \supseteq M$. $(P_L - P_M)$ projects $\mathcal{H}$ onto L/M!

Solution 3.2.18

1. CON-basis, therefore: $\mathbb{1} = |\varphi_1\rangle\langle\varphi_1| + |\varphi_2\rangle\langle\varphi_2|$:

$$A = A\mathbb{1} = -|\varphi_2\rangle\langle\varphi_1| - |\varphi_1\rangle\langle\varphi_2| \ .$$

2. With part 3. in Exercise 3.2.8:

$$A^+ = -(|\varphi_2\rangle\langle\varphi_1|)^+ - (|\varphi_1\rangle\langle\varphi_2|)^+ = -|\varphi_1\rangle\langle\varphi_2| - |\varphi_2\rangle\langle\varphi_1| = A$$
$$\Longrightarrow A \text{ Hermitian.}$$

3. $A A^+ = A^+ A = A^2$ because of 2.:

$$A^2 = (|\varphi_2\rangle\langle\varphi_1| + |\varphi_1\rangle\langle\varphi_2|)\,(|\varphi_2\rangle\langle\varphi_1| + |\varphi_1\rangle\langle\varphi_2|)$$
$$\Longrightarrow A^2 = |\varphi_2\rangle\langle\varphi_2| + |\varphi_1\rangle\langle\varphi_1| = \mathbb{1} \ .$$

4. Eigen-value equation:

$$A|a\rangle = a|a\rangle \implies A^2|a\rangle = a^2|a\rangle = \mathbb{1}|a\rangle = |a\rangle \ .$$

$\Longrightarrow$ eigen-values: $a_+ = +1;\ a_- = -1$.
eigen-states:

$$|a_\pm\rangle = \alpha_\pm^{(1)}|\varphi_1\rangle + \alpha_\pm^{(2)}|\varphi_2\rangle \ ,$$
$$A|a_\pm\rangle = -\left(\alpha_\pm^{(1)}\,|\varphi_2\rangle\ + \alpha_\pm^{(2)}\,|\varphi_1\rangle\right) = \pm\left(\alpha_\pm^{(1)}\,|\varphi_1\rangle\ + \alpha_\pm^{(2)}\,|\varphi_2\rangle\right)$$
$$\Longrightarrow\ \alpha_+^{(1)} = -\alpha_+^{(2)};\quad \alpha_-^{(1)} = \alpha_-^{(2)} \ .$$

Normalization: $\langle a_\pm|a_\pm\rangle = 1$

$$\Longrightarrow\ |a_\pm\rangle = \frac{1}{\sqrt{2}}\,(|\varphi_1\rangle \mp |\varphi_2\rangle) \ .$$

Solution 3.2.19

1. Hermiticity of A and B:
   Let $|\psi\rangle, |\varphi\rangle$ be arbitrary $\in \mathcal{H}$:

$$\langle\psi|A|\varphi\rangle \equiv \langle\varphi|A^\dagger|\psi\rangle^* \stackrel{!}{=} \langle\varphi|A|\psi\rangle^* \,.$$

   This means:

$$\begin{aligned}
|\varphi\rangle &= \sum_j \beta_j |\alpha_j\rangle \\
|\psi\rangle &= \sum_j \gamma_j |\alpha_j\rangle \\
A_{ij} &\equiv \langle\alpha_i|A|\alpha_j\rangle \\
\curvearrowright\ \langle\psi|A|\varphi\rangle &= \sum_{i,j} \gamma_i^* \beta_j A_{ij} \\
&\stackrel{!}{=} \langle\varphi|A|\psi\rangle^* \\
&= \sum_{n,m} \left(\beta_n^* \gamma_m\right)^* A_{nm}^* \\
&= \sum_{n,m} \beta_n \gamma_m^* A_{nm}^* \,.
\end{aligned}$$

   The assertion is proven, since $|\psi\rangle, |\varphi\rangle$ are arbitrary, if $A_{ij} = A_{ji}^*$.

$$A \equiv \begin{pmatrix} 3 & i\sqrt{2} & 1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ 1 & -i\sqrt{2} & 3 \end{pmatrix} \qquad \curvearrowright\ A_{ij} = A_{ji}^*$$

$$B \equiv \begin{pmatrix} 1 & -i\sqrt{2} & 1 \\ i\sqrt{2} & 0 & -i\sqrt{2} \\ 1 & i\sqrt{2} & 1 \end{pmatrix} \qquad \curvearrowright\ B_{ij} = B_{ji}^*$$

   $\curvearrowright$ A and B are Hermitian.

2. Eigen-values and eigen-states of A and B

   The homogeneous system of equations (3.115), following from the eigen-value equation of the operator A, has non-trivial solutions if

$$\det\{\langle\alpha_i|A|\alpha_j\rangle - a\delta_{ij}\} \stackrel{!}{=} 0 \,.$$

This means:

$$\det \begin{pmatrix} 3-a & i\sqrt{2} & 1 \\ -i\sqrt{2} & 2-a & i\sqrt{2} \\ 1 & -i\sqrt{2} & 3-a \end{pmatrix} \stackrel{!}{=} 0$$

$$\curvearrowright \quad (3-a)^2(2-a) - 2 - 2 - 2 + a - 2(3-a) - 2(3-a) \stackrel{!}{=} 0$$

$$\curvearrowright \quad -a(a-4)^2 \stackrel{!}{=} 0$$

Eigen-values of A:

$$a_1 = 0$$
$$a_2 = 4 \qquad \text{(twofold degenerate)}$$

Eigen-states to $a_1 = 0$:

$$\begin{pmatrix} 3 & i\sqrt{2} & 1 \\ -i\sqrt{2} & 2 & i\sqrt{2} \\ 1 & -i\sqrt{2} & 3 \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{13} \end{pmatrix} \stackrel{!}{=} 0$$

$$\begin{aligned} \curvearrowright \quad & 3a_{11} + i\sqrt{2}a_{12} + a_{13} = 0 \\ & -i\sqrt{2}a_{11} + 2a_{12} + i\sqrt{2}a_{13} = 0 \\ & a_{11} - i\sqrt{2}a_{12} + 3a_{13} = 0 \\ & \qquad \curvearrowright \quad a_{13} = -3a_{11} - i\sqrt{2}a_{12} \\ \curvearrowright \quad & -i\sqrt{2}a_{11} + 2a_{12} - 3i\sqrt{2}a_{11} + 2a_{12} = 0 \\ & \qquad \curvearrowright \quad a_{11} = -\frac{i}{\sqrt{2}}a_{12} \\ & \qquad \curvearrowright \quad a_{13} = \frac{i}{\sqrt{2}}a_{12} \end{aligned}$$

Normalization:

$$\begin{aligned} 1 &\stackrel{!}{=} |a_{11}|^2 + |a_{12}|^2 + |a_{13}|^2 \\ &= 2|a_{12}|^2 \,. \end{aligned}$$

The phase can be chosen arbitrarily $\curvearrowright$ w. l. o. g.: a_{12} real.

$$\curvearrowright \quad a_{12} = \frac{1}{\sqrt{2}} \qquad a_{11} = -\frac{i}{2} \qquad a_{13} = \frac{i}{2}$$

$$\curvearrowright \quad |a_1\rangle = -\frac{i}{2}|\alpha_1\rangle + \frac{1}{\sqrt{2}}|\alpha_2\rangle + \frac{i}{2}|\alpha_3\rangle$$

Eigen-states to $a_2 = 4$:

$$\begin{pmatrix} -1 & i\sqrt{2} & 1 \\ -i\sqrt{2} & -2 & i\sqrt{2} \\ 1 & -i\sqrt{2} & -1 \end{pmatrix} \begin{pmatrix} a_{21} \\ a_{22} \\ a_{23} \end{pmatrix} \stackrel{!}{=} 0$$

$$\curvearrowright \quad -a_{21} + i\sqrt{2}a_{22} + a_{23} = 0 \, .$$

The two other equations are identically fulfilled

$$\curvearrowright \quad a_{23} = a_{21} - i\sqrt{2}a_{22} \, .$$

Let $|a_2\rangle$ and $|a_3\rangle$ be arbitrary, linearly independent states from the two-dimensional eigen-space to $a_2 = 4$.
Therefore it can be assumed $a_{22} = 0$.
Normalization:

$$a_{23} = a_{21} = \frac{1}{\sqrt{2}}$$

$$\curvearrowright \quad |a_2\rangle = \frac{1}{\sqrt{2}} \left(|\alpha_1\rangle + |\alpha_3\rangle\right) \, .$$

Obviously $\langle a_1|a_2\rangle = 0$.
For $|a_3\rangle$ it must now be:

$$-a_{31} + i\sqrt{2}a_{32} + a_{33} = 0$$

$$0 = \langle a_1|a_3\rangle = \frac{i}{2}a_{31} + \frac{1}{\sqrt{2}}a_{32} - \frac{i}{2}a_{33}$$

$$0 = \langle a_2|a_3\rangle = \frac{1}{\sqrt{2}}a_{31} + \frac{1}{\sqrt{2}}a_{33}$$

$$\curvearrowright \quad a_{33} = -a_{31}$$

$$a_{31} = \frac{i}{\sqrt{2}}a_{32} \, .$$

Normalization:

$$1 = |a_{31}|^2 + |a_{32}|^2 + |a_{33}|^2 = 4|a_{31}|^2 \, .$$

The phase is freely selectable.
$\curvearrowright a_{31}$ can be chosen to be real.

$$\curvearrowright \; a_{31} = \frac{1}{2} = -a_{33} \qquad a_{32} = -\frac{i}{\sqrt{2}}$$

$$\curvearrowright \; |a_3\rangle = \frac{1}{2}|\alpha_1\rangle - \frac{i}{\sqrt{2}}|\alpha_2\rangle - \frac{1}{2}|\alpha_3\rangle \, .$$

Operator B

$$\det\{\langle\alpha_i|B|\alpha_j\rangle - b\delta_{ij}\rangle \stackrel{!}{=} 0$$

$$\det \begin{pmatrix} 1-b & -i\sqrt{2} & 1 \\ i\sqrt{2} & -b & -i\sqrt{2} \\ 1 & i\sqrt{2} & 1-b \end{pmatrix} \stackrel{!}{=} 0 \, .$$

Eigen-values of B:

$$\begin{aligned} & -b(1-b)^2 - 2 - 2 + b - 2(1-b) - 2(1-b) = 0 \\ \curvearrowright \; & -(b-2)^2(b+2) = 0 \\ \curvearrowright \; & b_1 = 2 \qquad b_2 = 2 \qquad b_3 = -2 \, . \end{aligned}$$

Eigen-states of B:
to the eigen-value $b_3 = -2$:

$$\begin{pmatrix} 3 & -i\sqrt{2} & 1 \\ i\sqrt{2} & 2 & -i\sqrt{2} \\ 1 & i\sqrt{2} & 3 \end{pmatrix} \begin{pmatrix} b_{31} \\ b_{32} \\ b_{33} \end{pmatrix} = 0$$

$$\begin{aligned} \curvearrowright \; & 3b_{31} - i\sqrt{2}b_{32} + b_{33} = 0 \\ & \qquad \curvearrowright \; b_{33} = -3b_{31} + i\sqrt{2}b_{32} \\ & i\sqrt{2}b_{31} + 2b_{32} - i\sqrt{2}b_{33} = 0 \\ \curvearrowright \; & i\sqrt{2}b_{31} + 2b_{32} + 3i\sqrt{2}b_{31} + 2b_{32} = 0 \\ & \qquad \curvearrowright \; b_{32} = -i\sqrt{2}b_{31} \\ & \qquad\qquad b_{33} = -b_{31} \, . \end{aligned}$$

Normalization:

$$1 = |b_{31}|^2 + 2|b_{31}|^2 + |b_{31}|^2 = 4|b_{31}|^2 \ .$$

The phase is freely selectable.

$$\curvearrowright \ b_{31} = \frac{1}{2} \qquad b_{32} = -\frac{i}{\sqrt{2}} \qquad b_{33} = -\frac{1}{2}$$

$$|b_3\rangle = \frac{1}{2}|\alpha_1\rangle - \frac{i}{\sqrt{2}}|\alpha_2\rangle - \frac{1}{2}|\alpha_3\rangle \ .$$

To the eigen-values $b_{1,2} = 2$ (degeneracy):

$$\begin{pmatrix} -1 & -i\sqrt{2} & 1 \\ i\sqrt{2} & -2 & -i\sqrt{2} \\ 1 & i\sqrt{2} & -1 \end{pmatrix} \begin{pmatrix} b_{11} \\ b_{12} \\ b_{13} \end{pmatrix} = 0$$

$$\curvearrowright \quad -b_{11} - i\sqrt{2}b_{12} + b_{13} = 0 \ .$$

The two other equations are identically fulfilled:

$$b_{13} = b_{11} + i\sqrt{2}b_{12}$$

$|b_1\rangle, |b_2\rangle$ not unique, linearly independent states of the two-dimensional eigenspace to $b = 2$.
We can therefore choose:

$$b_{12} = 0$$

Normalization:

$$b_{13} = b_{11} = \frac{1}{\sqrt{2}}$$

$$\curvearrowright \ |b_1\rangle = \frac{1}{\sqrt{2}} \left(|\alpha_1\rangle + |\alpha_3\rangle\right) \ .$$

Obviously $\langle b_1|b_3\rangle = 0$.
For $|b_2\rangle$ it is now to require:

$$-b_{21} - i\sqrt{2}b_{22} + b_{23} = 0 \ ,$$

$$0 = \langle b_3|b_2\rangle \ = \frac{1}{2}b_{21} + \frac{i}{\sqrt{2}}b_{22} - \frac{1}{2}b_{23}$$

$$0 = \langle b_1|b_2\rangle = \frac{1}{\sqrt{2}}b_{21} + \frac{1}{\sqrt{2}}b_{23}$$
$$\curvearrowright \quad b_{21} = -b_{23}$$
$$b_{21} = -\frac{i}{\sqrt{2}}b_{22} \; .$$

Normalization:

$$1 = |b_{21}|^2 + |b_{22}|^2 + |b_{23}|^2 = 4|b_{21}|^2 \; .$$

The phase can be chosen arbitrarily.
$\curvearrowright$ b_{21} can be assumed to be real.

$$\curvearrowright \quad b_{21} = \frac{1}{2} = -b_{23} \qquad b_{22} = \frac{i}{\sqrt{2}}$$
$$\curvearrowright \quad |b_2\rangle = \frac{1}{2}|\alpha_1\rangle + \frac{i}{\sqrt{2}}|\alpha_2\rangle - \frac{1}{2}|\alpha_3\rangle \; .$$

3. Therefore:

$$|b_1\rangle = |a_2\rangle$$
$$|b_2\rangle = i|a_1\rangle$$
$$|b_3\rangle = |a_3\rangle \; .$$

$\curvearrowright$ A and B have a common set of eigen-states.
$\curvearrowright$ $[A, B]_- = 0$.

Solution 3.2.20

1.

$$A|a_i\rangle = a_i\,|a_i\rangle \qquad i = 1, 2, 3, \ldots$$
$$\text{spectral representation} \quad (3.68): \qquad A = \sum_i a_i\,|a_i\rangle\langle a_i|$$
$$\text{expansion law} \quad (3.66): \qquad |\psi\rangle = \sum_i |a_i\rangle\langle a_i|\psi\rangle \quad \in \mathcal{H}$$

$$|\psi\rangle \neq |0\rangle \;\curvearrowright\; \text{for at least one } i\text{:} \quad \langle a_i|\psi\rangle \neq 0 \;\text{ with }\; |\langle a_i|\psi\rangle|^2 > 0 \; .$$

We use this to prove the assertion:

(a) $\underline{a_i > 0 \ \forall i}$
Then:

$$\begin{aligned}\langle\psi|A|\psi\rangle &= \sum_i \langle\psi|A|a_i\rangle\langle a_i|\psi\rangle \\ &= \sum_i a_i \langle\psi|a_i\rangle\langle a_i|\psi\rangle \\ &= \sum_i a_i \, |\langle a_i|\psi\rangle|^2 \\ &> 0 \, .\end{aligned}$$

(b) $\underline{\langle\psi|A|\psi\rangle > 0 \ ; \ \forall|\psi\rangle \in \mathcal{H} \ ; \ |\psi\rangle \neq |0\rangle}$
Then:

$$\langle\psi|A|\psi\rangle = \sum_i a_i |\langle a_i|\psi\rangle|^2 > 0 \quad \forall|\psi\rangle \neq |0\rangle$$

Choose in particular:

$$|\psi\rangle = |a_j\rangle \quad \curvearrowright \quad \langle\psi|A|\psi\rangle = a_j > 0 \ \ \forall j$$

The assertion is therewith proven!

2. Operator A in 'φ-representation':

$$A = \begin{pmatrix} 1 & 0 & -\sqrt{2} \\ 0 & 3 & 0 \\ -\sqrt{2} & 0 & 5 \end{pmatrix} .$$

From that one reads off:

$$\left(A^+\right)_{ij} \overset{(3.120)}{=} A^\star_{ji} = A_{ij} \quad \curvearrowright \ A = A^+$$

The operator A is thus Hermitian!
Eigen-values of A:

$$\det \begin{pmatrix} 1-a & 0 & -\sqrt{2} \\ 0 & 3-a & 0 \\ -\sqrt{2} & 0 & 5-a \end{pmatrix} \overset{!}{=} 0 = (3-a)\big((1-a)(5-a)-2\big) \, .$$

First eigen-value:

$$\underline{a_1 = 3}$$

The two others from

$$(1-a)(5-a) = 2 = a^2 - 6a + 5 \;\curvearrowright\; (a-3)^2 = 6$$
$$\curvearrowright \qquad \underline{a_2 = 3 - \sqrt{6}} \;;\; \underline{a_3 = 3 + \sqrt{6}}\,.$$

All eigen-values are greater than zero. The operator is therefore *positive-definite*!
Checking:
Arbitrary state in the 'φ-representation':

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

$|\psi\rangle \neq |0\rangle \;\curvearrowright$ at least one $\psi_i \neq 0$.

$$\begin{aligned}
\langle\psi|A|\psi\rangle &= \begin{pmatrix} \psi_1^\star & \psi_2^\star & \psi_3^\star \end{pmatrix} \begin{pmatrix} 1 & 0 & -\sqrt{2} \\ 0 & 3 & 0 \\ -\sqrt{2} & 0 & 5 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \\
&= \begin{pmatrix} \psi_1^\star & \psi_2^\star & \psi_3^\star \end{pmatrix} \begin{pmatrix} \psi_1 - \sqrt{2}\psi_3 \\ 3\psi_2 \\ -\sqrt{2}\psi_1 + 5\psi_3 \end{pmatrix} \\
&= |\psi_1|^2 - \sqrt{2}\psi_1^\star\psi_3 + 3|\psi_2|^2 - \sqrt{2}\psi_3^\star\psi_1 + 5|\psi_3|^2 \\
&= \left(|\psi_1|^2 - \sqrt{2}\psi_1^\star\psi_3 - \sqrt{2}\psi_1\psi_3^\star + 2|\psi_3|^2\right) + 3|\psi_2|^2 + 3|\psi_3|^2 \\
&= \left(\psi_1 - \sqrt{2}\psi_3\right)\left(\psi_1^\star - \sqrt{2}\psi_3^\star\right) + 3|\psi_2|^2 + 3|\psi_3|^2 \\
&= \left|\psi_1 - \sqrt{2}\psi_3\right|^2 + 3|\psi_2|^2 + 3|\psi_3|^2\,.
\end{aligned}$$

Since at least one ψ_i is unequal zero, it follows:

$$\langle\psi|A|\psi\rangle > 0 \;\text{ for arbitrary }\; |\psi\rangle \neq |0\rangle\,.$$

That was to be shown!

Solution 3.2.21

$$A^{-1}A|a\rangle = \mathbb{1}|a\rangle = aA^{-1}|a\rangle$$
$$a \neq 0 \implies A^{-1}|a\rangle = a^{-1}|a\rangle \ .$$

Solution 3.2.22 No, because there is no one-to-one mapping. All $|\psi\rangle \in \mathcal{H}$ with the same $\langle\alpha|\psi\rangle$ are mapped by $P(|\alpha\rangle)$ onto the same vector:

$$P(|\alpha\rangle)|\psi\rangle = |\alpha\rangle\langle\alpha|\psi\rangle \ .$$

Solution 3.2.23

1.

$$U|u\rangle = u|u\rangle$$
$$\implies \langle u|U^+U|u\rangle = u\langle u|U^+|u\rangle = u^*u\langle u|u\rangle = \langle u|\mathbb{1}|u\rangle = \langle u|u\rangle$$
$$\implies |u| = 1 \ .$$

2.

$$A = A^+ \ ; \qquad \overline{A} = UAU^+$$
$$(\overline{A})^+ = (UAU^+)^+ = (U^+)^+(UA)^+ = UA^+U^+ = UAU^+, \text{ since } A \text{ Hermitian}$$
$$\implies \overline{A}^+ = \overline{A} \implies \overline{A} \text{ Hermitian} \ .$$

3.

$$\overline{A} = UAU^+ \ ; \quad \overline{B} = UBU^+ \ ; \quad [A,B]_- = 0$$
$$[\overline{A},\overline{B}]_- = \overline{A}\,\overline{B} - \overline{B}\,\overline{A} = UAU^+UBU^+ - UBU^+UAU^+$$
$$= UABU^+ - UBAU^+ = U[A,B]_-U^+ = 0 \ .$$

Solution 3.2.24

1. We use directly the definition (3.103):

$$\frac{d}{dA}(f(A)+g(A)) = \lim_{\varepsilon\to 0}\frac{[f(A+\varepsilon\mathbb{1})+g(A+\varepsilon\mathbb{1})]-(f(A)+g(A))}{\varepsilon} =$$
$$= \lim_{\varepsilon\to 0}\left\{\frac{f(A+\varepsilon\mathbb{1})-f(A)}{\varepsilon} + \frac{g(A+\varepsilon\mathbb{1})-g(A)}{\varepsilon}\right\} =$$
$$= \frac{d}{dA}f(A) + \frac{d}{dA}g(A) \qquad \text{q.e.d.}$$

2.

$$\begin{aligned}
&\frac{d}{dA}\left(f(A)\,g(A)\right) = \\
&= \lim_{\varepsilon\to 0} \frac{f(A+\varepsilon\mathbb{1})\,g(A+\varepsilon\mathbb{1}) - f(A)\,g(A)}{\varepsilon} = \\
&= \lim_{\varepsilon\to 0} \left\{ \frac{[f(A+\varepsilon\mathbb{1}) - f(A)]\,g(A)}{\varepsilon} + \frac{f(A+\varepsilon\mathbb{1})\,[g(A+\varepsilon\mathbb{1}) - g(A)]}{\varepsilon} \right\} = \\
&= \frac{df}{dA}\,g(A) + f(A)\,\frac{dg}{dA}\,.
\end{aligned}$$

3. Complete induction.
   $\underline{n=1}$

$$\frac{d}{dA}A = \lim_{\varepsilon\to 0}\frac{A+\varepsilon\mathbb{1}-A}{\varepsilon} = \mathbb{1}\,.$$

   $\underline{n=2}$

$$\frac{d}{dA}A^2 \overset{2)}{=} \frac{dA}{dA}A + A\,\frac{dA}{dA} = 2A\,.$$

   $\underline{n \implies n+1}$
   Let the assertion be correct for n:

$$\begin{aligned}
\frac{d}{dA}A^{n+1} = \frac{d}{dA}\left(A\,A^n\right) &\overset{2.}{=} \frac{dA}{dA}A^n + A\,\frac{dA^n}{dA} = \\
&= \mathbb{1}\,A^n + A\,n\,A^{n-1} = (n+1)\,A^n \quad \text{q.e.d.}
\end{aligned}$$

Solution 3.2.25

1. We use the definition (3.102):

$$\begin{aligned}
&\frac{d}{d\eta}A(\eta)\,B(\eta) = \\
&= \lim_{\varepsilon\to 0} \frac{A(\eta+\varepsilon)B(\eta+\varepsilon) - A(\eta)\,B(\eta)}{\varepsilon} = \\
&= \lim_{\varepsilon\to 0} \left\{ \frac{[A(\eta+\varepsilon) - A(\eta)]\,B(\eta)}{\varepsilon} + \frac{A(\eta+\varepsilon)\,[B(\eta+\varepsilon) - B(\eta)]}{\varepsilon} \right\} = \\
&= \frac{dA(\eta)}{d\eta}\,B(\eta) + A(\eta)\,\frac{dB(\eta)}{d\eta}\,.
\end{aligned}$$

2. Complete induction:
   $\underline{n = 1}$

$$\frac{dA}{d\eta} = \mathbb{1}\frac{dA}{d\eta}\mathbb{1} \ .$$

   $\underline{n = 2}$

$$\frac{dA^2}{d\eta} \overset{1.)}{=} \frac{dA}{d\eta}A + A\frac{dA}{d\eta} = \sum_{\mu=1}^{2} A^{\mu-1}\frac{dA}{d\eta}A^{2-\mu} \ .$$

   $\underline{n \implies n+1}$
   Let the assertion be correct for n:

$$\frac{d}{d\eta}A^{n+1} \overset{1.}{=} \frac{dA^n}{d\eta}A + A^n\frac{dA}{d\eta} = \sum_{\mu=1}^{n} A^{\mu-1}\frac{dA}{d\eta}A^{n-\mu}A + A^n\frac{dA}{d\eta} =$$

$$= \sum_{\mu=1}^{n+1} A^{\mu-1}\frac{dA}{d\eta}A^{n+1-\mu} \qquad \text{q.e.d.}$$

3.

$$0 = \frac{d}{d\eta}(A\,A^{-1}) \overset{1.)}{=} \frac{dA}{d\eta}A^{-1} + A\frac{dA^{-1}}{d\eta} \implies \frac{dA^{-1}}{d\eta} = -A^{-1}\frac{dA}{d\eta}A^{-1} \ .$$

Solution 3.2.26 Functions of operators are defined only as polynomials or power series.

$$f(B) = \sum_{\mu=0}^{\dots} \beta_\mu B^\mu$$

$$g(A) = \sum_{\mu=0}^{\dots} \alpha_\mu A^\mu \ .$$

Assertion:

$$[A, B^n]_- = nCB^{n-1} = C\frac{\mathrm{d}}{\mathrm{d}B}B^n \ .$$

Proof: complete induction

$$n = 1: \quad [A, B]_- = C$$

$$n = 2: \quad \left[A, B^2\right]_- = B[A, B]_- + [A, B]_- B$$

$$
\begin{aligned}
&= BC + CB \\
&= 2CB \ ,
\end{aligned}
$$

$$
\begin{aligned}
n \ &\curvearrowright \ n+1 \\
\left[A, B^{n+1}\right]_- &= [A, B^n]_- \, B + B^n [A, B]_- \\
&= nCB^{n-1}B + B^n C \\
&= (n+1)CB^n
\end{aligned}
$$

therewith:

$$
\begin{aligned}
[A, f(B)]_- &= \sum_\mu \beta_\mu \, [A, B^\mu]_- \\
&= C \sum_\mu \beta_\mu \mu B^{\mu-1} \\
&= C \frac{\mathrm{d}}{\mathrm{d}B} \sum_\mu \beta_\mu B^\mu \\
&= C \frac{\mathrm{d}}{\mathrm{d}B} f(B) \ .
\end{aligned}
$$

Assertion:

$$
[A^n, B]_- = CnA^{n-1} \ .
$$

Proof:

$$
\begin{aligned}
n = 1: \qquad [A, B]_- &= C \\
n \to n+1: \left[A^{n+1}, B\right]_- &= [A, B]A^n + A \, [A^n, B]_- \\
&= CA^n + \underbrace{AC}_{=CA} nA^{n-1} \\
&= (n+1)CA^n
\end{aligned}
$$

therewith:

$$
\begin{aligned}
[g(A), B]_- &= \sum_\mu \alpha_\mu \, [A^\mu, B]_- \\
&= \sum_\mu \alpha_\mu \mu C A^{\mu-1}
\end{aligned}
$$

$$= C \sum_{\mu} \alpha_\mu \mu A^{\mu-1}$$

$$= C \frac{\mathrm{d}}{\mathrm{d}A} g(A) \; .$$

Solution 3.2.27

1.

$$\langle e_1|\rho\rangle = 1 \; ; \quad \langle e_2|\rho\rangle = 1 \; ; \quad \langle e_3|\rho\rangle = 0 \; ,$$
$$\langle \psi|e_1\rangle = 1 \; ; \quad \langle \psi|e_2\rangle = 0 \; ; \quad \langle \psi|e_3\rangle = 1$$
$$\Longrightarrow \; |\rho\rangle\langle\psi| = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = D \; .$$

2.

$$D^+ = |\psi\rangle\langle\rho| = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix} \neq D \; .$$

$\Longrightarrow D$ is **not** Hermitian!

3. Eigen-values d_i are determined via the secular determinant:

$$0 \stackrel{!}{=} \det\left(D - d\,\mathbb{1}\right) = \det \begin{pmatrix} 1-d & 0 & 1 \\ 1 & -d & 1 \\ 0 & 0 & -d \end{pmatrix} = d^2(1-d)$$
$$\Longrightarrow \; d_1 = d_2 = 0 \; , \quad d_3 = 1 \; .$$

4.

$$\langle \psi|\rho\rangle = (1\,0\,1) \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = 1$$
$$\Longrightarrow \; D^2 = |\rho\rangle\langle\psi|\rho\rangle\langle\psi| = |\rho\rangle\langle\psi| = D \; .$$

D is thus idempotent, and has, in addition, according to 3. the same eigen-values as a projection operator. D is nevertheless not a projection operator, since not Hermitian!

Solution 3.2.28

1. Eigen-values:

$$H_{21} = H_{12}^* \; ; \quad H_{11},\, H_{22} \text{ real because } H \text{ Hermitian.}$$

Secular determinant:

$$\begin{aligned} 0 &= \begin{vmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{vmatrix} = (H_{11} - E)\,(H_{22} - E) - |H_{12}|^2 \\ &\Longrightarrow \; E^2 - E(H_{11} + H_{22}) = |H_{12}|^2 - H_{11}\,H_{22} \\ &\Longrightarrow \; E_{1,2} = \frac{1}{2}\,(H_{11} + H_{22}) \mp \sqrt{\frac{1}{4}\,(H_{11} - H_{22})^2 + |H_{12}|^2}\,. \end{aligned}$$

2. Eigen-states:

$$|E_1\rangle = \begin{pmatrix} E_{11} \\ E_{12} \end{pmatrix}\,.$$

Eigen-value equation:

$$\begin{pmatrix} H_{11} - E_1 & H_{12} \\ H_{21} & H_{22} - E_1 \end{pmatrix} \begin{pmatrix} E_{11} \\ E_{12} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \; \Longrightarrow \; E_{11} = E_{12}\,\frac{H_{12}}{E_1 - H_{11}}\,.$$

Normalization:

$$\langle E_1 | E_1 \rangle = |E_{11}|^2 + |E_{12}|^2 \stackrel{!}{=} 1 = \frac{|H_{12}|^2 + (E_1 - H_{11})^2}{(E_1 - H_{11})^2}\,|E_{12}|^2\,.$$

Abbreviation:

$$\begin{aligned} \alpha^2 &= |H_{12}|^2 + (E_1 - H_{11})^2 = |H_{12}|^2 + (H_{22} - E_2)^2 \\ \Longrightarrow \; |E_{12}| &= \frac{1}{\alpha}\,(E_1 - H_{11})\,, \\ |E_{11}| &= \frac{1}{\alpha}|H_{12}|\,. \end{aligned}$$

We have then, except for an unimportant phase factor:

$$|E_1\rangle = \frac{1}{\alpha}\begin{pmatrix} |H_{12}| \\ E_1 - H_{11} \end{pmatrix}\,.$$

Analogously, we find the second eigen-state:

$$|E_2\rangle = \frac{1}{\alpha}\begin{pmatrix} |H_{12}| \\ E_2 - H_{22} \end{pmatrix} .$$

One easily checks the orthogonality:

$$\langle E_1 | E_2 \rangle = 0 .$$

Solution 3.2.29

1. Eigen-values:
   Matrix A is Hermitian, the e4igen-values are therefore real!
   Secular determinant:

$$0 = \begin{vmatrix} 3-a & 2i \\ -2i & -a \end{vmatrix} = -a(3-a) - 4$$

$$\Longleftrightarrow \; a^2 - 3a = 4 \; \Longleftrightarrow \; \left(a - \frac{3}{2}\right)^2 = \frac{25}{4} ,$$

$$a_1 = -1 ; \qquad a_2 = 4 .$$

2. Eigen-states:

$$\begin{pmatrix} 4 & 2i \\ -2i & 1 \end{pmatrix}\begin{pmatrix} a_{11} \\ a_{12} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \; \Longrightarrow \; a_{11} = -\frac{1}{2}\, i\, a_{12}$$

$$\Longrightarrow \; |a_1\rangle = c\begin{pmatrix} 1 \\ 2i \end{pmatrix} .$$

   Assumption: c real. It follows then from the normalization:

$$c = \frac{1}{\sqrt{5}} .$$

   For the determination of $|a_2\rangle$ we have to evaluate:

$$\begin{pmatrix} -1 & 2i \\ -2i & -4 \end{pmatrix}\begin{pmatrix} a_{21} \\ a_{22} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \; \Longleftrightarrow \; a_{21} = 2i\, a_{22}$$

$$\Longrightarrow \; |a_2\rangle = c'\begin{pmatrix} 2i \\ 1 \end{pmatrix} .$$

c' real, it follows then from the normalization:

$$c' = c = \frac{1}{\sqrt{5}} \,.$$

One should check: $\langle a_1 | a_2 \rangle = 0$.

3.

$$\begin{aligned}
&\overline{A} = U A U^+ \,, \\
&U = c \begin{pmatrix} 1 & -2i \\ -2i & 1 \end{pmatrix} \implies U^+ = c \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix} \,, \\
&\overline{A} = \frac{1}{5} \begin{pmatrix} 1 & -2i \\ -2i & 1 \end{pmatrix} \begin{pmatrix} 3 & 2i \\ -2i & 0 \end{pmatrix} \begin{pmatrix} 1 & 2i \\ 2i & 1 \end{pmatrix} \\
&\quad = \frac{1}{5} \begin{pmatrix} 1 & -2i \\ -2i & 1 \end{pmatrix} \begin{pmatrix} -1 & 8i \\ -2i & 4 \end{pmatrix} = \\
&\quad = \frac{1}{5} \begin{pmatrix} -5 & 0 \\ 0 & 20 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 4 \end{pmatrix} = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix} \,.
\end{aligned}$$

Solution 3.2.30 Eigen-values of A:

$$0 = \begin{vmatrix} -a & -i \\ i & -a \end{vmatrix} = a^2 - 1 \implies a_1 = -1 \,; \quad a_2 = +1 \,.$$

Eigen-vectors of A:

$$\begin{aligned}
&\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{12} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies a_{11} = i\, a_{12} \,, \\
&\qquad |a_1\rangle = c \begin{pmatrix} 1 \\ -i \end{pmatrix} \,; \quad \text{normalization} \implies c = \frac{1}{\sqrt{2}} \,, \\
&\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} a_{21} \\ a_{22} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies a_{21} = -i\, a_{22} \,, \\
&\qquad |a_2\rangle = c' \begin{pmatrix} 1 \\ i \end{pmatrix} \,; \quad \text{normalization} \implies c' = \frac{1}{\sqrt{2}} \,.
\end{aligned}$$

Eigen-states are orthonormal, because A Hermitian! Unitary matrix, built up by the eigen-states of A (3.125):

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \implies U^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \,.$$

Checking:

$$
\begin{aligned}
U\,U^{+} &= \frac{1}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} = \mathbb{1}\,, \\
\overline{B} &= U\,B\,U^{+} = U\,U^{+} = \mathbb{1} = B\,, \\
\overline{A} &= \frac{1}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}\begin{pmatrix} -1 & 1 \\ i & i \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\,.
\end{aligned}
$$

The eigen-values of A stand on the diagonal of the transformed matrix $\overline{A}$.

Solution 3.2.31

1. Operator functions to be understood as power series:

$$
T(\alpha) = \sum_{n=0}^{\infty} \frac{(i\alpha)^n}{n!} A^n\,.
$$

now

$$
\begin{aligned}
A^2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \\
\curvearrowright \quad A^{2m} &= \mathbb{1}\,;\;\; A^{2m+1} = A \\
\curvearrowright \quad T(\alpha) &= \sum_{m=0}^{\infty} \frac{(i\alpha)^{2m}}{(2m)!}\mathbb{1} + \sum_{m=0}^{\infty} \frac{(i\alpha)^{2m+1}}{(2m+1)!} A \\
&= (\cos\alpha)\mathbb{1} + (i\sin\alpha)A \\
&= \cos\alpha \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\sin\alpha \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
\Longrightarrow \quad T(\alpha) &= \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}\,.
\end{aligned}
$$

2. Derivative of the operator:

$$
\begin{aligned}
\frac{d}{d\alpha}T(\alpha) &= iAT(\alpha) \\
&= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \\
&= \begin{pmatrix} -\sin\alpha & \cos\alpha \\ -\cos\alpha & -\sin\alpha \end{pmatrix}\,.
\end{aligned}
$$

On the other hand, if one differentiates $T(\alpha)$ element by element:

$$\left(\frac{dT_{ij}(\alpha)}{d\alpha}\right) = \begin{pmatrix} -\sin\alpha & \cos\alpha \\ -\cos\alpha & -\sin\alpha \end{pmatrix} .$$

Solution 3.2.32 The assertion is surely correct, when F represents a sum or a product:

$$U(A+B)\,U^+ = U\,A\,U^+ + U\,B\,U^+ = \overline{A} + \overline{B}\,,$$
$$U\,A\,B\,U^+ = U\,A\mathbb{1}B\,U^+ = U\,A\,U^+\,U\,B\,U^+ = \overline{A}\,\overline{B}\,.$$

It is therefore valid also for polynomials and power series!

Solution 3.2.33

1.

$$\text{Tr}\; AB = \sum_n \langle\varphi_n|AB|\varphi_n\rangle = \sum_{n,m}\langle\varphi_n|A|\varphi_m\rangle\langle\varphi_m|B|\varphi_n\rangle =$$
$$= \sum_m \sum_n \langle\varphi_m|B|\varphi_n\rangle\langle\varphi_n|A|\varphi_m\rangle = \sum_m \langle\varphi_m|B\,A|\varphi_m\rangle = \text{Tr}\; BA\,.$$

This holds also for the case that the operators A and B do not commute. The generalization of the cyclic invariance of the trace to products of more than two operators is obvious:

$$\text{Tr}\; ABC = \text{Sp}\; CAB = \text{Sp}\; BCA\,.$$

2. Because of $U^+\,U = \mathbb{1}$ it is very easy to show with part 1.:

$$\text{Tr}\overline{A} = \text{Tr}\; UAU^+ = \text{Tr}\; U^+UA = \text{Tr}\; A\,.$$

Solution 3.2.34 $\{|\varphi_n\rangle\}$: any CON-basis in $\mathcal{H}$. Then:

$$\text{Tr}\; D = \sum_n \langle\varphi_n|\alpha\rangle\langle\beta|\varphi_n\rangle = \langle\beta|\left\{\sum_n |\varphi_n\rangle\langle\varphi_n|\right\}|\alpha\rangle$$
$$= \langle\beta|\mathbb{1}|\alpha\rangle = \langle\beta|\alpha\rangle = 0, \text{ because orthogonal.}$$

Solution 3.2.35 That the three operators are just the Cartesian components of the angular momentum $\mathbf{L} = (L_x, L_y, L_z)$ with the quantum number $l = 1$ (see (1.134)), is not relevant for the solution of the exercise. The angular momentum will be extensively discussed in Chap. 5 of Vol. 7.

1. **Eigen-values:**
   To L_x

$$0 = \hbar^3 \begin{vmatrix} -m & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -m & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -m \end{vmatrix} = \hbar^3 \left(-m^3 + \frac{m}{2} + \frac{m}{2} \right)$$
$$\Longrightarrow \; m_1 = 0 \; ; \quad m_2 = -1 \; ; \quad m_3 = +1 \; .$$

   Zu L_y

$$0 = \hbar^3 \begin{vmatrix} -\overline{m} & \frac{-i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & -\overline{m} & \frac{-i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & -\overline{m} \end{vmatrix} = \hbar^3 \left(-\overline{m}^3 + \frac{\overline{m}}{2} + \frac{\overline{m}}{2} \right)$$
$$\Longrightarrow \; \overline{m}_1 = 0 \; ; \quad \overline{m}_2 = -1 \; ; \quad \overline{m}_3 = +1 \; .$$

   L_z is already diagonal. In the diagonal we find the eigen-values. We recognize that all the three operators L_x, L_y, L_z possess the same eigen-values

$$\hbar m_l = -\hbar, \, 0, \, +\hbar \; .$$

2. **Eigen-vectors of** L_y:
   To $m_l = -1$

$$\begin{pmatrix} \sqrt{2} & -i & 0 \\ i & \sqrt{2} & -i \\ 0 & i & \sqrt{2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$
$$\Longrightarrow \; \sqrt{2}\,\alpha - i\,\beta = 0 \; ,$$
$$i\,\alpha + \sqrt{2}\,\beta - i\,\gamma = 0 \; ,$$
$$i\,\beta + \sqrt{2}\,\gamma = 0$$
$$\Longrightarrow \; \alpha = \frac{i}{\sqrt{2}}\,\beta \; ; \qquad \gamma = -\frac{i}{\sqrt{2}}\,\beta \; .$$

   Normalization (w.l.o.g.: β real):

$$1 = |\alpha|^2 + |\beta|^2 + |\gamma|^2 = \left(\frac{1}{2} + 1 + \frac{1}{2} \right) \beta^2 \; ,$$
$$\beta = \frac{1}{\sqrt{2}}$$

$$\Longrightarrow \left|L_y^{(-)}\right\rangle = \begin{pmatrix} \frac{i}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{-i}{2} \end{pmatrix} .$$

To $m_l = 0$

$$\begin{aligned} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} \overline{\alpha} \\ \overline{\beta} \\ \overline{\gamma} \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\ \Longrightarrow -i\,\overline{\beta} &= 0 , \\ i\,\overline{\alpha} - i\,\overline{\gamma} &= 0 , \\ i\,\overline{\beta} &= 0 \\ \Longrightarrow \overline{\beta} &= 0 ; \quad \overline{\alpha} = \overline{\gamma} . \end{aligned}$$

Normalization (w.l.o.g.: $\overline{\gamma}$ real):

$$\begin{aligned} 1 &= |\overline{\alpha}|^2 + |\overline{\beta}|^2 + |\overline{\gamma}|^2 = 2\,\overline{\gamma}^2 \\ \Longrightarrow \left|L_y^{(0)}\right\rangle &= \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} . \end{aligned}$$

To $m_l = +1$

$$\begin{aligned} \begin{pmatrix} -\sqrt{2} & -i & 0 \\ i & -\sqrt{2} & -i \\ 0 & i & -\sqrt{2} \end{pmatrix} \begin{pmatrix} \alpha' \\ \beta' \\ \gamma' \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\ \Longrightarrow -\sqrt{2}\,\alpha' - i\,\beta' &= 0 , \\ i\,\alpha' - \sqrt{2}\,\beta' - i\,\gamma' &= 0 , \\ i\,\beta' - \sqrt{2}\,\gamma' &= 0 \\ \Longrightarrow \alpha' = -\frac{i}{\sqrt{2}}\,\beta' &; \quad \gamma' = \frac{i}{\sqrt{2}}\,\beta' . \end{aligned}$$

Normalization (w.l.o.g.: β' real):

$$\begin{aligned} 1 = |\alpha'|^2 + |\beta'|^2 + |\gamma'|^2 &= \left(\frac{1}{2} + 1 + \frac{1}{2}\right) \beta'^2 \\ \Longrightarrow \beta' &= \frac{1}{\sqrt{2}} \end{aligned}$$

$$\Longrightarrow \left|L_y^{(+)}\right\rangle = \begin{pmatrix} -\frac{i}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{i}{2} \end{pmatrix} .$$

Unitary matrix:

$$U = \frac{1}{2}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix} \Longrightarrow U^+ = \frac{1}{2}\begin{pmatrix} -i & \sqrt{2} & i \\ \sqrt{2} & 0 & \sqrt{2} \\ i & \sqrt{2} & -i \end{pmatrix}$$

$$U\,U^+ = \mathbb{1}\,?$$

$$\frac{1}{4}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} -i & \sqrt{2} & i \\ \sqrt{2} & 0 & \sqrt{2} \\ i & \sqrt{2} & -i \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 4&0&0 \\ 0&4&0 \\ 0&0&4 \end{pmatrix} = \mathbb{1} .$$

Transformed operator $\overline{L}_y$:

$$\overline{L}_y = \frac{1}{4}\frac{\hbar}{\sqrt{2}}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} 0&-i&0 \\ i&0&-i \\ 0&i&0 \end{pmatrix}\begin{pmatrix} -i & \sqrt{2} & i \\ \sqrt{2} & 0 & \sqrt{2} \\ i & \sqrt{2} & -i \end{pmatrix} =$$

$$= \frac{\hbar}{4\sqrt{2}}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} -i\sqrt{2}&0&-i\sqrt{2} \\ 2&0&-2 \\ i\sqrt{2}&0&i\sqrt{2} \end{pmatrix}$$

$$= \frac{\hbar}{4\sqrt{2}}\begin{pmatrix} 4\sqrt{2}&0&0 \\ 0&0&0 \\ 0&0&-4\sqrt{2} \end{pmatrix} = \hbar\begin{pmatrix} 1&0&0 \\ 0&0&0 \\ 0&0&-1 \end{pmatrix} \Longrightarrow \overline{L}_y = L_z .$$

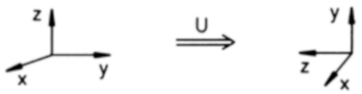
3.

$$\overline{L}_x = \frac{1}{4}\frac{\hbar}{\sqrt{2}}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} 0&1&0 \\ 1&0&1 \\ 0&1&0 \end{pmatrix}\begin{pmatrix} -i & \sqrt{2} & i \\ \sqrt{2} & 0 & \sqrt{2} \\ i & \sqrt{2} & -i \end{pmatrix} =$$

$$= \frac{\hbar}{4\sqrt{2}}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} \sqrt{2}&0&\sqrt{2} \\ 0&2\sqrt{2}&0 \\ \sqrt{2}&0&\sqrt{2} \end{pmatrix} =$$

$$= \frac{\hbar}{4\sqrt{2}}\begin{pmatrix} 0&4&0 \\ 4&0&4 \\ 0&4&0 \end{pmatrix} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0&1&0 \\ 1&0&1 \\ 0&1&0 \end{pmatrix} \Longrightarrow \overline{L}_x = L_x ,$$

Fig. A.7



$$\overline{L}_z = \frac{\hbar}{4}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} 1\,0 & 0 \\ 0\,0 & 0 \\ 0\,0 & -1 \end{pmatrix}\begin{pmatrix} -i & \sqrt{2} & i \\ \sqrt{2} & 0 & \sqrt{2} \\ i & \sqrt{2} & -i \end{pmatrix} =$$

$$= \frac{\hbar}{4}\begin{pmatrix} i & \sqrt{2} & -i \\ \sqrt{2} & 0 & \sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}\begin{pmatrix} -i & \sqrt{2} & i \\ 0 & 0 & 0 \\ -i & -\sqrt{2} & +i \end{pmatrix}$$

$$= \frac{\hbar}{4}\begin{pmatrix} 0 & 2i\sqrt{2} & 0 \\ -2i\sqrt{2} & 0 & 2i\sqrt{2} \\ 0 & -2i\sqrt{2} & 0 \end{pmatrix}$$

$$= \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix} \implies \overline{L}_z = -L_y \,.$$

$U \equiv$ rotation around the x-axis by 90° (Fig. A.7)!

Solution 3.2.36

1.

$$|\beta_j\rangle \stackrel{!}{=} U\,|\alpha_j\rangle$$

Because of

$$\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$$

it is simply

$$U = \sum_i |\beta_i\rangle\langle\alpha_i|$$

U unitary?

$$\left(|\beta_i\rangle\langle\alpha_i|\right)^+ = |\alpha_i\rangle\langle\beta_i|$$

$$\curvearrowright \quad U^+ = \sum_i |\alpha_i\rangle\langle\beta_i|$$

$$\curvearrowright \quad UU^+ = \sum_{i,j} |\beta_i\rangle \underbrace{\langle\alpha_i|\alpha_j\rangle}_{\delta_{ij}} \langle\beta_j|$$

$$= \sum_i |\beta_i\rangle\langle\beta_i|$$
$$= \mathbb{1} \qquad \text{(completeness)}$$

analogously:

$$U^+U = \mathbb{1}$$

2.

$$U_\alpha = \begin{pmatrix} \langle\alpha_1|U|\alpha_1\rangle & \langle\alpha_1|U|\alpha_2\rangle \\ \langle\alpha_2|U|\alpha_1\rangle & \langle\alpha_2|U|\alpha_2\rangle \end{pmatrix}$$
$$(U_\alpha)_{ij} = \langle\alpha_i| \sum_m |\beta_m\rangle\langle\alpha_m|\alpha_j\rangle = \langle\alpha_i|\beta_j\rangle$$
$$U_\alpha = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \quad \curvearrowright \quad U_\alpha^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

3.

$$\langle\alpha_1|\psi\rangle = \frac{1}{\sqrt{2}} = \langle\alpha_2|\psi\rangle$$
$$\langle\beta_j|\psi\rangle = \langle\alpha_j|U^\dagger|\psi\rangle$$
$$= \sum_m \langle\alpha_j|U^\dagger|\alpha_m\rangle\langle\alpha_m\ |\psi\rangle$$
$$= \frac{1}{\sqrt{2}} \sum_m \langle\alpha_j|U^+|\alpha_m\rangle$$
$$\curvearrowright \quad \langle\beta_1|\psi\rangle = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}}(1-i) \right)$$
$$\langle\beta_2|\psi\rangle = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}}(1+i) \right)$$
$$\curvearrowright \quad |\psi\rangle_\beta = \frac{1}{2} \begin{pmatrix} 1-i \\ 1+i \end{pmatrix}$$

4.

$$\left(A_\beta\right)_{ij} = \langle\beta_i|A|\beta_j\rangle$$
$$= \langle\alpha_i|U^+AU|\alpha_j\rangle$$

$$
\begin{aligned}
&= \sum_{m,n} \langle\alpha_i|U^+|\alpha_m\rangle\langle\alpha_m|A|\alpha_n\rangle\langle\alpha_n|U|\alpha_j\rangle \\
&= \left(U_\alpha^+ A_\alpha U_\alpha\right)_{ij} \\
\curvearrowright \quad A_\beta &= U_\alpha^+ A_\alpha U_\alpha \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\ 1 & i\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & 1\\ i & -i\end{pmatrix}\frac{1}{\sqrt{2}} \\
&= \frac{1}{2}\begin{pmatrix}1 & -i\\ 1 & i\end{pmatrix}\begin{pmatrix}1 & 1\\ -i & i\end{pmatrix} = \frac{1}{2}\begin{pmatrix}0 & 2\\ 2 & 0\end{pmatrix} \\
\Longrightarrow \quad A_\beta &= \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}
\end{aligned}
$$

Solution 3.2.37

1.

$$
\begin{aligned}
L &= \sum_{n=1}^{\infty} |\beta_{n+1}\rangle\langle\alpha_n| \\
L^+ &= \sum_{n=1}^{\infty} \left(|\beta_{n+1}\rangle\langle\alpha_n|\right)^+ \overset{(3.76)}{=} \sum_{n=1}^{\infty} |\alpha_n\rangle\langle\beta_{n+1}|
\end{aligned}
$$

Therewith:

$$
L^+L = \sum_{m,n=1}^{\infty} |\alpha_m\rangle \underbrace{\langle\beta_{m+1}|\beta_{n+1}\rangle}_{\delta_{mn}} \langle\alpha_n| = \underbrace{\sum_{n=1}^{\infty} |\alpha_n\rangle\langle\alpha_n|}_{(3.69)} = \mathbb{1} \ .
$$

Otherwise:

$$
\begin{aligned}
LL^+ &= \sum_{m,n=1}^{\infty} |\beta_{m+1}\rangle \underbrace{\langle\alpha_m|\alpha_n\rangle}_{\delta_{mn}} \langle\beta_{n+1}| \\
&= \sum_{m=1}^{\infty} |\beta_{m+1}\rangle\langle\beta_{m+1}| = \mathbb{1} - |\beta_1\rangle\langle\beta_1| \ .
\end{aligned}
$$

L is therefore obviously **not** unitary in $\mathcal{H}$!

2. Identity in $\mathcal{H}'$:

$$
\mathbb{1} = \sum_{m=2}^{\infty} |\beta_m\rangle\langle\beta_m| \ .
$$

Regard the beginning of the summation, which also brings about the fact that for each $|\gamma\rangle \in \mathcal{H}'$ we have:

$$|\beta_1\rangle\langle\beta_1|\gamma\rangle = 0 \ .$$

For all $|\gamma\rangle \in \mathcal{H}' \subset \mathcal{H}$ it must then be concluded, according to part 1.:

$$LL^+|\gamma\rangle = \left(\mathbb{1} - |\beta_1\rangle\langle\beta_1|\right)|\gamma\rangle = \mathbb{1}\,|\gamma\rangle \ .$$

The statement of part 1.

$$L^+L\,|\gamma\rangle = \mathbb{1}\,|\gamma\rangle$$

remains valid, so that it holds in $\mathcal{H}'$, other than in $\mathcal{H}$:

$$LL^+ = L^+L = \mathbb{1} \ .$$

L is therewith unitary in $\mathcal{H}'$!

Section 3.3.6

Solution 3.3.1 For probability-statements $|\psi\rangle$ has to be first normalized:

$$\begin{aligned} \langle\psi|\psi\rangle &= 1 + \frac{1}{4} = \frac{5}{4} \\ \Longrightarrow \ |\overline{\psi}\rangle &= \frac{|\psi\rangle}{\parallel \psi \parallel} = \frac{2}{\sqrt{5}}|a_1\rangle + \frac{i}{\sqrt{5}}|a_2\rangle \ . \end{aligned}$$

Probabilities:

$$\begin{aligned} w(a_2|\overline{\psi}) &= |\langle a_2|\overline{\psi}\rangle|^2 = \frac{1}{5} \ , \\ w(a_3|\overline{\psi}) &= |\langle a_3|\overline{\psi}\rangle|^2 = 0 \ . \end{aligned}$$

Solution 3.3.2

1. Condition:
   Schwarz's inequality must become an equality:

$$\parallel a\,\psi \parallel^2 \parallel b\,\psi \parallel^2 \stackrel{!}{=} |\langle a\,\psi|b\,\psi\rangle|^2 \ .$$

For this purpose, the vectors must be parallel (see the solution of Exercise 3.2.2):

$$|a\,\psi\rangle \stackrel{!}{=} \alpha|b\,\psi\rangle\;; \qquad \alpha \in \mathbb{C}\;.$$

It follows from that:

$$\begin{aligned} &\langle b\,\psi|a\,\psi\rangle = \alpha \parallel b\,\psi \parallel^2 \\ \Longrightarrow\;\; &|\langle a\,\psi|b\,\psi\rangle|^2 = |\alpha|^2 \parallel b\,\psi \parallel^4 = \parallel a\,\psi \parallel^2 \parallel b\,\psi \parallel^2 \\ \Longrightarrow\;\; &|\alpha| = \frac{\parallel a\,\psi \parallel}{\parallel b\,\psi \parallel} = \frac{\Delta A_\psi}{\Delta B_\psi}\;. \end{aligned}$$

2. Condition:
The *'neglect'* before (3.142) must be exact:

$$\langle\psi|(a\,b + b\,a)|\psi\rangle \stackrel{!}{=} 0\;.$$

a, b Hermitian:

$$\begin{aligned} \langle\psi|a\,b|\psi\rangle &= \alpha^* \parallel b\,\psi \parallel^2\;, \\ \langle\psi|b\,a|\psi\rangle &= \alpha \parallel b\,\psi \parallel^2\;. \end{aligned}$$

It is to require, since $\parallel b\,\psi \parallel > 0$:

$$\alpha^* + \alpha = 0 \;\Longrightarrow\; \alpha = \pm i|\alpha|\;.$$

$|\psi\rangle$ must therefore be such that

$$(A - \langle\psi|A|\psi\rangle\mathbb{1})|\psi\rangle = \pm i|\alpha|(B - \langle\psi|B|\psi\rangle\mathbb{1})|\psi\rangle$$

with

$$|\alpha| = \frac{\Delta A_\psi}{\Delta B_\psi}$$

is fulfilled.

Solution 3.3.3 Minimal uncertainty,

$$\Delta A\;\Delta B = \frac{\hbar}{2}|\langle C\rangle| \qquad \left([A,B]_- = \frac{\hbar}{i}C\right)\;.$$

also means:

$$0 \stackrel{!}{=} \mathrm{Tr}(\rho\, d_0\, d_0^+) = \sum_n \sum_m \langle\varphi_n|\psi_m\rangle\langle\psi_m|d_0\, d_0^+|\varphi_n\rangle p_m =$$

$$= \sum_m p_m \langle\psi_m|d_0\, d_0^+|\psi_m\rangle = \sum_m p_m \parallel d_0^+\, \psi_m \parallel^2 ,$$

$$d_0 = (a + i\,\lambda_0\, b)\,; \qquad \lambda_0 = \frac{\hbar\langle C\rangle}{2\langle b^2\rangle} = \frac{\Delta A}{\Delta B}\,.$$

Each summand itself must already be zero. Because of $\sum_m p_m = 1$, not all p_m can be equal to zero. For $p_m \neq 0$, however, it must be

$$(a - i\,\lambda_0\, b)|\psi_m\rangle = 0\,.$$

With $a = A - \langle A\rangle\mathbb{1}$, $b = B - \langle B\rangle\mathbb{1}$, this corresponds exactly to the result of Exercise 3.3.2!

Solution 3.3.4

1.

$$\mathrm{Tr}\,\widehat{\rho} = 2 \neq 1 \;\curvearrowright\; \text{no density matrix}\,.$$

2. Uncertainty relation:

$$\Delta A\;\Delta B \geq \frac{1}{2}\left|\langle [A, B]_-\rangle\right| .$$

We calculate each term separately:

- $$\rho \cdot A = \begin{pmatrix} \frac{1}{2} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{6} \\ -\frac{1}{6} & -\frac{1}{2} \end{pmatrix}$$
$$\langle A\rangle = \mathrm{Tr}\,(\rho A) = 0$$
$$A^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}$$
$$\Delta A = \sqrt{\langle (A - \langle A\rangle\mathbb{1})^2\rangle} = \sqrt{\langle A^2\rangle} = \sqrt{\langle \mathbb{1}\rangle} = 1$$

- $$\rho \cdot B = \begin{pmatrix} \frac{1}{2} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} -\frac{i}{6} & -\frac{i}{2} \\ \frac{i}{2} & \frac{i}{6} \end{pmatrix}$$

$$\langle B\rangle = \mathrm{Tr}\,(\rho B) = 0$$

$$B^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}$$

$$\Delta B = \sqrt{\langle (B - \langle B\rangle \mathbb{1})^2\rangle} = \sqrt{\langle B^2\rangle} = \sqrt{\langle \mathbb{1}\rangle} = 1\ .$$

- $$A \cdot B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$$

$$B \cdot A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

$$\curvearrowright \quad [A,B]_- = -2 \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

$$\rho \cdot [A,B]_- = -2 \begin{pmatrix} \frac{1}{2} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = \begin{pmatrix} \frac{i}{3} & -i \\ -i & \frac{i}{3} \end{pmatrix}$$

$$\curvearrowright \quad \frac{1}{2}\left|\langle [A,B]_-\rangle\right| = \frac{1}{2}\left|\mathrm{Tr}\big(\rho \cdot [A,B]_-\big)\right| = \frac{1}{3}\ .$$

- We see that the generalized Heisenberg uncertainty relation is obviously fulfilled:

$$\Delta A\, \Delta B \geq \frac{1}{2}\left|\langle [A,B]_-\rangle\right| \Longleftrightarrow 1 \cdot 1 > \frac{1}{3}\ .$$

Solution 3.3.5

1. **Eigen-values:**

$$\det\,(\sigma_z - \lambda\,\mathbb{1}) \stackrel{!}{=} 0 = \det \begin{pmatrix} 1-\lambda & 0 \\ 0 & -1-\lambda \end{pmatrix} = -\left(1-\lambda^2\right)$$

$$\Longrightarrow \quad \lambda_\pm = \pm 1\ .$$

Eigen-states:

$$\begin{pmatrix} 1-\lambda_\pm & 0 \\ 0 & -1-\lambda_\pm \end{pmatrix} \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Longrightarrow \quad b_+ = 0 = a_-\ ; \qquad a_+,\ b_- \text{ at first arbitrary!}$$

$$\text{Normalization} \Longrightarrow\ a_+ = b_- = 1:$$

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\ ; \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\ .$$

2.

$$\det(\sigma_x - x\mathbb{1}) \stackrel{!}{=} 0 = \det\begin{pmatrix} -x & 1 \\ 1 & -x \end{pmatrix}$$

$$\Longrightarrow\ x^2 = 1 \ \Longrightarrow\ x_\pm = \pm 1$$

$$\det(\sigma_y - y\mathbb{1}) \stackrel{!}{=} 0 = \det\begin{pmatrix} -y & -i \\ i & -y \end{pmatrix} = y^2 + i^2 \ \Longrightarrow\ y_\pm = \pm 1\ .$$

The eigen-states are not identical to those of σ_z:

$\underline{\sigma_x}$

$$\begin{pmatrix} -x_\pm & 1 \\ 1 & -x_\pm \end{pmatrix}\begin{pmatrix} \overline{a}_\pm \\ \overline{b}_\pm \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}\ ,$$

$$\mp\overline{a}_\pm + \overline{b}_\pm = 0 \ \Longrightarrow\ \overline{b}_\pm = \pm\overline{a}_\pm\ ,$$

$$|x_+\rangle = \overline{a}_+\begin{pmatrix} 1 \\ 1 \end{pmatrix}\ ;\quad |x_-\rangle = \overline{a}_-\begin{pmatrix} 1 \\ -1 \end{pmatrix}\ ,$$

$$\text{normalization: } \overline{a}_+ = \overline{a}_- = \frac{1}{\sqrt{2}}\ .$$

$\underline{\sigma_y}$

$$\begin{pmatrix} -y_\pm & -i \\ i & -y_\pm \end{pmatrix}\begin{pmatrix} \widehat{a}_\pm \\ \widehat{b}_\pm \end{pmatrix} = 0\ ,$$

$$\mp\widehat{a}_\pm = i\,\widehat{b}_\pm \ \Longrightarrow\ \widehat{b}_\pm = \pm i\,\widehat{a}_\pm\ ,$$

$$|y_+\rangle = \widehat{a}_+\begin{pmatrix} 1 \\ i \end{pmatrix}\ ;\quad |y_-\rangle = \widehat{a}_-\begin{pmatrix} 1 \\ -i \end{pmatrix}\ ,$$

$$\text{normalization: } \widehat{a}_+ = \widehat{a}_- = \frac{1}{\sqrt{2}}\ .$$

The components $\sigma_{x,y,z}$ of the spin operator have the same eigen-values, but different eigen-states. They are therefore not simultaneously sharply measurable.

3. Uncertainty relation:

$$\Delta A\ \Delta B \geq \frac{1}{2}|\langle [A,B]_-\rangle|\ .$$

We calculate the commutators!

$$\sigma_x\,\sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\,\sigma_z\ ,$$

$$\sigma_y\,\sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\,\sigma_z\ ,$$

$$\sigma_x\,\sigma_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\,\sigma_y\ ,$$

$$\sigma_z\,\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\,\sigma_y\ ,$$

$$\sigma_y\,\sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\,\sigma_x\ ,$$

$$\sigma_z\,\sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = -i\,\sigma_x\ .$$

That leads to the following commutators:

$$[\sigma_x, \sigma_y]_- = 2i\,\sigma_z, \quad [\sigma_y, \sigma_z]_- = 2i\,\sigma_x, \quad [\sigma_z, \sigma_x]_- = 2i\,\sigma_y\ .$$

Uncertainty relations:

$$\Delta\sigma_x\,\Delta\sigma_y \geq |\langle\sigma_z\rangle|\ ,$$
$$\Delta\sigma_y\,\Delta\sigma_z \geq |\langle\sigma_x\rangle|\ ,$$
$$\Delta\sigma_z\,\Delta\sigma_x \geq |\langle\sigma_y\rangle|\ .$$

Solution 3.3.6

1. ρ Hermitian, $\mathrm{Tr}\rho = 1$

$$\Longrightarrow\ \rho = \begin{pmatrix} a & b \\ b^* & 1-a \end{pmatrix}\ ;\quad a \text{ real}\ ,$$

$$\rho A = \begin{pmatrix} 3a & \dots \\ \dots & a-1 \end{pmatrix},$$

$$\rho B = \begin{pmatrix} a+b & \dots \\ \dots & b^*+a-1 \end{pmatrix}\ ,$$

$$\rho C = \begin{pmatrix} -2ib & \dots \\ \dots & 2ib^* \end{pmatrix}$$

$$\begin{aligned}
\Longrightarrow \quad \langle A\rangle &= \mathrm{Tr}\,(\rho A) = 4a - 1 \stackrel{!}{=} 2\,, \\
\langle B\rangle &= \mathrm{Tr}\,(\rho B) = 2a + b + b^* - 1 \stackrel{!}{=} \frac{1}{2}\,, \\
\langle C\rangle &= \mathrm{Tr}\,(\rho C) = 2i(b^* - b) \stackrel{!}{=} 0 \\
\Longrightarrow \quad a &= \frac{3}{4}\,; \quad b = b^* = 0\,, \\
\rho &= \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}\,.
\end{aligned}$$

2.

$$\begin{aligned}
\mathrm{Tr}\,\rho^2 &= \mathrm{Tr} \begin{pmatrix} \frac{9}{16} & 0 \\ 0 & \frac{1}{16} \end{pmatrix} = \frac{5}{8} < 1 \\
\Longrightarrow \quad & \text{mixed spin state.}
\end{aligned}$$

3. The eigen-value $+1$ belongs to the eigen-state $|+\rangle$ of the observable σ_z. The probability is therefore just the (1,1)-element of ρ or formally:

$$w(+1) = \langle + |\rho| + \rangle = (1\,0) \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\,.$$

4.

$$\begin{aligned}
\langle \sigma_x\rangle &= \mathrm{Tr} \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathrm{Tr} \begin{pmatrix} 0 & \frac{3}{4} \\ \frac{1}{4} & 0 \end{pmatrix} = 0\,, \\
\langle \sigma_y\rangle &= \mathrm{Tr} \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \mathrm{Tr} \begin{pmatrix} 0 & -\frac{3}{4}i \\ \frac{1}{4}i & 0 \end{pmatrix} = 0\,, \\
\langle \sigma_z\rangle &= \mathrm{Tr} \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \mathrm{Tr} \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & -\frac{1}{4} \end{pmatrix} = \frac{1}{2}\,.
\end{aligned}$$

Solution 3.3.7

1. The apparatus represents the observable

$$\boldsymbol{\sigma} \cdot \mathbf{e}\,.$$

Eigen-value equation:

$$(\boldsymbol{\sigma} \cdot \mathbf{e})|\mathbf{e}_\pm\rangle = \varepsilon_\pm |\mathbf{e}_\pm\rangle\,.$$

Matrix-representation (CON-basis = eigen-states of σ_z):

$$\boldsymbol{\sigma}\cdot\mathbf{e} = \sin\vartheta\cos\varphi\begin{pmatrix}0&1\\1&0\end{pmatrix} + \sin\vartheta\sin\varphi\begin{pmatrix}0&-i\\i&0\end{pmatrix} + \cos\vartheta\begin{pmatrix}1&0\\0&-1\end{pmatrix} =$$

$$= \begin{pmatrix}\cos\vartheta & e^{-i\varphi}\sin\vartheta\\ e^{i\varphi}\sin\vartheta & -\cos\vartheta\end{pmatrix} .$$

Secular determinant:

$$\det(\boldsymbol{\sigma}\cdot\mathbf{e} - \varepsilon\mathbb{1}) \stackrel{!}{=} 0 = -(\cos\vartheta - \varepsilon)(\cos\vartheta + \varepsilon) - \sin^2\vartheta =$$

$$= \varepsilon^2 - \cos^2\vartheta - \sin^2\vartheta = \varepsilon^2 - 1$$

$$\Longrightarrow\ \varepsilon_\pm = \pm 1 .$$

The eigen-values did **not** change as a consequence of the rotation of the apparatus!
Eigen-states:

$$\begin{pmatrix}\cos\vartheta \mp 1 & e^{-i\varphi}\sin\vartheta\\ e^{i\varphi}\sin\vartheta & -\cos\vartheta \mp 1\end{pmatrix}\begin{pmatrix}a_\pm\\ b_\pm\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$$

$$\Longrightarrow\ \frac{a_+}{b_+} = -e^{-i\varphi}\frac{\sin\vartheta}{\cos\vartheta - 1} = e^{-i\varphi}\frac{2\sin\frac{\vartheta}{2}\cos\frac{\vartheta}{2}}{2\sin^2\frac{\vartheta}{2}} = e^{-i\varphi}\cot\frac{\vartheta}{2} ,$$

$$\frac{a_-}{b_-} = -e^{-i\varphi}\frac{\sin\vartheta}{\cos\vartheta + 1} = -e^{-i\varphi}\frac{2\sin\frac{\vartheta}{2}\cos\frac{\vartheta}{2}}{2\cos^2\frac{\vartheta}{2}} = -e^{-i\varphi}\tan\frac{\vartheta}{2} .$$

Normalization and arbitrary phase:

$$|\mathbf{e}_+\rangle = \begin{pmatrix}\cos\frac{\vartheta}{2}\\ e^{i\varphi}\sin\frac{\vartheta}{2}\end{pmatrix} ; \quad |\mathbf{e}_-\rangle = \begin{pmatrix}-\sin\frac{\vartheta}{2}\\ e^{i\varphi}\cos\frac{\vartheta}{2}\end{pmatrix} .$$

Checking:

$$|\mathbf{e}_\pm\rangle \underset{\vartheta=0}{\longrightarrow} |\pm\rangle ; \quad \text{possibly except for a phase } e^{i\varphi} .$$

$\vartheta = 0$ means that the Stern-Gerlach apparatus is oriented in z-direction (Exercise 3.3.5, part 1.).

2. For pure states it is, according to (3.153):

$$\rho_{e_\pm} = P(e_\pm) = |\mathbf{e}_\pm\rangle\langle\mathbf{e}_\pm| .$$

a) **Basis** $|\mathbf{e}_\pm\rangle$
The basis states are orthonormalized:

$$\rho_{e_+} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \; ; \quad \rho_{e_-} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} .$$

b) **Basis** $|\pm\rangle$

$$\rho_{e_+} = \begin{pmatrix} \langle + |\mathbf{e}_+\rangle\langle \mathbf{e}_+|+\rangle & \langle + |\mathbf{e}_+\rangle\langle \mathbf{e}_+|-\rangle \\ \langle - |\mathbf{e}_+\rangle\langle \mathbf{e}_+|+\rangle & \langle - |\mathbf{e}_+\rangle\langle \mathbf{e}_+|-\rangle \end{pmatrix} =$$

$$= \begin{pmatrix} \cos^2 \frac{\vartheta}{2} & e^{-i\varphi} \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} \\ e^{i\varphi} \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} & \sin^2 \frac{\vartheta}{2} \end{pmatrix} .$$

We use:

$$\cos^2 \frac{\vartheta}{2} = \frac{1}{2}(1 + \cos\vartheta) \quad ; \quad \sin^2 \frac{\vartheta}{2} = \frac{1}{2}(1 - \cos\vartheta) \; ; \quad 2 \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} = \sin\vartheta$$

$$\Longrightarrow \quad \rho_{e_+} = \frac{1}{2} \begin{pmatrix} 1 + \cos\vartheta & e^{-i\varphi} \sin\vartheta \\ e^{i\varphi} \sin\vartheta & 1 - \cos\vartheta \end{pmatrix} ,$$

$$\rho_{e_-} = \begin{pmatrix} \sin^2 \frac{\vartheta}{2} & -e^{-\varphi} \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} \\ -e^{i\varphi} \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} & \cos^2 \frac{\vartheta}{2} \end{pmatrix} =$$

$$= \frac{1}{2} \begin{pmatrix} 1 - \cos\vartheta & -e^{-i\varphi} \sin\vartheta \\ -e^{i\varphi} \sin\vartheta & 1 + \cos\vartheta \end{pmatrix} .$$

3. $|\mathbf{e}_+\rangle$ is prepared:

$$P_x = \langle e_+|\sigma_x|e_+\rangle = \mathrm{Tr}(\rho_{e_+} \, \sigma_x) =$$

$$= \frac{1}{2} \mathrm{Tr} \begin{pmatrix} 1 + \cos\vartheta & e^{-i\varphi} \sin\vartheta \\ e^{i\varphi} \sin\vartheta & 1 - \cos\vartheta \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =$$

$$= \frac{1}{2} \mathrm{Tr} \begin{pmatrix} e^{-i\varphi} \sin\vartheta & \dots \\ \dots & e^{i\varphi} \sin\vartheta \end{pmatrix} = \sin\vartheta \cos\varphi$$

or with $|\mathbf{e}_+\rangle$ from part 1.:

$$P_x = \left(\cos \frac{\vartheta}{2} \; e^{-i\varphi} \sin \frac{\vartheta}{2} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos \frac{\vartheta}{2} \\ e^{i\varphi} \sin \frac{\vartheta}{2} \end{pmatrix} =$$

$$= \sin \frac{\vartheta}{2} \cos \frac{\vartheta}{2} \, (e^{i\varphi} + e^{-i\varphi}) = \sin\vartheta \cos\varphi \; ,$$

$$P_y = \mathrm{Tr}\,(\rho_{e_+}\,\sigma_y) = \frac{1}{2}\mathrm{Tr}\begin{pmatrix} 1+\cos\vartheta & e^{-i\varphi}\sin\vartheta \\ e^{i\varphi}\sin\vartheta & 1-\cos\vartheta \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} =$$

$$= \frac{1}{2}\mathrm{Tr}\begin{pmatrix} i\,e^{-i\varphi}\sin\vartheta & \dots \\ \dots & -i\,e^{i\varphi}\sin\vartheta \end{pmatrix} =$$

$$= \frac{1}{2i}\,(e^{i\varphi} - e^{-i\varphi})\sin\vartheta = \sin\vartheta\sin\varphi\ ,$$

$$P_z = \mathrm{Tr}\,(\rho_{e_+}\,\sigma_z) = \frac{1}{2}\mathrm{Tr}\begin{pmatrix} 1+\cos\vartheta & e^{-i\varphi}\sin\vartheta \\ e^{i\varphi}\sin\vartheta & 1-\cos\vartheta \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} =$$

$$= \frac{1}{2}\mathrm{Tr}\begin{pmatrix} 1+\cos\vartheta & \dots \\ \dots & -1+\cos\vartheta \end{pmatrix} = \cos\vartheta\ .$$

Solution 3.3.8

1. **Density matrix:**

$$\rho = p_+|\mathbf{e}_+\rangle\langle\mathbf{e}_+| + p_-|\mathbf{e}_-\rangle\langle\mathbf{e}_-| = p_+\,\rho_{e_+} + p_-\,\rho_{e_-} \text{ with } p_+ + p_- = 1.$$

The density matrices $\rho_{e_\pm}$ for the pure states $|\mathbf{e}_\pm\rangle$ have been calculated in Exercise 3.3.7, part 2.! We can therefore use the respective expressions:

$$\rho = \frac{1}{2}\begin{pmatrix} 1+(p_+-p_-)\cos\vartheta & (p_+-p_-)\,e^{-i\varphi}\sin\vartheta \\ (p_+-p_-)\,e^{i\varphi}\sin\vartheta & 1-(p_+-p_-)\cos\vartheta \end{pmatrix}\ .$$

Polarization:

$$\rho\,\sigma_x = \rho\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} (p_+-p_-)\,e^{-i\varphi}\sin\vartheta & \dots \\ \dots & (p_+-p_-)\,e^{i\varphi}\sin\vartheta \end{pmatrix}\ ,$$

$$\rho\,\sigma_y = \rho\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} i(p_+-p_-)\,e^{-i\varphi}\sin\vartheta & \dots \\ \dots & -i(p_+-p_-)\,e^{i\varphi}\sin\vartheta \end{pmatrix}\ ,$$

$$\rho\,\sigma_z = \rho\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+(p_+-p_-)\cos\vartheta & \dots \\ \dots & -1+(p_+-p_-)\cos\vartheta \end{pmatrix}\ .$$

From that we get:

$$P_x = \mathrm{Tr}(\rho\,\sigma_x) = (p_+-p_-)\cos\varphi\sin\vartheta\ ,$$
$$P_y = \mathrm{Tr}(\rho\,\sigma_y) = (p_+-p_-)\sin\varphi\sin\vartheta\ ,$$
$$P_z = \mathrm{Tr}(\rho\,\sigma_z) = (p_+-p_-)\cos\vartheta\ .$$

By comparison we have:

$$\rho = \frac{1}{2}\begin{pmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{pmatrix} = \frac{1}{2}(\mathbb{1} + \mathbf{P}\cdot\boldsymbol{\sigma}) \,.$$

2. **Eigen-values of ρ:**

$$0 \overset{!}{=} \det(\rho - \lambda\mathbb{1}) = \det\begin{pmatrix} \frac{1}{2}(1+P_z) - \lambda & \frac{1}{2}(P_x - iP_y) \\ \frac{1}{2}(P_x + iP_y) & \frac{1}{2}(1-P_z) - \lambda \end{pmatrix} =$$

$$= \lambda^2 - \lambda + \frac{1}{4}(1-P_z^2) - \frac{1}{4}(P_x^2 + P_y^2) \,.$$

We abbreviate:

$$P = \sqrt{P_x^2 + P_y^2 + P_z^2} \overset{1)}{=} |p_+ - p_-| \,.$$

It remains then to be solved:

$$0 = \left(\lambda - \frac{1}{2}\right)^2 - \frac{1}{4}P^2 \implies \lambda_\pm = \frac{1}{2}(1 \pm P) \,,$$

w.l.o.g: $p_+ \geq p_-$:

$$\lambda_\pm = \frac{1}{2}(1 \pm P) = p_\pm \,.$$

The fact that the eigen-values of ρ are equal to the weights of the mixed spin state, follows already from the general theory. The weights $p_\pm$ of the mixed state are thus determined by measuring the polarization P:

$$P = +1 \iff \textit{'totally polarized'},$$
$$P = 0 \iff \textit{'totally unpolarized'}.$$

3. Let $w(\pm)$ be the probabilities to find the eigen-values ± 1 , by a measurement in z-direction on the mixed spin state:

$$w(+) = \frac{N_\uparrow}{N} \,; \quad w(-) = \frac{N_\downarrow}{N} \,; \quad N = N_\uparrow + N_\downarrow \,.$$

On the other hand, it is also valid:

$$w(+) = \langle + |\rho| + \rangle = (1\,0)\,\rho \begin{pmatrix} 1 \\ 0 \end{pmatrix} =$$

$$\overset{1.}{=} (1\,0) \begin{pmatrix} \frac{1}{2}[1 + (p_+ - p_-)\cos\vartheta] \\ \frac{1}{2}(p_+ - p_-)\, e^{i\varphi} \sin\vartheta \end{pmatrix} = \frac{1}{2}[1 + (p_+ - p_-)\cos\vartheta] \,,$$

$$w(-) = \langle - |\rho| - \rangle = (0\,1)\,\rho \begin{pmatrix} 0 \\ 1 \end{pmatrix} =$$

$$\overset{1.}{=} \frac{1}{2}(0\,1) \begin{pmatrix} (p_+ - p_-)\, e^{-i\varphi} \sin\vartheta \\ 1 - (p_+ - p_-)\cos\vartheta \end{pmatrix} = \frac{1}{2}[1 - (p_+ - p_-)\cos\vartheta] \,.$$

It follows by comparison with the result for P_z from part 1.:

$$w(+) = \frac{1}{2}(1 + P_z) \,; \quad w(-) = \frac{1}{2}(1 - P_z) \,.$$

According to the general theory, we could have read this result directly off ρ from part 1. These probabilities are just the diagonal elements of ρ. We recognize:

$$P_z = w(+) - w(-) = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \quad \text{q.e.d.}$$

Solution 3.3.9

1.

$$\langle \sigma_x \rangle = \mathrm{Tr}(\rho\,\sigma_x) \,,$$
$$\rho\,\sigma_x = \frac{1}{2}\,[\sigma_x + (\mathbf{P}\cdot\boldsymbol{\sigma})\,\sigma_x] = \frac{1}{2}\,(\sigma_x + P_x\,\sigma_x^2 + P_y\,\sigma_y\,\sigma_x + P_z\,\sigma_z\,\sigma_x) \,.$$

It was shown in the solution of Exercise 3.3.5:

$$\sigma_x\,\sigma_y = i\,\sigma_z = -\sigma_y\,\sigma_x \,,$$
$$\sigma_x\,\sigma_z = -i\,\sigma_y = -\sigma_z\,\sigma_x \,,$$
$$\sigma_y\,\sigma_z = i\,\sigma_x = -\sigma_z\,\sigma_y \,.$$

This means:

$$\rho\,\sigma_x = \frac{1}{2}\,(\sigma_x + P_x\,\sigma_x^2 - i\,P_y\,\sigma_z + i\,P_z\,\sigma_y) \,.$$

The Pauli spin matrices have the following properties:

$$\begin{aligned} \mathrm{Tr}\sigma_x = \mathrm{Tr}\sigma_y = \mathrm{Tr}\sigma_z = 0 \,, \\ \sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \mathbb{1} \,, \\ \mathrm{Tr}\sigma_x^2 = \mathrm{Tr}\sigma_y^2 = \mathrm{Tr}\sigma_z^2 = 2 \,. \end{aligned}$$

One should check the validity of these relations.

It follows therewith:

$$\mathrm{Tr}(\rho\,\sigma_x) = P_x \,.$$

2.

$$\begin{aligned} \langle\sigma_y\rangle &= \mathrm{Tr}(\rho\,\sigma_y) \,, \\ \rho\,\sigma_y &= \frac{1}{2}\,(\sigma_y + P_x\,\sigma_x\,\sigma_y + P_y\,\sigma_y^2 + P_z\,\sigma_z\,\sigma_y) = \\ &= \frac{1}{2}\,(\sigma_y + i\,P_x\,\sigma_z + P_y\,\sigma_y^2 - i\,P_z\,\sigma_x) \\ &\Longrightarrow\ \mathrm{Tr}(\rho\,\sigma_y) = P_y \,. \end{aligned}$$

3.

$$\begin{aligned} \langle\sigma_z\rangle &= \mathrm{Tr}(\rho\,\sigma_z) \,, \\ \rho\,\sigma_z &= \frac{1}{2}\,(\sigma_z + P_x\,\sigma_x\,\sigma_z + P_y\,\sigma_y\,\sigma_z + P_z\,\sigma_z^2) = \\ &= \frac{1}{2}\,(\sigma_z - i\,P_x\,\sigma_y + i\,P_y\,\sigma_x + P_z\,\sigma_z^2) \\ &\Longrightarrow\ \mathrm{Tr}(\rho\,\sigma_z) = P_z \,. \end{aligned}$$

All together we thus have:

$$\mathbf{P} = \mathrm{Tr}(\rho\,\boldsymbol{\sigma}) = \langle\boldsymbol{\sigma}\rangle \,.$$

Solution 3.3.10 According to Solution 3.3.7, we have for the general spin eigenstates:

$$\begin{aligned} +\frac{\hbar}{2}: \quad |\mathbf{e}_+(\vartheta,\varphi)\rangle &= \begin{pmatrix} \cos\frac{\vartheta}{2} \\ e^{i\varphi}\sin\frac{\vartheta}{2} \end{pmatrix} \,, \\ -\frac{\hbar}{2}: \quad |\mathbf{e}_-(\vartheta,\varphi)\rangle &= \begin{pmatrix} -\sin\frac{\vartheta}{2} \\ e^{i\varphi}\cos\frac{\vartheta}{2} \end{pmatrix} \,. \end{aligned}$$

The first apparatus is passed by

$$N_1 = N_0 \left| \left\langle \mathbf{e}_+ \left(\frac{\pi}{2}, 0 \right) \middle| \psi_0 \right\rangle \right|^2$$

particles, the second by

$$N_2 = N_1 \left| \left\langle \mathbf{e}_-(\pi, 0) \middle| \mathbf{e}_+ \left(\frac{\pi}{2}, 0 \right) \right\rangle \right|^2$$

particles.

$$\left| \mathbf{e}_+ \left(\frac{\pi}{2}, 0 \right) \right\rangle = \begin{pmatrix} \cos \frac{\pi}{4} \\ \sin \frac{\pi}{4} \end{pmatrix} = \frac{1}{2} \sqrt{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} ,$$

$$|\mathbf{e}_-(\pi, \pi)\rangle = \begin{pmatrix} -1 \\ 0 \end{pmatrix} .$$

This means:

$$\left| \left\langle \mathbf{e}_+ \left(\frac{\pi}{2}, 0 \right) \middle| \psi_0 \right\rangle \right|^2 = \left(\frac{1}{2} \sqrt{2} \, \frac{1}{5} (3 + 4) \right)^2 = \frac{49}{50} ,$$

$$\left| \left\langle \mathbf{e}_-(\pi, \pi) \middle| e_+ \left(\frac{\pi}{2}, 0 \right) \right\rangle \right|^2 = \left(-\frac{1}{2} \sqrt{2} \right)^2 = \frac{1}{2} .$$

From that it follows:

$$N_1 = N_0 \, \frac{49}{50} ; \qquad N_2 = \frac{1}{2} N_1 \implies \frac{N_2}{N_0} = 0.49 .$$

Solution 3.3.11

$$\rho^2 = \frac{1}{9} \begin{pmatrix} 2 & \dots & \dots \\ \dots & 1 & \dots \\ \dots & \dots & 2 \end{pmatrix} \implies \mathrm{Tr} \rho^2 = \frac{5}{9} < 1 .$$

It is therefore **not** a pure state!

$$\rho A = \frac{1}{3} \begin{pmatrix} +i & \dots & \dots \\ \dots & 0 & \dots \\ \dots & \dots & -i \end{pmatrix} \implies \langle A \rangle = \mathrm{Tr}(\rho A) = 0 .$$

Solution 3.3.12

$$\rho = \sum_m p_m |\psi_m\rangle\langle\psi_m| \;\; ; \;\; \sum_m p_m = 1 \; ; \quad \langle\psi_m|\psi_m\rangle = 1$$

$\{|\psi_m\rangle\}$: not orthogonal

1. $\{|\varphi_i\rangle\}$: CON-System

$$\begin{aligned}
\langle A\rangle &\overset{(3.146)}{=} \sum_m p_m \langle\psi_m|A|\psi_m\rangle \\
&= \sum_m \sum_{i,j} p_m \langle\psi_m|\varphi_i\rangle\langle\varphi_i|A|\varphi_j\rangle\langle\varphi_j|\psi_m\rangle \\
&= \sum_{i,j} \langle\varphi_i|A|\varphi_j\rangle\langle\varphi_j| \left(\sum_m p_m |\psi_m\rangle\langle\psi_m| \right) |\varphi_i\rangle \\
&= \sum_{i,j} A_{ij}\, \rho_{ji} = \sum_i (A\,\rho)_{ii} \\
&= \mathrm{Tr}(\rho A) \; .
\end{aligned}$$

That is the statement (3.149). The orthogonality of the states was not used!

2. ρ is Hermitian since the projector $|\psi_m\rangle\langle\psi_m|$ is Hermitian and the p_m are all real.
3. $|\chi\rangle$ arbitrary state of the Hilbert space.

$$\langle\chi|\rho|\chi\rangle = \sum_m p_m \langle\chi|\psi_m\rangle\langle\psi_m|\chi\rangle = \sum \underbrace{p_m}_{\geq 0} \underbrace{|\langle\chi|\psi_m\rangle|^2}_{\geq 0} \geq 0 \; .$$

That is the statement of (3.150). ρ is positive-definite.

4.

$$\mathrm{Tr}\,\rho = 1 \qquad (3.152)$$

follows from 1. for $A = \mathbb{1}$

5. Eigen-value equation:

$$\rho|\rho_n\rangle = \rho_n|\rho_n\rangle \; .$$

Because of 2. all eigen-values ρ_n are real, and because of 3. non-negative (see Exercise 3.2.20). The eigen-states are orthonormal:

$$\langle\rho_n|\rho_{n'}\rangle = \delta_{nn'} \; .$$

The trace is independent of the applied basis. If one uses the eigen-basis of ρ for the representation of $\mathrm{Tr}\rho$, then it follows from 4.:

$$\sum_n \rho_n = 1 \quad \text{and therewith:} \quad 0 \leq \rho_n \leq 1 \ \forall n \ .$$

But bear in mind that:

$$\rho_m \not\equiv p_m \ .$$

6. Spectral representation:

$$\rho = \sum_n \rho_n |\rho_n\rangle\langle\rho_n| \ .$$

7. Pure state:

$$\begin{aligned} & p_1 = 1 \ ; \ p_m = 0 \ \forall m \neq 1 \\ & \curvearrowright \ \rho = |\psi_1\rangle\langle\psi_1| \ \curvearrowright \ \rho^2 = |\psi_1\rangle \underbrace{\langle\psi_1|\psi_1\rangle}_{=1}\langle\psi_1| = \rho \\ & \curvearrowright \ \mathrm{Tr}\rho^2 = \mathrm{Tr}\rho = 1 \ . \end{aligned}$$

8. Mixed state:

$$\mathrm{Tr}\rho^2 = \sum_n \langle\rho_n|\rho^2|\rho_n\rangle = \sum_n \rho_n^2 \langle\rho_n|\rho_n\rangle = \sum_n \rho_n^2 \ .$$

According to 6., at least two ρ_n are unequal zero for the mixed state. Otherwise, it would be a pure state. It is then, because of 5.:

$$\sum_n \rho_n^2 < \sum_n \rho_n = 1 \ .$$

(3.154) is therefore valid for a mixed state:

$$\mathrm{Tr}\rho^2 < 1 \ .$$

All properties of the density matrix are therewith reproduced, and that without being obliged to use the orthogonality of the states $|\psi_m\rangle$.

Section 3.4.7

Solution 3.4.1 The von Neumann's series

$$U(t,t_0) = \mathbb{1} + \sum_{n=1}^{\infty} U^{(n)}(t,t_0)$$

reads, according to (3.172), for this special case:

$$U^{(n)}(t,t_0) = \left(-\frac{i}{\hbar}\right)^n H^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \ .$$

The proof is thus done if it can be shown that

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \stackrel{!}{=} \frac{(t-t_0)^n}{n!}$$

That succeeds by the use of *'complete induction'*!

- $n = 2$

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 = \int_{t_0}^{t} dt_1 (t_1 - t_0) = \frac{1}{2}\left(t^2 - t_0^2\right) - t_0(t-t_0) = \frac{1}{2}(t-t_0)^2 \ .$$

- $n \curvearrowright n+1$

$$\begin{aligned}
\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n \int_{t_0}^{t_n} dt_{n+1} &= \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n (t_n - t_0) \\
&= -t_0 \frac{(t-t_0)^n}{n!} + \\
&\quad + \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-2}} dt_{n-1} \frac{1}{2}\left(t_{n-1}^2 - t_0^2\right) \\
&= -t_0 \frac{(t-t_0)^n}{n!} - \frac{1}{2} t_0^2 \frac{(t-t_0)^{n-1}}{(n-1)!} + \\
&\quad + \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-3}} dt_{n-2} \frac{1}{3!}(t_{n-2}^3 - t_0^3)
\end{aligned}$$

$$= -\sum_{\alpha=1}^{n} \frac{t_0^\alpha}{(n+1-\alpha)!\alpha!}(t-t_0)^{n+1-\alpha} + \frac{1}{n!}\int_{t_0}^{t} dt_1\, t_1^n \,.$$

That can be combined:

$$\begin{aligned}
\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_n} dt_{n+1} &= -\frac{1}{(n+1)!}\sum_{\alpha=1}^{n}\binom{n+1}{\alpha} t_0^\alpha (t-t_0)^{n+1-\alpha} \\
&\quad + \frac{1}{(n+1)!}\left(t^{n+1} - t_0^{n+1}\right) \\
&= -\frac{1}{(n+1)!}\sum_{\alpha=0}^{n+1}\binom{n+1}{\alpha} t_0^\alpha (t-t_0)^{n+1-\alpha} + \\
&\quad + \frac{1}{(n+1)!}(t-t_0)^{n+1} + \frac{1}{(n+1)!}t_0^{n+1} + \\
&\quad + \frac{1}{(n+1)!}t^{n+1} - \frac{1}{(n+1)!}t_0^{n+1} \\
&= -\frac{1}{(n+1)!}t^{n+1} + \\
&\quad + \frac{1}{(n+1)!}(t-t_0)^{n+1} + \frac{1}{(n+1)!}t_0^{n+1} + \\
&\quad + \frac{1}{(n+1)!}t^{n+1} - \frac{1}{(n+1)!}t_0^{n+1} \\
&= \frac{1}{(n+1)!}(t-t_0)^{n+1} \,.
\end{aligned}$$

That was to be shown!

Solution 3.4.2

$$\frac{\partial H}{\partial t} = 0 \iff \text{closed system} \,,$$

$$\sigma_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \;; \quad \sigma_z \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} \,,$$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle = e^{-i\omega\sigma_z t}\,\frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] =$$

$$= \frac{1}{\sqrt{2}}\left[e^{-i\omega t}\begin{pmatrix}1\\0\end{pmatrix} + e^{+i\omega t}\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\omega t}\\ e^{i\omega t}\end{pmatrix}$$
$$\Longleftrightarrow \text{ pure state .}$$

Expectation values:

$$\langle\sigma_x\rangle_t = \langle\psi(t)|\sigma_x|\psi(t)\rangle = \frac{1}{2}\left(e^{i\omega t}\, e^{-i\omega t}\right)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}e^{-i\omega t}\\ e^{i\omega t}\end{pmatrix} =$$
$$= \frac{1}{2}\left(e^{i\omega t}\, e^{-i\omega t}\right)\begin{pmatrix}e^{i\omega t}\\ e^{-i\omega t}\end{pmatrix} = \cos(2\omega t)\ ,$$
$$\langle\sigma_y\rangle_t = \langle\psi(t)|\sigma_y|\psi(t)\rangle = \frac{1}{2}\left(e^{i\omega t}\, e^{-i\omega t}\right)\begin{pmatrix}0&-i\\i&0\end{pmatrix}\begin{pmatrix}e^{-i\omega t}\\ e^{i\omega t}\end{pmatrix} =$$
$$= \frac{1}{2}\left(e^{i\omega t}\, e^{-i\omega t}\right)\begin{pmatrix}-i\, e^{i\omega t}\\ i\, e^{-i\omega t}\end{pmatrix} = \frac{1}{2i}\left(e^{2i\omega t} - e^{-2i\omega t}\right) = \sin(2\omega t)\ ,$$
$$\langle\sigma_z\rangle_t = \frac{1}{2}\left(e^{i\omega t}\, e^{-i\omega t}\right)\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}e^{-i\omega t}\\ e^{i\omega t}\end{pmatrix} =$$
$$= \frac{1}{2}\left(e^{i\omega t}\, e^{-i\omega t}\right)\begin{pmatrix}e^{-i\omega t}\\ -e^{i\omega t}\end{pmatrix} = \frac{1}{2}(1-1) = 0\ ,$$
$$t_1 = 0: \quad \langle\sigma_x\rangle = 1\ ; \quad \langle\sigma_y\rangle = 0\ ; \quad \langle\sigma_z\rangle = 0\ ,$$
$$t_2 = \frac{\pi\, m}{q\, B} = \frac{\pi}{2\omega}: \quad \langle\sigma_x\rangle = -1\ ; \quad \langle\sigma_y\rangle = 0\ ; \quad \langle\sigma_z\rangle = 0\ .$$

Solution 3.4.3 The time-dependence of ρ is tucked into $\mathbf{P} = \mathbf{P}(t)$.
Schrödinger picture:

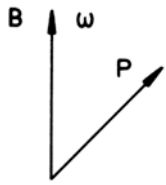
$$\dot\rho = \frac{i}{\hbar}[\rho, H]_- = \frac{1}{2}\dot{\mathbf{P}}\cdot\boldsymbol{\sigma}\ ,$$

$$[\rho, H]_- = \frac{1}{2}\hbar\omega\,[\mathbf{P}\cdot\boldsymbol{\sigma}\,,\, \mathbf{e}\cdot\boldsymbol{\sigma}]_-$$
$$= \frac{1}{2}\hbar\,\omega\,\{P_x\,[\sigma_x, e_y\,\sigma_y + e_z\,\sigma_z]_- + P_y\,[\sigma_y, e_x\,\sigma_x + e_z\,\sigma_z]_- +$$
$$+P_z\,[\sigma_z, e_x\,\sigma_x + e_y\,\sigma_y]_-\}\ .$$

Commutator relations according to the solution of Exercise 3.3.9:

$$[\sigma_x, \sigma_y]_- = 2i\,\sigma_z\ ; \quad [\sigma_x, \sigma_z]_- = -2i\,\sigma_y\ , \quad [\sigma_y, \sigma_z]_- = 2i\,\sigma_x$$
$$\Longrightarrow\ [\rho, H]_- =$$

Fig. A.8



$$= i\hbar\,\omega\,\{P_x\,e_y\,\sigma_z - P_x\,e_z\,\sigma_y - P_y\,e_x\,\sigma_z + P_y\,e_z\,\sigma_x + P_z\,e_x\,\sigma_y - P_z\,e_y\,\sigma_x\} =$$
$$= i\hbar\,\omega\,\{(P_x\,e_y - P_y\,e_x)\,\sigma_z + (P_z\,e_x - P_x\,e_z)\,\sigma_y + (P_y\,e_z - P_z\,e_y)\,\sigma_x\} =$$
$$= i\hbar\,\omega\,(\mathbf{P}\times\mathbf{e})\cdot\boldsymbol{\sigma}\ .$$

It follows therewith:

$$\dot{\rho} = -\omega(\mathbf{P}\times\mathbf{e})\cdot\boldsymbol{\sigma} = \frac{1}{2}\,\dot{\mathbf{P}}\cdot\boldsymbol{\sigma}$$
$$\Longrightarrow\ \dot{\mathbf{P}} = 2\,\boldsymbol{\omega}\times\mathbf{P} \qquad (\boldsymbol{\omega} = \omega\,\mathbf{e})\ .$$

This is the velocity, with which the vector of polarization rotates around the direction of the field (Fig. A.8). It is typical for spin-$\frac{1}{2}$-particles (Sect. 1.3.2) that the angular velocity corresponds to twice the Larmor frequency $\omega_{\mathrm{L}} = q\,B/(2m)$!

Solution 3.4.4

$$t = 0:\ A|\psi(0)\rangle = a|\psi(0)\rangle\ ,$$
$$t > 0:\ A_{\mathrm{H}}(t) = U^{+}(t,t_0)\,A\,U(t,t_0)\ ;\quad t_0 = 0\ .$$

Schrödinger-state:

$$|\psi(t)\rangle = U(t,0)|\psi(0)\rangle\ ,$$
$$\frac{\partial H}{\partial t} = 0:\ U(t,0) = e^{-\frac{i}{\hbar}Ht} = U(0,-t)\ .$$

Then:

$$A_{\mathrm{H}}(-t)|\psi(t)\rangle = U^{+}(-t,0)\,A\,\underbrace{U(-t,0)\,U(t,0)}_{=\mathbb{1}}\,|\psi(0)\rangle$$
$$= U^{+}(-t,0)\,A|\psi(0)\rangle = a\,U^{+}(-t,0)|\psi(0)\rangle =$$
$$= a\,U(t,0)|\psi(0)\rangle = a|\psi(t)\rangle \quad \text{q.e.d.}$$

Solution 3.4.5

1. Equation of motion for not explicitly time-dependent observables:

$$i\hbar\frac{d}{dt}q_{\mathrm{H}}(t) = [q_{\mathrm{H}}(t), H_{\mathrm{H}}]_- = e^{\frac{i}{\hbar}Ht}\,[q,H]_-\,e^{-\frac{i}{\hbar}Ht}\,,$$

$$\frac{\partial H}{\partial t} = 0 \implies H_{\mathrm{H}} = H\,,$$

$$[q,H]_- = \frac{1}{2m}\,[q,p^2] = \frac{1}{2m}\,\{[q,p]_-\,p + p[q,p]_-\} = \frac{i\hbar}{m}\,p\,.$$

Intermediate result:

$$\frac{d}{dt}\,q_{\mathrm{H}}(t) = \frac{1}{m}\,p_{\mathrm{H}}(t)\,.$$

2.

$$i\hbar\frac{d}{dt}\,p_{\mathrm{H}}(t) = [p_{\mathrm{H}}(t), H] = e^{\frac{i}{\hbar}Ht}\,[p,H]_-\,e^{-\frac{i}{\hbar}Ht}$$

$$[p,H]_- = \frac{1}{2}\,m\omega^2\,[p,q^2]_- = \frac{1}{2}\,m\omega^2\{q\,[p,q]_- + [p,q]_-\,q\} = -i\hbar m\omega^2 q\,.$$

Intermediate result:

$$\frac{d}{dt}\,p_{\mathrm{H}}(t) = -m\omega^2 q_{\mathrm{H}}(t)\,.$$

3. Combination of the two intermediate results:

$$\frac{d^2}{dt^2}\,q_{\mathrm{H}}(t) = \frac{1}{m}\,\frac{d}{dt}\,p_{\mathrm{H}}(t) = -\omega^2 q_{\mathrm{H}}(t)\,,$$

$$\frac{d^2}{dt^2}\,p_{\mathrm{H}}(t) = -m\omega^2\,\frac{d}{dt}\,q_{\mathrm{H}}(t) = -\omega^2\,p_{\mathrm{H}}(t) \qquad \text{q.e.d.}$$

Solution 3.4.6

$$H = \frac{1}{2m}\,p^2; \quad \frac{\partial H}{\partial t} = 0 \implies H_{\mathrm{H}} = H\,.$$

1. Equations of motion:

$$
\begin{aligned}
i\hbar\dot{q}_{\mathrm{H}}(t) &= [q_{\mathrm{H}}(t), H_{\mathrm{H}}]_- = e^{\frac{i}{\hbar}Ht}\,[q,H]_-\,e^{-\frac{i}{\hbar}Ht}\ ,\ (t_0=0)\ ,\\
[q,H]_- &= \frac{1}{2m}\,[q,p^2] = \frac{1}{2m}\,\{p[q,p]_- + [q,p]_-\,p\} = \frac{i\,\hbar}{m}\,p\\
\Longrightarrow\ \dot{q}_{\mathrm{H}}(t) &= \frac{1}{m}\,p_{\mathrm{H}}(t)\ ,\\
i\hbar\dot{p}_{\mathrm{H}}(t) &= [p_{\mathrm{H}}(t), H_{\mathrm{H}}]_- = 0\\
\Longrightarrow\ p_{\mathrm{H}}(t) &= \mathrm{const} = p(0) = p \qquad \text{(integral of motion)}\\
\Longrightarrow\ q_{\mathrm{H}}(t) &= q_{\mathrm{H}}(0) + \frac{1}{m}\,p\,t = q + \frac{p}{m}\,t\ .
\end{aligned}
$$

2.

$$
\begin{aligned}
[q_{\mathrm{H}}(t_1), q_{\mathrm{H}}(t_2)]_- &= \left[q + \frac{p}{m}\,t_1, q + \frac{p}{m}\,t_2\right]_- =\\
&= [q,q]_- + \frac{1}{m^2}\,t_1\,t_2\,[p,p]_- + \frac{t_1}{m}[p,q]_- + \frac{t_2}{m}[q,p]_- =\\
&= \frac{i\,\hbar}{m}\,(t_2 - t_1)
\end{aligned}
$$

$$
[p_{\mathrm{H}}(t_1), p_{\mathrm{H}}(t_2)]_- = [p,p]_- = 0
$$

$$
[q_{\mathrm{H}}(t_1), p_{\mathrm{H}}(t_2)]_- = \left[q + \frac{p}{m}\,t_1, p\right]_- = [q,p]_- + \frac{t_1}{m}\,[p,p]_- = i\,\hbar\ .
$$

Solution 3.4.7

1. $H = \frac{p^2}{2m} - \alpha q$.
   Equation of motion in the Heisenberg picture

$$
\begin{aligned}
i\hbar\,\dot{q} &= [q,H]_-\\
&= \left[q, \frac{p^2}{2m}\right]_- - \alpha\,\underbrace{[q,q]_-}_{=0}\\
&= \frac{1}{2m}(\underbrace{[q,p]_-}_{=i\hbar}p + p[q,p]_-)\\
&= \frac{i\hbar}{m}p\\
\curvearrowright\ \dot{q}(t) &= \frac{1}{m}p(t) \qquad \text{(see Classical Physics)}
\end{aligned}
$$

$$
\begin{aligned}
i\hbar\,\dot{p} &= [p, H]_- \\
&= -\alpha [p, q]_- \\
&= i\hbar\alpha \\
\curvearrowright\ \dot{p}(t) &= \alpha \\
\curvearrowright\ p(t) &= \alpha t + p_0 \\
\dot{q}(t) &= \frac{\alpha}{m} t + \frac{1}{m} p_0 \\
\curvearrowright\ q(t) &= \frac{\alpha}{2m} t^2 + \frac{p_0}{m} t + q_0 \ .
\end{aligned}
$$

2.

$$
\begin{aligned}
[q(t_1), q(t_2)]_- &= \left[\frac{\alpha}{2m} t_1^2 + \frac{1}{m} p_0 t_1 + q_0, \frac{\alpha}{2m} t_2^2 + \frac{1}{m} p_0 t_2 + q_0 \right]_- \\
&= \left[\frac{1}{m} p_0 t_1, q_0 \right]_- + \left[q_0, \frac{1}{m} p_0 t_2 \right]_- \\
&= \frac{1}{m} t_1 \underbrace{[p_0, q_0]_-}_{=-i\hbar} + \frac{1}{m} t_2 \underbrace{[q_0, p_0]_-}_{=i\hbar} \\
&= \frac{i\hbar}{m} (t_2 - t_1) \ ,
\end{aligned}
$$

$$
\begin{aligned}
\left[q(t_1), p^2(t_2) \right]_- &= p(t_2) \, [q(t_1), p(t_2)]_- + [q(t_1), p(t_2)]_- \, p(t_2) \\
&= p(t_2) \left[\frac{1}{m} p_0 t_1 + q_0, p_0 \right]_- + \left[\frac{1}{m} p_0 t_1 + q_0, p_0 \right]_- p(t_2) \\
&= p(t_2) \, [q_0, p_0]_- + [q_0, p_0]_- \, p(t_2) \\
&= 2i\hbar \, p(t_2) \ ,
\end{aligned}
$$

$$
\begin{aligned}
\left[p(t_1), q^2(t_2) \right]_- &= q(t_2) \, [p(t_1), q(t_2)]_- + [p(t_1), q(t_2)]_- \, q(t_2) \\
&= q(t_2) \left[p_0, \frac{1}{m} p_0 t_2 + q_0 \right]_- + \left[p_0, \frac{1}{m} p_0 t_2 + q_0 \right]_- q(t_2) \\
&= q(t_2) \underbrace{[p_0, q_0]_-}_{=-i\hbar} + \underbrace{[p_0, q_0]_-}_{=-i\hbar} q(t_2) \\
&= -2i\hbar \, q(t_2) \ .
\end{aligned}
$$

Solution 3.4.8

1. **Schrödinger picture:**
   Pure state::

$$\begin{aligned}\frac{d}{dt}\langle A\rangle &= \frac{d}{dt}\langle\psi(t)|A|\psi(t)\rangle = \\ &= \left\langle\dot{\psi}(t)|A|\psi(t)\right\rangle + \left\langle\psi(t)\left|\frac{\partial A}{\partial t}\right|\psi(t)\right\rangle + \left\langle\psi(t)|A|\dot{\psi}(t)\right\rangle = \\ &= \frac{-1}{i\hbar}\left\langle\psi(t)|(HA - AH)|\psi(t)\right\rangle + \left\langle\psi(t)\left|\frac{\partial A}{\partial t}\right|\psi(t)\right\rangle \\ \Longrightarrow\quad i\hbar\frac{d}{dt}\langle A\rangle &= \langle[A,H]_-\rangle + i\hbar\left\langle\frac{\partial A}{\partial t}\right\rangle .\end{aligned}$$

   Mixed state:

$$\begin{aligned}\frac{d}{dt}\langle A\rangle &= \frac{d}{dt}\mathrm{Tr}(\rho A) \\ &= \mathrm{Tr}(\dot{\rho}A) + \mathrm{Tr}(\rho\dot{A}) \\ &= \frac{i}{\hbar}\mathrm{Tr}([\rho,\, H]_- A) + \mathrm{Tr}\left(\rho\frac{\partial A}{\partial t}\right) \\ &= \frac{i}{\hbar}\mathrm{Tr}(\rho HA - H\rho A) + \left\langle\frac{\partial A}{\partial t}\right\rangle \\ &= \frac{i}{\hbar}\mathrm{Tr}(\rho HA - \rho AH) + \left\langle\frac{\partial A}{\partial t}\right\rangle\end{aligned}$$

   In the last step we have used the cyclic invariance of the trace:

$$\Longrightarrow\quad i\hbar\frac{d}{dt}\langle A\rangle = \mathrm{Tr}(\rho[A,H]_-) + i\hbar\left\langle\frac{\partial A}{\partial t}\right\rangle = \langle[A,H]_-\rangle + i\hbar\left\langle\frac{\partial A}{\partial t}\right\rangle .$$

2. **Heisenberg picture:**
   Pure state:

$$\begin{aligned}\frac{d}{dt}\langle A_{\mathrm{H}}\rangle &= \left\langle\psi_{\mathrm{H}}\left|\frac{d}{dt}A_{\mathrm{H}}\right|\psi_{\mathrm{H}}\right\rangle \\ &\overset{(3.191)}{=} \frac{1}{i\hbar}\left\langle\psi_{\mathrm{H}}\left|[A_{\mathrm{H}},H_{\mathrm{H}}]_-\right|\psi_{\mathrm{H}}\right\rangle + \left\langle\psi_{\mathrm{H}}\left|\frac{\partial A_{\mathrm{H}}}{\partial t}\right|\psi_{\mathrm{H}}\right\rangle \\ \Longrightarrow\quad i\hbar\frac{d}{dt}\langle A_{\mathrm{H}}\rangle &= \langle[A_{\mathrm{H}},H_{\mathrm{H}}]_-\rangle + i\hbar\left\langle\frac{\partial A_{\mathrm{H}}}{\partial t}\right\rangle .\end{aligned}$$

Mixed state:

$$\frac{d}{dt}\langle A_{\rm H}\rangle = {\rm Tr}\left(\rho_{\rm H}\,\frac{d}{dt}A_{\rm H}\right)\,.$$

With (3.191) it follows immediately the same equation as for the pure state.

3. **Dirac picture:**
   Pure state:

$$\begin{aligned}
\frac{d}{dt}\langle A_{\rm D}\rangle &= \langle\dot{\psi}_{\rm D}(t)|A_{\rm D}|\psi_{\rm D}(t)\rangle \\
&\quad +\langle\psi_{\rm D}(t)|\dot{A}_{\rm D}|\psi_{\rm D}(t)\rangle + \langle\psi_{\rm D}(t)|A_{\rm D}|\dot{\psi}_{\rm D}(t)\rangle \\
&= \frac{-1}{i\hbar}\langle\psi_{\rm D}(t)|(H_{1\rm D}\,A_{\rm D} - A_{\rm D}\,H_{1\rm D})|\psi_{\rm D}(t)\rangle \\
&\quad +\frac{1}{i\hbar}\langle\psi_{\rm D}(t)|[A_{\rm D},H_0]_-|\psi_{\rm D}(t)\rangle + \left\langle\psi_{\rm D}(t)|\frac{\partial A_{\rm D}}{\partial t}|\psi_{\rm D}(t)\right\rangle \\
\Longrightarrow\ i\hbar\,\frac{d}{dt}\langle A_{\rm D}\rangle &= \langle\psi_{\rm D}(t)|[A_{\rm D},H_{\rm D}]_-|\psi_{\rm D}(t)\rangle + i\hbar\left\langle\frac{\partial A_{\rm D}}{\partial t}\right\rangle \\
&= \langle[A_{\rm D},H_{\rm D}]_-\rangle + i\hbar\left\langle\frac{\partial A_{\rm D}}{\partial t}\right\rangle\,.
\end{aligned}$$

   Mixed state:

$$\begin{aligned}
\frac{d}{dt}\langle A_D\rangle &= \\
&= {\rm Tr}(\dot{\rho}\,A_D) + {\rm Tr}(\rho\dot{A_D}) \\
&= {\rm Tr}\left(\frac{i}{\hbar}[\rho_D,\,H_{1D}]_-A_D\right) + {\rm Tr}\left(\rho_D\frac{1}{i\hbar}[A_D,\,H_0]_-\right) + {\rm Tr}\left(\rho_D\frac{\partial A_D}{\partial t}\right) \\
&= \frac{1}{i\hbar}{\rm Tr}(\rho_D\,A_D\,H_0 - \rho_D\,H_0\,A_D - \rho_D\,H_{1D}\,A_D + H_{1D}\,\rho_D\,A_D) + \left\langle\frac{\partial A_D}{\partial t}\right\rangle \\
&\quad \text{(cyclic invariance of the trace!)} \\
&= \frac{1}{i\hbar}{\rm Tr}\,(\rho_D\,[A_D,\,H_0+H_{1D}]_-) + \left\langle\frac{\partial A_D}{\partial t}\right\rangle \\
\Longrightarrow i\hbar\frac{d}{dt}\langle A_D\rangle &= \langle[A_D,\,H_D]_-\rangle + \left\langle\frac{\partial A_D}{\partial t}\right\rangle
\end{aligned}$$

Conclusion:
The equation of motion of $\langle A\rangle$ is form-invariant, i.e., independent of the representation. $\Longrightarrow$ Ehrenfest's theorem (3.211).

Solution 3.4.9 Force:

$$F(q) = -\frac{d}{dq}V(q) \equiv F = \text{const}$$
$$\Longrightarrow \quad V(q) = -F\,q + C\ .$$

The constant is inconsequential and can therefore be neglected. q is the position **operator**, while F is a c-number. Hamilton operator:

$$H = \frac{p^2}{2m} - F\,q\ .$$

The momentum is not explicitly time-dependent! (3.211) $\Longrightarrow$

$$\frac{d}{dt}\langle p\rangle = \frac{1}{i\,\hbar}\langle [p,H]_-\rangle = -\frac{1}{i\,\hbar}F\langle [p,q]_-\rangle = F$$
$$\Longrightarrow \quad \langle p\rangle_t = \langle p\rangle_0 + F\,t\ .$$

Solution 3.4.10

1. Hamilton's equations of motion:

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}\ ; \quad \dot{p} = -\frac{\partial H}{\partial q} = -m\omega^2 q$$
$$\Longrightarrow \qquad \ddot{q}(t) + \omega^2 q(t) = 0\ ,$$
$$\ddot{p}(t) + \omega^2 p(t) = 0\ .$$

2. $\hat{q}$, $\hat{p}$ are not explicitly time-dependent. It holds therefore with (3.211):

$$i\,\hbar\,\frac{d}{dt}\langle\hat{q}\rangle = \langle [\hat{q},\widehat{H}]_-\rangle\ ,$$
$$i\,\hbar\,\frac{d}{dt}\langle\,\hat{p}\rangle = \langle\,[\hat{p},\,\widehat{H}]_-\rangle\ .$$

With (3.215), (3.216) we come to the conclusion:

$$[\hat{p},\,\widehat{H}]_- = \frac{\hbar}{i}\,\frac{d}{d\hat{q}}\,V(\hat{q}) = \frac{\hbar}{i}\,m\omega^2\hat{q}\ ,$$

$$[\hat{q},\widehat{H}]_- = \frac{i\,\hbar}{m}\,\hat{p}\ .$$

This means:

$$\begin{aligned} & \frac{d}{dt}\langle\hat{q}\rangle = \frac{1}{m}\langle\hat{p}\rangle \,, \\ & \frac{d}{dt}\langle\hat{p}\rangle = -m\omega^2\langle\hat{q}\rangle \\ \Longrightarrow \quad & \frac{d^2}{dt^2}\langle\hat{q}\rangle + \omega^2\langle\hat{q}\rangle = 0 \,, \\ & \frac{d^2}{dt^2}\langle\hat{p}\rangle + \omega^2\langle\hat{p}\rangle = 0 \,. \end{aligned}$$

3. The quantum-mechanical equation of motion reads according to (3.220):

$$m\,\frac{d^2}{dt^2}\langle\hat{q}\rangle = -\left\langle\frac{d}{d\hat{q}}\,V(\hat{q})\right\rangle \,.$$

Agreement with the classical result if

$$\left\langle\frac{d}{d\hat{q}}\,V(\hat{q})\right\rangle = \frac{d}{d\langle\hat{q}\rangle}\,V(\langle\hat{q}\rangle) \,.$$

In part 2.:

$$\begin{aligned} & V(\hat{q}) = \frac{1}{2}\,m\omega^2\,\hat{q}^2 \\ \Longrightarrow \quad & \left\langle\frac{d}{d\hat{q}}\,V(\hat{q})\right\rangle = m\omega^2\langle\hat{q}\rangle = \frac{d}{d\langle\hat{q}\rangle}\,V(\langle\hat{q}\rangle) \,. \end{aligned}$$

Now:

$$\begin{aligned} & V(\hat{q}) = \alpha\,\hat{q}^4 \\ \Longrightarrow \quad & \langle\frac{d}{d\hat{q}}\,V(\hat{q})\rangle = 4\alpha\langle\hat{q}^3\rangle \,, \\ & \frac{d}{d\langle\hat{q}\rangle}\,V(\langle\hat{q}\rangle) = 4\alpha\langle\hat{q}\rangle^3 \\ & \text{in general:} \quad \langle\hat{q}^3\rangle \neq \langle\hat{q}\rangle^3 \\ \Longrightarrow \quad & \left\langle\frac{d}{d\hat{q}}\,V(\hat{q})\right\rangle \neq \frac{d}{d\langle\hat{q}\rangle}\,V(\langle\hat{q}\rangle) \,. \end{aligned}$$

No match of classical and quantum-mechanical equations of motion!

Section 3.5.3

Solution 3.5.1

1. Classical angular momentum:

$$L_i = \sum_{m,\,n} \varepsilon_{imn}\, x_m p_n \ ,$$

$$\varepsilon_{imn} = \begin{cases} +1, & \text{if } (i,m,n) \text{ cyclic from (1,2,3)} \ , \\ -1, & \text{if } (i,m,n) \text{ anti-cyclic from (1,2,3)} \ , \\ 0 & \text{otherwise} \ , \end{cases}$$

fully antisymmetric unit tensor of third rank (see (1.193), Vol. 1).

a)

$$\begin{aligned} \{L_i, L_j\} &= \sum_{m,\,n} \sum_{s,\,t} \varepsilon_{imn}\, \varepsilon_{jst}\, \{x_m p_n, x_s\, p_t\} \\ &= \sum_{m,\,n} \sum_{s,\,t} \varepsilon_{imn}\, \varepsilon_{jst}\, (x_m \{\, p_n, x_s\} p_t + x_s \{x_m, p_t\} p_n) \\ &= \sum_{\substack{m,\,n \\ s,\,t}} \varepsilon_{imn}\, \varepsilon_{jst}\, (-\delta_{ns}\, x_m p_t + \delta_{mt}\, x_s\, p_n) \ . \end{aligned}$$

We have here applied the properties of the Poisson bracket as listed in Sect. 3.5.1.

$$\begin{aligned} \{L_i, L_j\} &= \sum_{m,\,n,\,s} \varepsilon_{imn}\, (\varepsilon_{jsm}\, x_s\, p_n - \varepsilon_{jns}\, x_m p_s) = \\ &= \sum_{m,n,s} \varepsilon_{imn}\, \varepsilon_{jsm}\, (x_s\, p_n - x_n\, p_s) \ . \end{aligned}$$

It is easily realized that

$$\sum_m \varepsilon_{imn}\, \varepsilon_{jsm} = -\sum_m \varepsilon_{inm}\, \varepsilon_{jsm} = -(\delta_{ij}\, \delta_{ns} - \delta_{is}\, \delta_{nj}) \ .$$

This means:

$$\begin{aligned} \underline{\{L_i, L_j\}} &= \sum_{n,s} (\delta_{is}\, \delta_{nj} - \delta_{ij}\, \delta_{ns})\, (x_s\, p_n - x_n\, p_s) = x_i\, p_j - x_j\, p_i \\ &= \underline{\sum_k \varepsilon_{ijk}\, L_k} \ . \end{aligned}$$

In detail, the following important Poisson brackets are found:

$$\begin{aligned}\{L_x, L_y\} &= -\{L_y, L_x\} = L_z \ , \\ \{L_x, L_z\} &= -\{L_z, L_x\} = -L_y \ , \\ \{L_y, L_z\} &= -\{L_z, L_y\} = L_x \ .\end{aligned}$$

We calculate in the next step:

$$\begin{aligned}\underline{\{L_i, \mathbf{L}^2\}} &= \sum_j \left\{L_i, L_j^2\right\} = \sum_j \left(L_j \{L_i, L_j\} + \{L_i, L_j\} L_j\right) \\ &= \sum_{j,k} \varepsilon_{ijk} \left(L_j L_k + L_k L_j\right) = \sum_{j,k} \underbrace{\left(\varepsilon_{ijk} + \varepsilon_{ikj}\right)}_{=0} L_j L_k \underline{= 0 \ .}\end{aligned}$$

b)

$$\begin{aligned}\underline{\{L_i, x_j\}} &= \sum_{m,n} \varepsilon_{imn} \{x_m p_n, x_j\} = \sum_{m,n} \varepsilon_{imn} x_m \{p_n, x_j\} = \\ &= \sum_{m,n} \varepsilon_{imn} x_m (-\delta_{nj}) = \underline{\sum_m \varepsilon_{ijm} x_m} \ , \\ \underline{\{L_i, \mathbf{r}^2\}} &= \sum_j \{L_i, x_j^2\} = \sum_j (x_j \{L_i, x_j\} + \{L_i, x_j\} x_j) = \\ &= \sum_{jm} \varepsilon_{ijm} (x_j x_m + x_m x_j) = \sum_{jm} \underbrace{\left(\varepsilon_{ijm} + \varepsilon_{imj}\right)}_{=0} x_j x_m \underline{= 0 \ .}\end{aligned}$$

c)

$$\begin{aligned}\underline{\{L_i, p_j\}} &= \sum_{m,n} \varepsilon_{imn} \{x_m p_n, p_j\} = \sum_{m,n} \varepsilon_{imn} \{x_m, p_j\} p_n = \underline{\sum_n \varepsilon_{ijn} p_n} \ , \\ \underline{\{L_i, \mathbf{p}^2\}} &= \sum_j \{L_i, p_j^2\} = \sum_j \left(p_j \{L_i, p_j\} + \{L_i, p_j\} p_j\right) = \\ &= \sum_{jn} \varepsilon_{ijn} \left(p_j p_n + p_n p_j\right) = \sum_{j,n} \underbrace{\left(\varepsilon_{ijn} + \varepsilon_{inj}\right)}_{=0} p_j p_n \underline{= 0 \ .}\end{aligned}$$

2. Transition to quantum-mechanical operators:

$$\widehat{L}_i = \sum_{m,n} \varepsilon_{imn} \widehat{x}_m \hat{p}_n \ .$$

Symmetrization **not** necessary, since $\widehat{x}_m$ and $\widehat{p}_n$ commute for $n \neq m$.
Principle of correspondence (3.229):

$$[\widehat{L}_i, \widehat{L}_j]_- = i\hbar \sum_k \varepsilon_{ijk} \widehat{L}_k$$

$$[\widehat{L}_i, \widehat{\mathbf{L}}^2]_- = 0$$

$$[\widehat{L}_i, \widehat{x}_j]_- = i\hbar \sum_m \varepsilon_{ijm} \widehat{x}_m$$

$$[\widehat{L}_i, \hat{\mathbf{r}}^2]_- = 0$$

$$[\widehat{L}_i, \hat{p}_j]_- = i\hbar \sum_m \varepsilon_{ijm} \hat{p}_m$$

$$[\widehat{L}_i, \hat{\mathbf{p}}^2]_- = 0\,.$$

Solution 3.5.2

1.

$$\begin{aligned} i\hbar \frac{d}{dt}(A+B) &= [A+B, H]_- + i\hbar \frac{\partial}{\partial t}(A+B) \\ &= [A, H]_- + [B, H]_- + i\hbar \frac{\partial}{\partial t} A + i\hbar \frac{\partial}{\partial t} B \\ &= i\hbar \frac{d}{dt} A + i\hbar \frac{d}{dt} B \qquad \text{q.e.d.} \end{aligned}$$

2.

$$\begin{aligned} i\hbar \frac{d}{dt}(A\,B) &= [A\,B, H]_- + i\hbar \frac{\partial}{\partial t}(A\,B) \\ &= A[B, H]_- + [A, H]_- B + i\hbar \left(\frac{\partial}{\partial t} A\right) B + i\hbar A \left(\frac{\partial}{\partial t} B\right) \\ &= i\hbar \left(\frac{d}{dt} A\right) B + i\hbar A \left(\frac{d}{dt} B\right) \qquad \text{q.e.d.} \end{aligned}$$

3.

$$
\begin{aligned}
i\hbar\,\frac{d}{dt}\,(\alpha A) &= [\alpha A, H]_- + i\hbar\,\frac{\partial}{\partial t}\,(\alpha A) \\
&= \alpha[A, H]_- + i\hbar\,\dot{\alpha}\,A + i\hbar\,\alpha\,\frac{\partial}{\partial t}A \\
&= \alpha\, i\hbar\,\frac{d}{dt}A + i\hbar\,\dot{\alpha}\,A \qquad \text{q.e.d.}
\end{aligned}
$$

Solution 3.5.3 Equation of motion:

$$
\begin{aligned}
& i\hbar\,\frac{d}{dt}\,q = [q, H]_- \,; \qquad \frac{\partial}{\partial t}\,q = 0 \\
\Longrightarrow\ & \dot{q} = \frac{1}{i\hbar}[q, H]_- \,.
\end{aligned}
$$

Equation of motion for the operator of the velocity:

$$
\begin{aligned}
& i\hbar\ddot{q} = [\dot{q}, H]_- + i\hbar\,\frac{\partial \dot{q}}{\partial t} = \frac{1}{i\hbar}\big[[q, H]_-, H\big]_- + \frac{\partial}{\partial t}[q, H]_- \\
\Longrightarrow\ & \ddot{q} = \frac{1}{(i\hbar)^2}\big[[q, H]_-, H\big]_- + \frac{1}{i\hbar}\left[q, \frac{\partial H}{\partial t}\right]_- \,.
\end{aligned}
$$

Solution 3.5.4

1.

$$
A = \frac{1}{2}\sum_{i=1}^{3}(x_i\,p_i + p_i\,x_i) = \frac{1}{2}\sum_{i=1}^{3}\left(2x_i\,p_i + \frac{\hbar}{i}\mathbb{1}\right) = \mathbf{r}\cdot\mathbf{p} + \frac{3\hbar}{2i}\mathbb{1}\,.
$$

V is homogeneous of degree n: $V(\alpha\,\mathbf{r}) = \alpha^n\,V(\mathbf{r})$:

$$
\begin{aligned}
\frac{d}{d\alpha}\,V(\alpha\,\mathbf{r}) &= (\mathbf{r}\cdot\nabla_{\alpha\,\mathbf{r}})\,V(\alpha\,\mathbf{r}) = \sum_i x_i\,\frac{\partial V(\alpha\,\mathbf{r})}{\partial(\alpha\,x_i)}, \\
\frac{d}{d\alpha}\,V(\alpha\,\mathbf{r}) &= \frac{d}{d\alpha}\,\alpha^n\,V(\mathbf{r}) = n\,\alpha^{n-1}\,V(\mathbf{r})\,.
\end{aligned}
$$

The comparison yields:

$$
\sum_i x_i\,\frac{\partial V(\alpha\,\mathbf{r})}{\partial(\alpha\,x_i)} = n\,\alpha^{n-1}\,V(\mathbf{r})\,.
$$

This is valid for all $\alpha \in \mathbb{R}^+$, therefore also for $\alpha = 1$:

$$\sum_{i=1}^{3} x_i \frac{\partial V}{\partial x_i} = n\,V\ .$$

2. Equation of motion:

$$\begin{aligned} i\hbar\dot{A} &= [A,H]_- = [\mathbf{r}\cdot\mathbf{p},H]_- + \frac{3\hbar}{2i}\,[\mathbb{1},H]_- \\ \Longrightarrow\quad i\hbar\dot{A} &= [\mathbf{r}\cdot\mathbf{p},T]_- + [\mathbf{r}\cdot\mathbf{p},V]_- \end{aligned}$$

$$\begin{aligned} [\mathbf{r}\cdot\mathbf{p},T]_- &= \sum_{i=1}^{3}[x_i\,p_i,T(\mathbf{p})]_- = \sum_{i=1}^{3}[x_i,T(\mathbf{p})]_-\,p_i = \sum_{i,j}[x_i,\,p_j^2]_-\,\frac{p_i}{2m} \\ &= \sum_{i,j}\left(p_j[x_i,p_j]_- + [x_i,p_j]_-\,p_j\right)\frac{p_i}{2m} \\ &= i\,\hbar\sum_{i,j}2p_j\,\delta_{ij}\,\frac{p_i}{2m} = i\,\hbar\,2\sum_i\frac{p_i^2}{2m} = i\,\hbar\,2\,T \end{aligned}$$

$$[\mathbf{r}\cdot\mathbf{p},V]_- = \sum_{i=1}^{3}[x_i\,p_i,V(\mathbf{r})]_- = \sum_{i=1}^{3}x_i\,[p_i,V(\mathbf{r})]_-\ .$$

It is according to Exercise 3.2.26:

$$\begin{aligned} [p_i,V(\mathbf{r})]_- &= \frac{\hbar}{i}\,\frac{\partial V(\mathbf{r})}{\partial x_i} \\ \Longrightarrow\quad [\mathbf{r}\cdot\mathbf{p},V]_- &= -i\,\hbar\sum_{i=1}^{3}x_i\,\frac{\partial V}{\partial x_i} = -i\,\hbar\,n\,V\ . \end{aligned}$$

This yields eventually the virial theorem:

$$\dot{A} = 2\,T - n\,V\ .$$

3.

$$\begin{aligned} \langle E|[A,H]_-|E\rangle &= \langle E|A\,H|E\rangle - \langle E|H\,A|E\rangle \\ &= E(\langle E|A|E\rangle - \langle E|A|E\rangle) = 0 \\ \Longrightarrow\quad \langle E|\dot{A}|E\rangle &= 0\ . \end{aligned}$$

The virial theorem therewith reads:

$$2\langle T\rangle = n\langle V\rangle \ .$$

a) Coulomb potential $\sim 1/r$:

$$\begin{aligned} &\Longrightarrow\ V(\alpha\,\mathbf{r}) = \alpha^{-1}\,V(\mathbf{r}) \ \Longrightarrow\ n=-1 \\ &\Longrightarrow\ 2\langle T\rangle = -\langle V\rangle \ . \end{aligned}$$

b) Oscillator potential $\sim r^2$:

$$\Longrightarrow\ \langle T\rangle = \langle V\rangle,\ \text{since } n=2 \ .$$

Solution 3.5.5 Eigen-value equation:

$$\hat{p}|p\rangle = p|p\rangle \ .$$

Multiplication by the bra-state $\langle q|$:

$$\langle q|\hat{p}|p\rangle = p\langle q|p\rangle \ .$$

Position representation:

$$\frac{\hbar}{i}\,\frac{d}{dq}\,\psi_p(q) = p\,\psi_p(q) \ .$$

Solution:

$$\psi_p(q) = \alpha\,\exp\left(\frac{i}{\hbar}\,p\,q\right) \ .$$

For normalization (α) look up Sect. 2.2.5.

Solution 3.5.6

1.

$$\begin{aligned} &T(a)\,T(-a)|q\rangle = T(a)|q-a\rangle = |q\rangle \qquad \forall|q\rangle \\ &\Longrightarrow\ T(a)\,T(-a) = \mathbb{1} \ \Longrightarrow\ T^{-1}(a) = T(-a) \ . \end{aligned}$$

2.

$$\begin{aligned} \langle q|T(a)|\overline{q}\rangle &\overset{\text{Def.}}{=} \langle\overline{q}|T^{+}(a)|q\rangle^{*} \ , \\ \langle q|T(a)|\overline{q}\rangle &= \langle q|\overline{q}+a\rangle = \delta(q-\overline{q}-a) = \langle q-a|\overline{q}\rangle \end{aligned}$$

$$
\begin{aligned}
&= \langle \overline{q}|q-a\rangle^* = \langle \overline{q}|T(-a)|q\rangle^* \\
\Longrightarrow\ T^+(a) &= T(-a) \overset{1.}{=} T^{-1}(a)\ .
\end{aligned}
$$

3.

$$
\begin{aligned}
&T(a)\,T(b)|q\rangle = T(a)|q+b\rangle = |q+a+b\rangle = T(a+b)|q\rangle \qquad \forall |q\rangle \\
\Longrightarrow\ &T(a)\,T(b) = T(a+b)\ .
\end{aligned}
$$

4.

$$
\begin{aligned}
T(a)\,\hat{q}\,T^+(a)|q\rangle &= T(a)\,\hat{q}\,T(-a)|q\rangle = T(a)\,\hat{q}|q-a\rangle \\
&= (q-a)\,T(a)|q-a\rangle = \\
&= (q-a)|q\rangle = (\hat{q}-a\mathbb{1})|q\rangle \qquad \forall |q\rangle \\
&\Longrightarrow\ T(a)\,\hat{q}\,T^+(a) = \hat{q}-a\mathbb{1}\ .
\end{aligned}
$$

5.

$$
\begin{aligned}
T(a)\,\hat{p}\,T^+(a)|q\rangle &= T(a)\,\hat{p}\,T(-a)|q\rangle = T(a)\,\hat{p}|q-a\rangle = \\
&= T(a)\Big(\underbrace{\int d\,q'|q'\rangle\langle q'|}_{\mathbb{1}}\Big)\Big(\underbrace{\int dp\,p|p\rangle\langle p|}_{\hat{p}}\Big)|q-a\rangle = \\
&= \int dq' \int dp|q'+a\rangle\langle q'|p\rangle\langle p|q-a\rangle p\ .
\end{aligned}
$$

According to Exercise 3.5.5 we have:

$$
\begin{aligned}
&\langle q'|p\rangle\langle p|q-a\rangle = |\alpha|^2 \exp\Big[\frac{i}{\hbar}\big(p(q'+a-q)\big)\Big] = \langle q'+a|p\rangle\langle p|q\rangle \\
\Longrightarrow\ &T(a)\,\hat{p}\,T^+(a)|q\rangle = \Big(\underbrace{\int dq'|q'+a\rangle\langle q'+a|}_{\mathbb{1}}\Big)\Big(\underbrace{\int dp\,p|p\rangle\langle p|}_{\hat{p}}\Big)|q\rangle \\
&\qquad = \mathbb{1}\hat{p}|q\rangle \qquad \forall |q\rangle \\
\Longrightarrow\ &T(a)\,\hat{p}\,T^+(a) = \hat{p} \quad \Big(\overset{2.}{\Longrightarrow}\ [T(a),\hat{p}]_- = 0\Big)\ .
\end{aligned}
$$

Solution 3.5.7

1.

$$\begin{aligned}
\Pi^2|q\rangle = \Pi|-q\rangle = |q\rangle \qquad \forall|q\rangle \\
\Longrightarrow\ \Pi^2 = \mathbb{1} \iff \Pi^{-1} = \Pi\ , \\
\langle q|\Pi|\overline{q}\rangle = \langle q|-\overline{q}\rangle = \delta(q+\overline{q}) = \delta(-q-\overline{q}) = \langle -q|\overline{q}\rangle \\
= \langle \overline{q}|-q\rangle^* = \langle \overline{q}|\Pi|q\rangle^* \overset{!}{=} \langle \overline{q}|\Pi^+|q\rangle^*\ .
\end{aligned}$$

Π is thus unitary and Hermitian:

$$\Pi^+ = \Pi = \Pi^{-1}\ .$$

2. Eigen-value equation:

$$\begin{aligned}
\Pi|\pi\rangle = \pi|\pi\rangle\ , \\
\Pi^2 = \mathbb{1} \ \Longrightarrow\ \Pi^2|\pi\rangle = \pi^2|\pi\rangle = |\pi\rangle\ .
\end{aligned}$$

Eigen-values: $\pi_\pm = \pm 1$.

3.

$$\begin{aligned}
\Pi|\alpha\rangle = \pi|\alpha\rangle\ ; \quad \Pi|\beta\rangle = \pi|\beta\rangle\ , \\
\Pi A\,\Pi^+ = -A\ ; \quad \Pi^+ = \Pi \text{ because of 1.}
\end{aligned}$$

We calculate therewith:

$$\begin{aligned}
\langle\alpha|A|\beta\rangle &= -\langle\alpha|\Pi A\,\Pi|\beta\rangle = -\pi^2\langle\alpha|A|\beta\rangle \overset{2.}{=} -\langle\alpha|A|\beta\rangle \\
&\Longrightarrow\ \langle\alpha|A|\beta\rangle = 0\ .
\end{aligned}$$

4.

$$\Pi\,\hat{q}\Pi^+|q\rangle = \Pi\,\hat{q}\,\Pi|q\rangle = \Pi\,\hat{q}|-q\rangle = -q\,\Pi|-q\rangle = -q|q\rangle = -\hat{q}|q\rangle\ .$$

This is valid for **all** $|q\rangle$, which, on the other hand, build a complete system.

$$\Pi\,\hat{q}\,\Pi^+ = -\hat{q}\ .$$

Treat $|q\rangle$ and $|-q\rangle$ as **different** eigen-states; i.e. in particular, they are linearly independent.

5.

$$\begin{aligned}
\Pi\,\hat{p}\,\Pi^{+}|q\rangle &= \Pi\Bigg(\underbrace{\int dq'|q'\rangle\langle q'|}_{\mathbb{1}}\Bigg)\Bigg(\underbrace{\int dp\, p|p\rangle\langle p|}_{\hat{p}}\Bigg)\Pi|q\rangle \\
&\qquad\qquad \text{(spectral representations)} \\
&= \int dq' \int dp\, p|-q'\rangle\langle q'|p\rangle\langle p|-q\rangle\ , \\
\langle q'|p\rangle &= \psi_p(q') \overset{(3.5.5)}{=} \psi_{-p}(-q') = \langle -q'|-p\rangle\ , \\
\langle p|-q\rangle &= \psi_p^*(-q) \overset{(3.5.5)}{=} \psi_{-p}^*(q) = \langle -p|q\rangle \\
\Longrightarrow\ \Pi\,\hat{p}\,\Pi^{+}|q\rangle &= \left(\int dq'|-q'\rangle\langle -q'|\right)\left(\int dp\, p|-p\rangle\langle -p|\right)|q\rangle\ ,
\end{aligned}$$

$$\int_{-\infty}^{+\infty} dq'|-q'\rangle\langle -q'| \underbrace{=}_{q''=-q'} \int_{-\infty}^{+\infty} dq''|q''\rangle\langle q''| = \mathbb{1}\ ,$$

$$\begin{aligned}
\int_{-\infty}^{+\infty} dp\, p|-p\rangle\langle -p| &\underbrace{=}_{p'=-p} \int_{+\infty}^{-\infty} dp'\, p'|p'\rangle\langle p'| \\
&= -\int_{-\infty}^{+\infty} dp'\, p'|p'\rangle\langle p'| = -\hat{p}\ .
\end{aligned}$$

It remains therewith:

$$\Pi\,\hat{p}\,\Pi^{+}|q\rangle = \mathbb{1}(-\hat{p})|q\rangle = -\hat{p}|q\rangle\ .$$

That holds for all $|q\rangle$, therefore:

$$\Pi\,\hat{p}\,\Pi^{+} = -\hat{p}\ .$$

The momentum operator, too, possesses odd parity!

Solution 3.5.8 Condition for Hermiticity:

$$\langle\psi|\hat{p}|\varphi\rangle \overset{!}{=} \langle\varphi|\hat{p}|\psi\rangle^* \qquad \forall|\varphi\rangle, |\psi\rangle\ .$$

This is equivalent to:

$$\int dq\langle\psi|q\rangle\langle q|\hat{p}|\varphi\rangle \overset{!}{=} \int dq(\langle\varphi|q\rangle\langle q|\hat{p}|\psi\rangle)^*\ .$$

Position representation (3.253):

$$\int dq\, \psi^*(q) \left(\frac{\hbar}{i} \frac{\partial}{\partial q} \varphi(q) \right) \stackrel{!}{=} \int dq \left(\frac{\hbar}{i} \frac{\partial}{\partial q} \psi(q) \right)^* \varphi(q) \; .$$

That agrees with the requirement:

$$\int dq\, \psi^*(q) \frac{\partial}{\partial q} \varphi(q) = - \int dq \left(\frac{\partial}{\partial q} \psi(q) \right)^* \varphi(q) = - \int dq \left(\frac{\partial}{\partial q} \psi^*(q) \right) \varphi(q) \; .$$

Integration by parts:

$$\int_{-\infty}^{+\infty} dq\, \psi^*(q) \frac{\partial}{\partial q} \varphi(q) = \psi^*(q) \varphi(q) |_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} dq \left(\frac{\partial}{\partial q} \psi^*(q) \right) \varphi(q) \; .$$

The Hermiticity thus requires:

$$\psi^*(q)\, \varphi(q) |_{-\infty}^{+\infty} = 0 \; .$$

That is guaranteed by the square-integrability of the wave functions! In the case of non-square integrable wave functions, periodic boundary conditions, as explained in Sect. 2.2.5, can take care for the Hermiticity of the momentum operator.

Solution 3.5.9

$$\begin{array}{ll} \textit{position:} & \hat{q}|q\rangle = q|q\rangle \; q \in \mathbb{R} \; , \\ \textit{momentum:} & \hat{p}|p\rangle = p|p\rangle \; p \in \mathbb{R} \; . \end{array}$$

We define an *infinitesimal momentum-translation operator* D_{dp} by:

$$D_{dp}|p\rangle = |p + dp\rangle \; .$$

Conservation of the norm

$$\langle p|p\rangle = \langle p + dp|p + dp\rangle$$

requires that D_{dp} mediates, as in (3.94), an infinitesimal unitary transformation. The following ansatz is therefore reasonable:

$$D_{dp} = \mathbb{1} + i\, dp\, S \quad \text{with } S = S^+ \; .$$

What is S?

$$
\begin{aligned}
D_{dp}\,\hat{p}|p\rangle &= p|p+dp\rangle\ , \\
\hat{p}\,D_{dp}|p\rangle &= (p+dp)|p+dp\rangle \\
\Longrightarrow\ [\hat{p}, D_{dp}]_-|p\rangle &= dp|p+dp\rangle = dp\,(\mathbb{1} + i\,dp\,S)|p\rangle = dp|p\rangle + \mathcal{O}(dp)^2\ .
\end{aligned}
$$

This is valid for all $|p\rangle$, which, on the other hand, build a complete system.

$$
\Longrightarrow\ [\hat{p}, D_{dp}]_- = dp\mathbb{1} = i\,dp[\hat{p}, S]_-\ .
$$

Therefore it must be

$$
[\hat{p}, S]_- = -i\mathbb{1}\ .
$$

Together with $[\hat{p}, \hat{q}]_- = -i\,\hbar$ we then have:

$$
[\hat{p}, \hbar\,S - \hat{q}]_- = 0\ . \tag{A.6}
$$

A shifting of the momentum-scale does of course not influence the position-measurement. Therefore we can assume:

$$
[\hat{q}, D_{dp}]_- = 0\ \Longrightarrow\ [\hat{q}, S]_- = 0\ \Longrightarrow\ [\hat{q}, \hbar S - \hat{q}]_- = 0\ . \tag{A.7}
$$

(A.6) and (A.7) can be combined to:

$$
[\hat{p}^n\,\hat{q}^m,\ \hbar\,S - \hat{q}]_- = 0\ .
$$

Let $B(\hat{q}, \hat{p})$ be an arbitrary operator function, which can always be brought, by applying the commutator relation $[\hat{q}, \hat{p}]_- = i\,\hbar$, into the form

$$
B(\hat{q}, \hat{p}) = \sum_{n,m} \beta_{nm}\,\hat{p}^n\,\hat{q}^m\ .
$$

This means, however:

$$
[B(\hat{q}, \hat{p}),\ \hbar\,S - \hat{q}]_- = 0\ .
$$

Since B is arbitrary, it must be concluded that $\hbar\,S - \hat{q} = d\mathbb{1}\quad (d \in \mathbb{R})$. d can be chosen to be zero:

$$
\begin{aligned}
\hbar\,S &= \hat{q} \\
\Longrightarrow\ D_{dp} &= \mathbb{1} + \frac{i}{\hbar}\,dp\,\hat{q}\ .
\end{aligned}
$$

($d \neq 0$ would lead to $D_{dp} = \mathbb{1}\,(1 + i(d/\hbar)\,dp) + (i/\hbar)\,dp\,\hat{q}$, where the second summand in the bracket can be, because of dp, neglected with respect to the first summand.) We multiply

$$\frac{\partial}{\partial p}\langle p| = \frac{1}{dp}\left(\langle p + dp| - \langle p|\right) = -\frac{i}{\hbar}\langle p|\hat{q}$$

from the right scalarly by the ket-state $|\psi\rangle$:

$$\begin{aligned} \frac{\partial}{\partial p}\,\overline{\psi}(p) &= -\frac{i}{\hbar}\langle p|\hat{q}|\psi\rangle \\ \Longrightarrow\quad \langle p|\hat{q}|\psi\rangle &= -\frac{\hbar}{i}\,\frac{\partial}{\partial p}\,\overline{\psi}(p)\,. \end{aligned}$$

We conclude recursively onto $\hat{q}^m$:

$$\begin{aligned} \langle p|\hat{q}^m|\psi\rangle &= \langle p|\hat{q}\Bigg(\underbrace{\int dp'|p'\rangle\langle p'|}_{\mathbb{1}}\Bigg)\hat{q}^{m-1}|\psi\rangle \\ &= -\frac{\hbar}{i}\,\frac{\partial}{\partial p}\int dp'\langle p|p'\rangle\left\langle p'\left|\hat{q}^{m-1}\right|\psi\right\rangle \\ &= -\frac{\hbar}{i}\,\frac{\partial}{\partial p}\left\langle p\left|\hat{q}^{m-1}\right|\psi\right\rangle \\ &\;\;\vdots \\ &= \left(-\frac{\hbar}{i}\,\frac{\partial}{\partial p}\right)^m\overline{\psi}(p)\,. \end{aligned}$$

From that it follows immediately:

$$\begin{aligned} \langle p|\hat{p}^n\,\hat{q}^m|\psi\rangle &= p^n\left(-\frac{\hbar}{i}\,\frac{\partial}{\partial p}\right)^m\overline{\psi}(p)\,, \\ \langle p|B(\hat{q},\hat{p})|\psi\rangle &= B\left(-\frac{\hbar}{i}\,\frac{\partial}{\partial p},p\right)\overline{\psi}(p)\,. \end{aligned}$$

Solution 3.5.10

1.

$$\begin{aligned} [H,\hat{q}]_- &= \frac{1}{2m}\,[\hat{p}^2,\hat{q}]_- + \underbrace{[V(\hat{q}),\hat{q}]_-}_{=0} = \frac{1}{2m}\,(\hat{p}\,[\hat{p},\hat{q}]_- + [\hat{p},\hat{q}]_-\,\hat{p}) = \frac{\hbar}{i\,m}\,\hat{p} \\ \Longrightarrow\quad \big[[H,\hat{q}]_-,\hat{q}\big]_- &= \frac{\hbar}{i\,m}\,[\hat{p},\hat{q}]_- = -\frac{\hbar^2}{m}\,. \end{aligned}$$

2. With the result of part 1.:

$$\frac{\hbar^2}{2m} = -\frac{1}{2}\left[[H,\hat{q}]_-,\hat{q}\right]_- = -\frac{1}{2}\left(H\,\hat{q}^2 - 2\hat{q}\,H\,\hat{q} + \hat{q}^2\,H\right)$$

$$\frac{\hbar^2}{2m} = \langle E_n' \left| \frac{\hbar^2}{2m} \right| E_{n'}\rangle = -\frac{1}{2}\langle E_{n'}|(H\,\hat{q}^2 + \hat{q}^2\,H)|E_{n'}\rangle + \langle E_{n'}|\hat{q}\,H\,\hat{q}|E_{n'}\rangle$$

$$= -E_{n'}\langle E_{n'}|\hat{q}^2|E_{n'}\rangle + \langle E_{n'}|\hat{q}\,H\mathbb{1}\hat{q}|E_{n'}\rangle\ ,$$

$$\mathbb{1} = \sum_n |E_n\rangle\langle E_n|$$

$$\Longrightarrow \quad \frac{\hbar^2}{2m} =$$

$$= -E_{n'}\sum_n \langle E_{n'}|\hat{q}|E_n\rangle\langle E_n|\hat{q}|E_{n'}\rangle + \sum_n \langle E_{n'}|\hat{q}\,H|E_n\rangle\langle E_n|\hat{q}|E_{n'}\rangle$$

$$= \sum_n (E_n - E_{n'})|\langle E_{n'}|\hat{q}|E_n\rangle|^2 \qquad \text{q.e.d.}$$

Section 4.1.5

Solution 4.1.1 Solutions of the discrete spectrum must fulfill asymptotically the boundary conditions

$$\varphi_{1,2}\,(q \to \pm\infty) = 0\ .$$

This means for the Wronski determinant:

$$W(\varphi_1,\varphi_2;q)|_{-\infty}^{+\infty} = \left(\varphi_1(q)\,\varphi_2'(q) - \varphi_2(q)\,\varphi_1'(q)\right)\Big|_{-\infty}^{+\infty} = 0\ .$$

It is then according to (4.12):

$$\frac{2m}{\hbar^2}\,(E_1 - E_2)\int_{-\infty}^{+\infty} dq\,\varphi_1(q)\,\varphi_2(q) = 0\ .$$

Because of $E_1 \neq E_2$, it follows with

$$\int_{-\infty}^{+\infty} dq\,\varphi_1(q)\,\varphi_2(q) = 0$$

the assertion (φ_1, φ_2 real!).

Solution 4.1.2

1. Let $W(\varphi_1, \varphi_2; q) \equiv 0$ in $[q_0, q_1]_-$. Consider then the following homogeneous system of equations for $\alpha_1, \alpha_2 \in \mathbb{C}$:

$$\begin{aligned} \alpha_1\, \varphi_1(q) + \alpha_2\, \varphi_2(q) &= 0\,, \\ \alpha_1\, \varphi_1'(q) + \alpha_2\, \varphi_2'(q) &= 0\,. \end{aligned}$$

   Its coefficient-determinant is identical to the Wronski determinant:

$$W = \det A\,.$$

   But $\det A = 0$ means, ((1.352), Vol. 1), that the homogeneous system of equations has a non-trivial solution:

$$(\alpha_1, \alpha_2) \neq (0, 0)$$

   The first row then indicates the linear dependence of $\varphi_1(q)$ and $\varphi_2(q)$!
2. Let $\varphi_1(q)$, $\varphi_2(q)$ be linearly dependent in the interval $[q_0, q_1]_-$. That means for all q from this interval:

$$\begin{aligned} &\varphi_2(q) = c\, \varphi_1(q) \\ \Longrightarrow\ &W = \varphi_1(q)\, \varphi_2'(q) - \varphi_2(q)\, \varphi_1'(q) \equiv 0 \quad \text{q.e.d.} \end{aligned}$$

Solution 4.1.3 We know from Sect. 4.1.3 that eigen-functions of non-degenerate energy-eigen values have a well-defined parity, if $\Pi\, H\, \Pi^+ = H$, i.e., $V(q) = V(-q)$. The discrete eigen-value spectrum of H is non-degenerate. **Each** eigen-function $\varphi_n(q)$ has therefore a definite parity, being either even or odd with respect to a space inversion:

$$\Pi\, \varphi_n(q) = \varphi_n(-q) = \pm \varphi_n(q)\,.$$

$\varphi_0(q)$ has no zero and must therefore necessarily have odd parity. In general it is:

$$\Pi\, \varphi_n(q) = \varphi_n(-q) = (-1)^n\, \varphi_n(q)\,.$$

Solution 4.1.4 Eigen-value equation and differential equation for the parity operator:

$$\Pi\, p_\pm(q) = \pm\, p_\pm(q) \stackrel{!}{=} p_\pm(-q)\,.$$

Therewith:

$$\begin{aligned}\int_{-\infty}^{+\infty} dq\, p_+(q)\, p_-(q) &\overset{q\to -q}{=} \int_{-\infty}^{+\infty} dq\, p_+(-q)\, p_-(-q)\\ &= \int_{-\infty}^{+\infty} dq\, p_+(q)\, (-p_-(q))\\ &= -\int_{-\infty}^{+\infty} dq\, p_+(q)\, p_-(q)\\ &= 0\,.\end{aligned}$$

That was to be shown.

Section 4.2.3

Solution 4.2.1

1. We divide the q-axis in the same manner as in Sect. 4.2.1 for the finitely deep potential well:

$$\begin{aligned}\text{Region A:}\quad & -\infty < q \le -q_0\,,\\ & k^2(q) \equiv -\kappa^2 \to -\infty\,,\\ \text{region B:}\quad & -q_0 < q < +q_0\,,\\ & k^2(q) = \tfrac{2m}{\hbar^2}\, E \equiv k^2\,,\\ \text{Region C:}\quad & +q_0 \le q < +\infty\,,\\ & k^2(q) \equiv -\kappa^2 \to -\infty\,.\end{aligned}$$

$E < 0$ yields only the trivial solution $\varphi \equiv 0$. In the following it is therefore always $E > 0$.

Schrödinger equation:

$$\varphi''(q) + k^2(q)\, \varphi(q) = 0\,.$$

Because of $\kappa = +\infty$, the wave function must vanish in the regions A and C (see (4.32) and (4.35)).
$\Longrightarrow$ ansatz for the solution:

$$\begin{aligned}&\varphi(q) \equiv 0 \quad \text{for} \quad |q| \ge q_0\,,\\ &\varphi(q) = \beta_+\, e^{ikq} + \beta_-\, e^{-ikq} \quad \text{for } |q| < q_0.\end{aligned}$$

Boundary conditions:

a) $\varphi(\pm q_0) = 0$,
b) Eigen-functions have definite parities because

$$[\Pi, H]_- = 0 \,.$$

2. Schrödinger equation:

$$H\,\varphi(q) = E\,\varphi(q) \underset{\text{region B}}{=} -\frac{\hbar^2}{2m}\,\frac{d^2}{dq^2}\,\varphi(q)$$
$$\Longrightarrow\; E = \frac{\hbar^2 k^2}{2m} \,.$$

a) Even parity:

$$\begin{aligned}
\beta_+ &= \beta_- = \beta \\
\Longrightarrow\; \varphi^{(+)}(q) &= 2\beta \cos kq \,, \\
\varphi^{(+)}(q_0) = \varphi^{(+)}(-q_0) = 0 \;&\Longleftrightarrow\; kq_0 = (2n+1)\frac{\pi}{2} \\
\Longleftrightarrow\; k_n^{(+)} &= \frac{\pi}{2q_0}\,(2n+1) \quad n \in \mathbb{Z} \,, \\
E_n^{(+)} &= \frac{\hbar^2 \pi^2}{8m\,q_0^2}\,(2n+1)^2 \,.
\end{aligned}$$

Normalization:

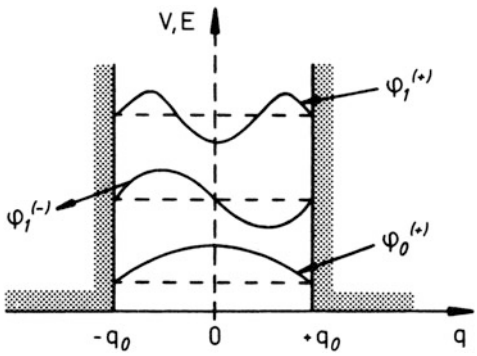
$$1 = 4\,\beta^2 \int\limits_{-q_0}^{+q_0} dq \cos^2 kq = 4\beta^2 \left(\frac{1}{2}q + \frac{1}{4k}\sin 2qk\right)\Big|_{-q_0}^{+q_0} = 4\beta^2 q_0 \,,$$

$$\varphi_n^{(+)} = \frac{1}{\sqrt{q_0}} \cos\left(\frac{\pi}{2q_0}\,(2n+1)\,q\right) \,.$$

b) Odd parity:

$$\begin{aligned}
\beta_+ &= -\beta_- = b \\
\Longrightarrow\; \varphi^{(-)}(q) &= 2ib \sin kq \,, \\
\varphi^{(-)}(\pm q_0) = 0 \;&\Longleftrightarrow\; kq_0 = n\,\pi \,, \\
k_n^{(-)} = \frac{\pi}{q_0}\,n \qquad & n = \pm 1, \pm 2, \pm 3, \ldots
\end{aligned}$$

Fig. A.9



$n = 0$ drops out because it would then be $\varphi^{(-)} \equiv 0$.

$$E_n^{(-)} = \frac{\hbar^2 \pi^2}{2m\, q_0^2}\, n^2 \ .$$

Normalized eigen-functions:

$$\varphi_n^{(-)} = \frac{1}{\sqrt{q_0}} \sin\left(\frac{\pi}{q_0}\, n\, q\right) \ .$$

The ground state has therefore even parity (Fig. A.9)!

3. Probabilities:

$$w_n^{(\pm)} = \int\limits_{-q_0/2}^{+q_0/2} dq\, (\varphi_n^{(\pm)}(q))^2 \ ,$$

$$w_n^{(+)} = \frac{1}{q_0} \int\limits_{-q_0/2}^{+q_0/2} dq \cos^2\left[\frac{\pi}{2q_0}\,(2n+1)q\right] =$$

$$= \frac{1}{q_0}\left\{\frac{1}{2}q + \frac{1}{4\frac{\pi}{2q_0}\,(2n+1)} \sin\left[\frac{\pi}{q_0}\,(2n+1)q\right]\right\}\Bigg|_{-\frac{q_0}{2}}^{+\frac{q_0}{2}} =$$

$$= \frac{1}{2} + \frac{1}{2\pi(2n+1)}\left\{\sin\left[\frac{\pi}{2}\,(2n+1)\right] - \sin\left[-\frac{\pi}{2}\,(2n+1)\right]\right\}$$

$$\Longrightarrow \quad w_n^{(+)} = \frac{1}{2} + \frac{(-1)^n}{\pi(2n+1)} \ ,$$

$$w_n^{(-)} = \frac{1}{q_0} \int\limits_{-q_0/2}^{+q_0/2} dq \sin^2\left(\frac{\pi}{q_0} n\, q\right) = \frac{1}{q_0}\left[\frac{1}{2} q - \frac{1}{4\,\frac{\pi}{q_0} n} \sin\left(\frac{2\pi}{q_0} n\, q\right)\right]\Bigg|_{-\frac{q_0}{2}}^{+\frac{q_0}{2}}$$

$$\Longrightarrow \quad w_n^{(-)} = \frac{1}{2} \,.$$

Solution 4.2.2 Let the motion of the particle be restricted to the interval $-q_0 \leq q \leq q_0$. For this region, exactly the same considerations are valid as in the preceding exercise. We can therefore adopt:

$$\varphi^{(+)}(q) = 2\beta \cos kq \,,$$
$$\varphi^{(-)}(q) = 2i\, b \sin kq \,.$$

Periodic boundary conditions:

$$k\, 2q_0 = 2\pi\, n \qquad n \in \mathbb{Z}$$
$$\Longrightarrow \quad k_n = \frac{\pi}{q_0} n \,.$$

Eigen-energies:

$$E_n = \frac{\hbar^2 \pi^2}{2m\, q_0^2} n^2 \,.$$

These energies are now, in contrast to those in the case of homogeneous boundary conditions, doubly degenerate, since to each E_n belongs a symmetric as well as an antisymmetric function as solution.

Solution 4.2.3

1. Region A: classically forbidden

$$k_{\mathrm{A}}^2(q) = \frac{2m}{\hbar^2}(E - V_1) = -\kappa_1^2 < 0 \,,$$
$$\varphi''(q) - \kappa_1^2\, \varphi(q) = 0 \,.$$

Ansatz: $\varphi_{\mathrm{A}}(q) = a \exp(\kappa_1\, q)$.

Region B: classically allowed

$$k_{\mathrm{B}}^2(q) = \frac{2m}{\hbar^2} E = k^2 > 0 \,,$$
$$\varphi''(q) + k^2\, \varphi(q) = 0 \,.$$

Ansatz: $\varphi_{\mathrm{B}}(q) = b_+ \exp(i\, k\, q) + b_- \exp(-i\, k\, q)$.

Region C: classically forbidden

$$k_C^2(q) = \frac{2m}{\hbar^2}(E - V_3) = -\kappa_3^2 < 0 \,,$$
$$\varphi''(q) - \kappa_3^2 \varphi(q) = 0 \,.$$

Ansatz: $\varphi_C(q) = c \exp(-\kappa_3 q)$.

Fitting conditions:

a) Continuity of φ :

$$a \exp(-\kappa_1 q_0) = b_+ \exp(-i k q_0) + b_- \exp(i k q_0) \,,$$
$$b_+ \exp(i k q_0) + b_- \exp(-i k q_0) = c \exp(-\kappa_3 q_0) \,.$$

b) Continuity of φ':

$$a \kappa_1 \exp(-\kappa_1 q_0) = i k [b_+ \exp(-i k q_0) - b_- \exp(i k q_0)]$$
$$i k [b_+ \exp(i k q_0) - b_- \exp(-i k q_0)] = -\kappa_3 c \exp(-\kappa_3 q_0) \,.$$

2. The fitting conditions lead to a homogeneous system of equations, whose secular determinant must vanish:

$$0 \stackrel{!}{=} \begin{vmatrix} e^{-\kappa_1 q_0} & -e^{-ikq_0} & -e^{ikq_0} & 0 \\ 0 & e^{ikq_0} & e^{-ikq_0} & -e^{-\kappa_3 q_0} \\ \kappa_1 e^{-\kappa_1 q_0} & -ik e^{-ikq_0} & ik e^{ikq_0} & 0 \\ 0 & ik e^{ikq_0} & -ik e^{-ikq_0} & \kappa_3 e^{-\kappa_3 q_0} \end{vmatrix} =$$

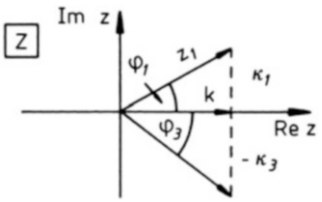
$$= e^{-\kappa_1 q_0} \begin{vmatrix} e^{ikq_0} & e^{-ikq_0} & -e^{-\kappa_3 q_0} \\ -ik e^{-ikq_0} & ik e^{ikq_0} & 0 \\ ik e^{ikq_0} & -ik e^{-ikq_0} & \kappa_3 e^{-\kappa_3 q_0} \end{vmatrix} +$$

$$+ e^{-ikq_0} \begin{vmatrix} 0 & e^{-ikq_0} & -e^{-\kappa_3 q_0} \\ \kappa_1 e^{-\kappa_1 q_0} & ik e^{ikq_0} & 0 \\ 0 & -ik e^{-ikq_0} & \kappa_3 e^{-\kappa_3 q_0} \end{vmatrix} -$$

$$- e^{ikq_0} \begin{vmatrix} 0 & e^{ikq_0} & -e^{-\kappa_3 q_0} \\ \kappa_1 e^{-\kappa_1 q_0} & -ik e^{-ikq_0} & 0 \\ 0 & ik e^{ikq_0} & \kappa_3 e^{-\kappa_3 q_0} \end{vmatrix} =$$

$$= e^{-\kappa_1 q_0} \left\{ (ik\kappa_3 - k^2) e^{-(\kappa_3 - 2ik)q_0} + (ik\kappa_3 + k^2) e^{-(\kappa_3 + 2ik)q_0} \right\} +$$
$$+ e^{-(\kappa_1 + \kappa_3 + 2ik)q_0} (ik\kappa_1 - \kappa_1\kappa_3) + e^{-(\kappa_1 + \kappa_3 - 2ik)q_0} (ik\kappa_1 + \kappa_1\kappa_3) \,.$$

Fig. A.10



This equation simplifies to:

$$0 \stackrel{!}{=} -e^{2ikq_0}\,(k - i\,\kappa_1)\,(k - i\,\kappa_3) + e^{-2ikq_0}\,(k + i\,\kappa_1)\,(k + i\,\kappa_3)$$

$$\Longrightarrow\quad 1 = e^{-4ikq_0}\,\frac{(k + i\,\kappa_1)\,(k + i\,\kappa_3)}{(k - i\,\kappa_1)\,(k - i\,\kappa_3)}\;.$$

Suitably extended, this relation yields, because of $(k^2 + \kappa_3^2)/(k^2 + \kappa_1^2) = V_3/V_1$, the assertion:

$$1 = e^{-4ikq_0}\,\frac{V_3}{V_1}\,\left(\frac{k + i\,\kappa_1}{k - i\,\kappa_3}\right)^2\;.$$

3. For the complex wave-vector combinations, we apply the polar representations (Fig. A.10) ((2.140), Vol. 1):

$$z_1 = k + i\,\kappa_1 = \sqrt{k^2 + \kappa_1^2}\;e^{i\varphi_1}\;,$$

$$z_3 = k - i\,\kappa_3 = \sqrt{k^2 + \kappa_3^2}\;e^{-i\varphi_3}\;.$$

$$\cos\varphi_1 = \frac{k}{\sqrt{k^2 + \kappa_1^2}} = \sqrt{\frac{E}{V_1}} = \sin\left(\frac{\pi}{2} - \varphi_1\right)\;,$$

$$\cos\varphi_3 = \frac{k}{\sqrt{k^2 + \kappa_3^2}} = \sqrt{\frac{E}{V_3}} = \sin\left(\frac{\pi}{2} - \varphi_3\right)\;.$$

The conditional equation in 2. now reads:

$$1 = \frac{V_3}{V_1}\,\frac{k^2 + \kappa_1^2}{k^2 + \kappa_3^2}\,e^{-2i(2q_0k - \varphi_1 - \varphi_3)} = e^{-2i(2q_0k - \varphi_1 - \varphi_3)}$$

$$\Longleftrightarrow\quad 2q_0k = n\,\pi + \varphi_1 + \varphi_3\;; \qquad n = 0, \pm1, \pm2, \ldots\;.$$

But this we can write also as follows:

$$2q_0k = (n+1)\pi - \arcsin\sqrt{\frac{E}{V_1}} - \arcsin\sqrt{\frac{E}{V_3}}\,.$$

Because of $q_0k > 0$ only non-negative n come into question as possible solution. Then it follows with $n' = n + 1$ the assertion:

$$f(E) = \arcsin\sqrt{\frac{E}{V_1}} + \arcsin\sqrt{\frac{E}{V_3}} = n'\pi - 2q_0k \qquad n' = 1, 2, 3, \ldots$$

4. We write for abbreviation:

$$x = \sqrt{\frac{E}{V_1}}\,; \quad R = q_0\sqrt{\frac{2m}{\hbar^2}V_1}\,; \quad \gamma = \arccos\sqrt{\frac{V_1}{V_3}}\,.$$

It then remains to discuss:

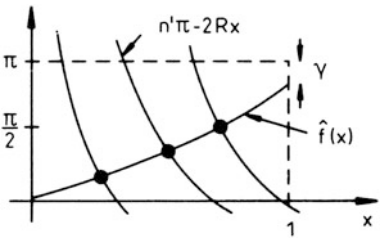
$$\widehat{f}(x) = \arcsin x + \arcsin(x\cos\gamma) = n'\pi - 2Rx\,.$$

We discuss both sides as functions of x:

$$\begin{aligned} 0 \le E < V_1 \implies 0 &\le \arcsin x \le \frac{\pi}{2}\,, \\ 0 &\le \arcsin(x\cos\gamma) \le \arcsin(\cos\gamma) = \frac{\pi}{2} - \gamma\,, \\ 0 &\le \widehat{f}(x) < \pi - \gamma\,. \end{aligned}$$

$\widehat{f}(x) = \arcsin x + \arcsin(x\cos\gamma)$ is a monotonously increasing function, from 0 to $\pi - \gamma$, when x increases from 0 to 1. In the same interval, $n'\pi - 2Rx$ is monotonously decreasing from $n'\pi$ to $n'\pi - 2R$ (Fig. A.11). The intersection points yield the solutions.

Fig. A.11



a) Intersections exist only if

$$n'\pi - 2R \leq \pi - \gamma \iff (n'-1)\,\pi + \gamma \leq 2R\,.$$

b) No solutions are possible if

$$2R < \gamma \iff 2q_0\sqrt{\frac{2m}{\hbar^2}V_1} < \arccos\sqrt{\frac{V_1}{V_3}}\,.$$

c) Exactly one solution appears if

$$\gamma \leq 2R \leq \gamma + \pi \qquad (n' = 1)\,.$$

d) Exactly two solutions are possible if

$$\gamma + \pi \leq 2R \leq \gamma + 2\pi \qquad (n' = 1, 2)$$

and so forth.

$\Longrightarrow$ discrete spectrum. Because of a), there is only a finite number of discrete energy-eigen values.

5.

$$V_1 = V_3 \implies \gamma = \arccos 1 = 0\,,$$
$$2V_1 = V_3 \Longrightarrow \gamma = \arccos\sqrt{\frac{1}{2}} = \frac{\pi}{4}\,.$$

We see in Fig. A.11 that the $\widehat{f}(x)$-curve shifts downwards, therewith becoming flatter. The intersection points lie at larger x-values: The energy-eigen values move higher with increasing V_3 (V_1 fixed)!

Solution 4.2.4

1. Abbreviations:

$$k^2 = \frac{2m}{\hbar^2}(E + V_0)\,; \qquad \kappa^2 = \frac{2m}{\hbar^2}|E|\,.$$

Bound states are to be expected only for

$$-V_0 \leq E < 0\,.$$

The following considerations therefore aim only at this case:
We start with the ansatz $(\varphi''(q) + k^2(q)\,\varphi(q) = 0)$:

$$\begin{aligned} \varphi_{\mathrm{A}}(q) &\equiv 0 && -\infty < q \le 0\,, \\ \varphi_{\mathrm{B}}(q) &= \alpha \sin(kq + \overline{\varphi}) && 0 < q < q_0\,, \\ \varphi_{\mathrm{C}}(q) &= \gamma\, e^{-\kappa q} && q_0 \le q < +\infty\,. \end{aligned}$$

Continuity of φ and φ':
At $q = 0$:

$$0 = \alpha \sin\overline{\varphi} \quad (\varphi' \text{ need not necessarily be continuous!})\,.$$

At $q = q_0$:

$$\begin{aligned} \alpha \sin(kq_0 + \overline{\varphi}) &= \gamma\, e^{-\kappa q_0}\,, \\ \alpha\, k \cos(kq_0 + \overline{\varphi}) &= -\gamma\,\kappa\, e^{-\kappa q_0}\,. \end{aligned}$$

It follows immediately:

$$\overline{\varphi} = 0\,; \qquad \frac{1}{k}\tan kq_0 = -\frac{1}{\kappa} \iff \cot kq_0 = -\frac{\kappa}{k} < 0\,.$$

2.

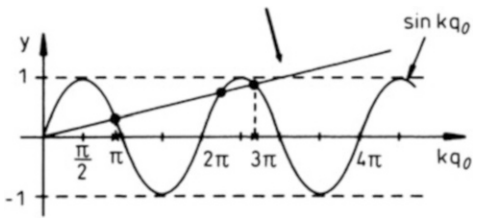
$$\begin{aligned} \cot^2 kq_0 &= \frac{1}{\sin^2 kq_0} - 1 \\ \Longrightarrow \quad \frac{\kappa^2}{k^2} + 1 &= \frac{1}{\sin^2 kq_0} \iff \frac{V_0}{V_0 + E} = \frac{1}{\sin^2 kq_0}\,. \end{aligned}$$

That can also be written as follows:

$$\sin kq_0 = \sqrt{\frac{\hbar^2}{2m\,q_0^2\,V_0}}\,(kq_0)\,; \quad q_0 = \text{const}\,.$$

Graphical solution (Fig. A.12): Only the intersection points, marked in Fig. A.12, come into question as solutions . However, it is still to respect that, according to

Fig. A.12



part 1., $\cot kq_0 < 0$ must be fulfilled. That means:

$$\frac{\pi}{2} + n\,\pi < k\,q_0 < \pi + n\,\pi\ ; \quad n = 0, \pm 1, \pm 2, \ldots$$

In order to have at least one bound state, the slope of the straight line

$$y = \sqrt{\frac{\hbar^2}{2m\,q_0^2\,V_0}}\,(kq_0)$$

must not be so large that the first, and then also the only, intersection point lies at

$$kq_0 \leq \frac{\pi}{2}\ .$$

For the slope it must therefore be:

$$\sqrt{\frac{\hbar^2}{2m\,q_0^2\,V_0}} < \frac{1}{\frac{\pi}{2}} = \frac{2}{\pi}\ .$$

That is the required, necessary condition for the existence of a bound state!

3. No, because then the last inequality reads:

$$\sqrt{\frac{1}{2}} < \frac{2}{\pi} \iff \frac{1}{2} < \frac{4}{\pi^2} \iff \pi^2 < 8 \implies \#\ .$$

Solution 4.2.5 Schrödinger equation (position representation):

$$-\frac{\hbar^2}{2m}\,\varphi''(q) - V_0\,\delta(q)\,\varphi(q) = E\,\varphi(q)\ .$$

$\varphi''(q)$ surely exists for $q \neq 0$ and is there continuous, along with $\varphi'(q)$ and $\varphi(q)$. We therefore can integrate the Schrödinger equation over a small interval around the zero point:

$\eta \to 0^+$:

$$-\frac{\hbar^2}{2m}\int\limits_{-\eta}^{+\eta}\varphi''(q)\,dq - V_0\int\limits_{-\eta}^{+\eta}\delta(q)\,\varphi(q) = E\int\limits_{-\eta}^{+\eta}\varphi(q)\,dq\ .$$

According to our general presumption, $|\varphi(q)|^2$ must be interpretable everywhere, maybe except for the critical point $q = 0$, as probability density. We can therefore assume that $\varphi(q)$, if discontinuous at all at $q = 0$, then exhibits there at most a finite

discontinuity-jump. But then it is

$$\lim_{\eta\to 0^+} \int_{-\eta}^{+\eta} \varphi(q)\, dq = 0 \,.$$

and therefore:

$$-\frac{\hbar^2}{2m}\left[\varphi'(\eta) - \varphi'(-\eta)\right] - V_0\,\varphi(0) = 0 \,.$$

The derivative of the wave function is thus discontinuous at the zero point, if $\varphi(0) \neq 0$. But since V_0 is finite we can conclude:

$\varphi(q)$ continuous, since $\varphi(0)$ finite (according to the presupposition).

Ansatz for the solution:
$q \neq 0 \implies$ *classically forbidden region:*

$$q < 0: \ \varphi_-(q) = \alpha_-\, e^{\kappa - q} \,,$$
$$q > 0: \ \varphi_+(q) = \alpha_+\, e^{-\kappa + q} \,;$$

Insertion into the Schrödinger equation yields ($q \neq 0$):

$$\kappa_+ = \kappa_- = \sqrt{-\frac{2m}{\hbar^2}\,E} \equiv \kappa \,.$$

Wave function:

$$\varphi(q) = \alpha \exp\left(-\kappa |q|\right)$$
$$(\alpha_- = \alpha_+ = \alpha \text{ because of continuity at } q = 0) \,.$$

Normalization:

$$1 \stackrel{!}{=} \int_{-\infty}^{+\infty} dq |\varphi(q)|^2 = |\alpha|^2 \left(\int_{-\infty}^{0} dq\, e^{2\kappa q} + \int_{0}^{\infty} dq\, e^{-2\kappa q} \right) =$$
$$= |\alpha|^2\, \frac{1}{\kappa}$$

$\implies$ except for a phase of magnitude 1: $\varphi(q) = \sqrt{\kappa}\exp\left(-\kappa|q|\right)$ (symmetric!) .

Are there bound states?

We exploit the discontinuity-jump of the first derivative:

$$\begin{aligned} & q < 0: \quad \varphi'(q) = \kappa^{3/2} \exp(\kappa\, q)\ , \\ & q > 0: \quad \varphi'(q) = -\kappa^{3/2} \exp(-\kappa\, q) \\ \Longrightarrow\ & 0 = -\frac{\hbar^2}{2m}\left[\varphi'(\eta) - \varphi'(-\eta)\right] - V_0\,\varphi(0) = -\frac{\hbar^2}{2m}\left(-2\kappa^{3/2}\right) - V_0\,\kappa^{1/2} \\ \Longrightarrow\ & \kappa = \frac{m\,V_0}{\hbar^2} = \sqrt{-\frac{2m}{\hbar^2}E}\ . \end{aligned}$$

Therefore, there exists exactly one bound state:

$$E = -\frac{m\,{V_0}^2}{2\hbar^2}\ .$$

Regard the analogy to the finitely broad and finitely deep potential well (see Sect. 4.2.1).

Solution 4.2.6

1.

$$V(q) = V(-q) \quad \curvearrowright \quad \left[\Pi,\, H\right]_- = 0\ .$$

Eigen-functions therefore have a definite parity:

$$\varphi(q) = \pm\varphi(-q)\ .$$

2. Integration of the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\int_{-\eta}^{+\eta}\varphi''(q)\,dq + \frac{\hbar^2}{2m}V_0\int_{-\eta}^{+\eta}\delta(q)\varphi(q)\,dq = E\int_{-\eta}^{+\eta}\varphi(q)\,dq \overset{\eta\to 0^+}{\longrightarrow} 0\ .$$

The last step is valid because $\varphi(q)$ can be assumed to be continuous. It remains therewith:

$$\varphi'(+0^+) - \varphi'(-0^+) = V_0\varphi(0)\ .$$

The wave function is thus continuous at $q = 0$ with a discontinuous first derivative if $\varphi(0) \neq 0$!

3. Ansatz for the solution:

$$\varphi(q) = \begin{cases} 0\,, & \text{if } |q| \geq q_0 \\ \beta_1 e^{ikq} + \beta_2 e^{-ikq}\,, & \text{if } -q_0 < q < 0 \\ \gamma_1 e^{ikq} + \gamma_2 e^{-ikq}\,, & \text{if } 0 < q < +q_0\ . \end{cases}$$

Here it is:

$$k^2 = \frac{2m}{\hbar^2} E \,.$$

Continuity of the wave function:

$$\varphi(-q_0) = \beta_1 e^{-ikq_0} + \beta_2 e^{ikq_0} = 0 \tag{A.8}$$

$$\varphi(0) = \beta_1 + \beta_2 = \gamma_1 + \gamma_2 \tag{A.9}$$

$$\varphi(q_0) = \gamma_1 e^{ikq_0} + \gamma_2 e^{-ikq_0} = 0 \,. \tag{A.10}$$

Derivative at $q = 0$:

$$ik(\gamma_1 - \gamma_2 - \beta_1 + \beta_2) = V_0(\beta_1 + \beta_2) \,. \tag{A.11}$$

(A.8) to (A.11) are the physical boundary conditions for $\varphi(q)$.

4. • Even parity $\Leftrightarrow \quad \beta_1 = \gamma_2 \; ; \; \beta_2 = \gamma_1$
From (A.8) and (A.11) follows a homogeneous system of equations:

$$0 = \beta_1 e^{-ikq_0} + \beta_2 e^{ikq_0}$$
$$0 = \beta_1(V_0 + 2ik) + \beta_2(V_0 - 2ik)$$

Non-trivial solution, if the secular determinant vanishes:

$$0 \stackrel{!}{=} e^{-ikq_0}(V_0 - 2ik) - e^{ikq_0}(V_0 + 2ik) = -2iV_0 \sin kq_0 - 4ik \cos kq_0 \,.$$

This means:

$$\cot kq_0 = -\frac{V_0}{2k} \,.$$

This is, because of $k^2 = 2m/\hbar^2 E$, the transcendental conditional equation for the energy-eigen values!

• Odd parity $\Leftrightarrow \quad \beta_1 = -\gamma_2 \; ; \; \beta_2 = -\gamma_1$
From (A.9):

$$2(\beta_1 + \beta_2) = 0 = 2\varphi(0) \,.$$

Hence, there is **no** jump of the derivative at $q = 0$. Combination of (A.8) and (A.9):

$$0 = \beta_1 e^{-ikq_0} + \beta_2 e^{ikq_0}$$
$$0 = \beta_1 + \beta_2 \,.$$

Secular determinant:

$$0 \stackrel{!}{=} e^{ikq_0} - e^{-ikq_0} \ .$$

From that it follows as conditional equation for the energy-eigen values:

$$\sin kq_0 = 0 \ .$$

This equation is identical to the corresponding conditional equation for the infinitely high potential well **without** δ-potential at $q = 0$ (see Exercise 4.2.1). This can be understood by the fact that for the odd functions the derivatives, too, are continuous at $q = 0$:

$$k_n^{(-)} = \frac{\pi}{q_0}\, n \quad \curvearrowright \quad E_n^{(-)} = \frac{\hbar^2\pi^2}{2mq_0^2}\, n^2 \ ; \quad n = \pm 1, \pm 2, \pm 3, \ldots$$

5. • Even parity $\Leftrightarrow \quad \beta_1 = \gamma_2 \ ; \ \beta_2 = \gamma_1$
Equation (A.8) is solved by:

$$\beta_1 = \beta\, e^{ikq_0} \ ; \quad \beta_2 = -\beta\, e^{-ikq_0} \ .$$

That yields:

$$\varphi^{(+)}(q) = 2\beta i \begin{cases} \sin(k(q+q_0)) & \text{for } -q_0 \le q \le 0 \\ -\sin(k(q-q_0)) & \text{for } 0 \le q \le q_0 \\ 0 & \text{for } |q| \ge q_0 \ . \end{cases}$$

β is found by the normalization condition.

• Odd parity $\Leftrightarrow \quad \beta_1 = -\gamma_2 \ ; \ \beta_2 = -\gamma_1$
It follows from $\varphi(0) = 0$ with (A.9): $\beta_1 = -\beta_2$ and therewith:

$$\beta_1 = \widehat{\beta} = -\gamma_2 \ ; \quad \beta_2 = -\widehat{\beta} = -\gamma_1 \ .$$

That leads to the same solution as for the infinitely high potential well **without** δ-potential at $q = 0$ (see Exercise 4.2.1):

$$\varphi^{(-)}(q) = 2\widehat{\beta} i \begin{cases} \sin kq & \text{for } -q_0 \le q \le +q_0 \\ 0 & \text{for } |q| \ge q_0 \ . \end{cases}$$

$\widehat{\beta}$ is found by the use of the normalization condition.

Solution 4.2.7

1. In the solution for Exercise 2.3.9 we found:

$$\frac{p^2}{2m}\overline{\psi}(p) + \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dp'\,\overline{V}(p-p')\overline{\psi}(p') = E\overline{\psi}(p)\,.$$

2. We have

$$\overline{V}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dq\,V(q)\,e^{-\frac{i}{\hbar}pq}$$

$$\to\ = \frac{V_0}{\sqrt{2\pi\hbar}}\,.$$

The Schrödinger equation therewith reads:

$$\frac{p^2}{2m}\overline{\psi}(p) + \frac{V_0}{2\pi\hbar}\int_{-\infty}^{+\infty} dp'\,\overline{\psi}(p') = E\overline{\psi}(p)\,.$$

The integral is independent of p:

$$\int_{-\infty}^{+\infty} dp'\,\overline{\psi}(p') = C$$

$$\curvearrowright\ \overline{\psi}(p) = \frac{V_0}{2\pi\hbar}\frac{C}{E-\frac{p^2}{2m}}\,.$$

Thereby:

$$C = -\frac{V_0}{2\pi\hbar}2mC\int_{-\infty}^{+\infty} dp'\,\frac{1}{p'^2-2mE} \qquad (E<0)$$

$$\curvearrowright\ 1 = -\frac{2V_0m}{\pi\hbar}\int_0^{\infty} dp'\frac{1}{p'^2+2m|E|}$$

$$= -\frac{2V_0m}{\pi\hbar}\frac{1}{2m|E|}\int_0^{\infty} dp'\frac{1}{\frac{p'^2}{2m|E|}+1}$$

$$
\begin{aligned}
&= -\frac{2V_0 m}{\pi\hbar}\frac{1}{\sqrt{2m|E|}}\int_0^\infty dx \frac{1}{x^2+1} \\
&= -\frac{2V_0 m}{\pi\hbar}\frac{1}{\sqrt{2m|E|}}\underbrace{\int_0^\infty dx \frac{d}{dx}\arctan x}_{\pi/2} \\
&= -\frac{V_0 m}{\hbar}\frac{1}{\sqrt{2m|E|}}
\end{aligned}
$$

$$
\curvearrowright \sqrt{2m\,|E|} = -V_0\frac{m}{\hbar} \qquad (V_0 < 0)
$$

$$
\curvearrowright |E| = \frac{m\,|V_0|^2}{2\hbar^2}
$$

Bound state:

$$
E = -\frac{m\,|V_0|^2}{2\hbar^2}\,.
$$

We obtain the constant C from the normalization condition for $\overline{\psi}(p)$. Let C be real:

$$
\begin{aligned}
1 &\stackrel{!}{=} \int_{-\infty}^{+\infty} dp\ \left|\overline{\psi}(p)\right|^2 \\
&= \frac{V_0^2}{4\pi^2\hbar^2}C^2\int_{-\infty}^{+\infty} dp\,\frac{1}{\left(E-\frac{p^2}{2m}\right)^2} \\
&= \frac{V_0^2}{4\pi^2\hbar^2}C^2\cdot 4m^2 \underbrace{\int_{-\infty}^{+\infty} dp\,\frac{1}{\left(p^2+2m\,|E|\right)^2}}_{-\frac{1}{2m}\frac{d}{d\,|E|}\underbrace{\int_{-\infty}^{+\infty} dp\frac{1}{p^2+2m\,|E|}}_{\frac{\pi}{2\sqrt{2m}}\cdot\frac{1}{\sqrt{E}}}}
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{V_0^2 C^2 m^2}{\pi^2 \hbar^2} \left(-\frac{\pi}{4m\sqrt{2m}} \right) \left(-\frac{1}{2} \frac{1}{|E|^{\frac{3}{2}}} \right) \\
&= \frac{V_0^2 C^2 m^{\frac{1}{2}}}{\pi \cdot 8\sqrt{2}} \cdot \frac{\left(2\hbar^2\right)^{\frac{3}{2}}}{m^{\frac{3}{2}} \left|V_0\right|^3} \\
&= C^2 \frac{\hbar^3}{\pi m \left|V_0\right| \cdot 4} \\
\curvearrowright \quad C &= \frac{2\sqrt{\pi m \left|V_0\right|}}{\hbar^{\frac{3}{2}}} \, .
\end{aligned}
$$

It follows eventually:

$$
\begin{aligned}
\overline{\psi}(p) &= V_0 \frac{\sqrt{\pi m \left|V_0\right|}}{\pi \hbar^{\frac{5}{2}}} \cdot \frac{1}{E - \frac{p^2}{2m}} \\
&= -V_0 \frac{2m\sqrt{m \left|V_0\right|}}{\sqrt{\pi} \cdot \hbar^{\frac{5}{2}}} \frac{1}{p^2 + \frac{m^2 |V_0|^2}{\hbar^2}} \, .
\end{aligned}
$$

Solution 4.2.8

$$
V(q) = V(-q) \implies [H, \Pi]_- = 0 \, .
$$

The eigen-functions have a definite parity.

Schrödinger equation:

$$
-\frac{\hbar^2}{2m} \varphi''(q) - V_0 \, \delta(q + q_0) \, \varphi(q) - V_0 \, \delta(q - q_0) \, \varphi(q) = E \, \varphi(q) \, .
$$

With the same restrictions as in Exercise 4.2.5, we integrate this equation over a small interval around $\pm q_0$:

At $q = -q_0 \ (\eta \to 0^+)$:

$$
\varphi'(-q_0 + \eta) - \varphi'(-q_0 - \eta) = -\frac{2m}{\hbar^2} V_0 \, \varphi(-q_0) \, .
$$

At $q = +q_0$:

$$
\varphi'(q_0 + \eta) - \varphi'(q_0 - \eta) = -\frac{2m}{\hbar^2} V_0 \, \varphi(q_0) \, .
$$

Since, according to the presupposition, V_0 and also $\varphi(\pm q_0)$ are finite, the derivative makes a finite jump at $\pm q_0$, but are otherwise everywhere continuous. $\varphi(q)$ is

therefore continuous on the whole q-axis, including the points $\pm q_0$.

$$\kappa^2 = -\frac{2m}{\hbar^2} E \; ; \quad \textit{classically forbidden region.}$$

Ansatz for the solution, which already takes into account symmetries (parity) and correct asymptotic behavior:

$$\varphi_\pm(q) = \begin{cases} \alpha_\pm e^{\kappa q} & -\infty < q < -q_0 \\ \beta\,(e^{\kappa q} \pm e^{-\kappa q}) & -q_0 < q < +q_0 \\ \pm\alpha_\pm e^{-\kappa q} & +q_0 < q < +\infty \end{cases}$$

Continuity at $\pm q_0$:

$$\alpha_\pm e^{-\kappa q_0} = \beta \left(e^{-\kappa q_0} \pm e^{+\kappa q_0}\right) .$$

Solving for β and inserting into the preceding equation:

$$\varphi_\pm(q) = \alpha_\pm \begin{cases} e^{\kappa q} & -\infty < q < -q_0 \, , \\ \pm e^{-\kappa q_0} \, \frac{e^{\kappa q} \pm e^{-\kappa q}}{e^{\kappa q_0} \pm e^{-\kappa q_0}} & -q_0 < q < +q_0 \, , \\ \pm e^{-\kappa q} & +q_0 < q < +\infty \, . \end{cases}$$

Normalization:

$$\begin{aligned} 1 &\stackrel{!}{=} \int_{-\infty}^{+\infty} dq |\varphi_\pm(q)|^2 \\ &= |\alpha_\pm|^2 \left\{ \frac{1}{2\kappa} e^{-2\kappa q_0} + \frac{e^{-2\kappa q_0}}{(e^{\kappa q_0} \pm e^{-\kappa q_0})^2} \left[\frac{1}{\kappa} \left(e^{2\kappa q_0} - e^{-2\kappa q_0}\right) \pm 4 q_0 \right] + \frac{1}{2\kappa} e^{-2\kappa q_0} \right\} \\ &= |\alpha_\pm|^2 \, \frac{e^{-2\kappa q_0} \, \frac{1}{\kappa}}{(e^{\kappa q_0} \pm e^{-\kappa q_0})^2} \left\{ (e^{\kappa q_0} \pm e^{-\kappa q_0})^2 + \left(e^{2\kappa q_0} - e^{-2\kappa q_0}\right) \pm 4\kappa \, q_0 \right\} \\ &= \frac{|\alpha_\pm|^2}{\kappa (e^{\kappa q_0} \pm e^{-\kappa q_0})^2} \left\{ 2 \pm 2\, e^{-2\kappa q_0} \pm 4\kappa \, q_0 \, e^{-2\kappa q_0} \right\} . \end{aligned}$$

We write for abbreviation:

$$\begin{aligned} c_\pm \;&=\; \sqrt{\frac{\kappa}{2}} \left\{ 1 \pm (1 + 2\kappa \, q_0) \, e^{-2\kappa q_0} \right\}^{-\frac{1}{2}} \\ &\Longrightarrow \; \alpha_\pm = c_\pm \, (e^{\kappa q_0} \pm e^{-\kappa q_0}) \\ &\qquad \textit{(except for an unimportant phase factor of the magnitude 1!)} \, . \end{aligned}$$

Therewith, the wave function can be brought for the whole q-axis into the following compact form:

$$\varphi_{\pm}(q) = c_{\pm} \left\{ e^{-\kappa|q+q_0|} \pm e^{-\kappa|q-q_0|} \right\} .$$

We still exploit the discontinuity-jumps of the first derivative at $\pm q_0$:

$$\varphi'(q) = c_{\pm}\,\kappa \begin{cases} e^{\kappa(q+q_0)} \pm e^{\kappa(q-q_0)} : & -\infty < q < -q_0 \,, \\ -e^{-\kappa(q+q_0)} \pm e^{\kappa(q-q_0)} : & -q_0 < q < +q_0 \,, \\ -e^{-\kappa(q+q_0)} \mp e^{-\kappa(q-q_0)} : & +q_0 < q < +\infty \,. \end{cases}$$

'Jump-conditions' at $q = -q_0$:

$$c_{\pm}\,\kappa(-1 \pm e^{-2\kappa q_0} - 1 \mp e^{-2\kappa q_0}) = -\frac{2m}{\hbar^2} V_0\, c_{\pm}\,(1 \pm e^{-2\kappa q_0})$$

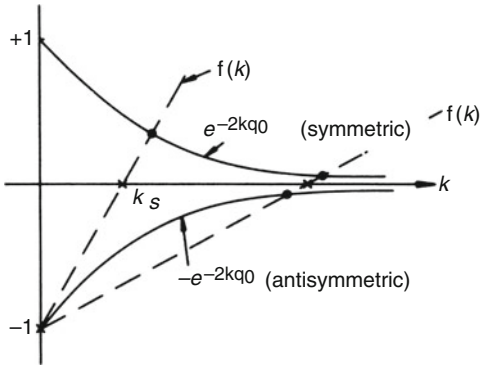
$$\Longrightarrow \quad \kappa = \frac{m}{\hbar^2} V_0\,(1 \pm e^{-2\kappa q_0}) \left(= \sqrt{-\frac{2m}{\hbar^2} E} \right) .$$

Exactly the same relation is found for $q = +q_0$. We discuss this expression graphically (Fig. A.13):

$$f(\kappa) = \kappa \left(\frac{\hbar^2}{m\,V_0} \right) - 1 = \pm e^{-2\kappa q_0} .$$

1. There is **always** a symmetric solution.
2. There are at most two solutions, one of which is symmetric, the other antisymmetric.

Fig. A.13



3. The intersection point of the straight line $f(\kappa)$ with the κ-axis appears at

$$\kappa_s = \frac{m\,V_0}{\hbar^2}\ .$$

$\Longrightarrow$ the larger V_0, the more probable an antisymmetric solution appears!

4. The larger q_0 the steeper $e^{-2\kappa q_0}$ decreases. $\Longrightarrow$ The larger q_0, the more probable an antisymmetric solution appears!
5. Eigen-energies:

$$E_\pm = -\frac{m\,V_0^2}{2\hbar^2}\,(1 \pm e^{-2\kappa q_0})^2\ ,$$
$$\textit{additional condition: } \kappa \geq 0.$$

6.

$$q_0 = 0 \implies E_- = 0\,; \quad E_+ = -\frac{2m\,V_0^2}{\hbar^2}\ .$$

That is exactly the result for the simple δ-potential of the preceding exercise, if one replaces V_0 by $V_0/2$.

Solution 4.2.9 We define:

$$k_1^2 = \frac{2m}{\hbar^2}\,(E - V_1)\ \ ; \quad k^2 = \frac{2m}{\hbar^2}\,E\,; \quad k_3^2 = \frac{2m}{\hbar^2}\,(E - V_3)\ ,$$
$$x = \frac{k_1}{k} = \sqrt{\frac{E - V_1}{E}}\ \ ; \quad y = \frac{k_3}{k} = \sqrt{\frac{E - V_3}{E}}\ .$$

Ansatz for the solution:

$$\varphi(q) = \begin{cases} \varphi_1(q) + \varphi_\mathrm{r}(q) & -\infty < q \leq -q_0\ , \\ \beta_+\,e^{ikq} + \beta_-\,e^{-ikq} & -q_0 < q < +q_0\ , \\ \varphi_\mathrm{d}(q) & +q_0 \leq q < +\infty\ , \end{cases}$$
$$\varphi_1(q) = e^{ik_1 q}\,; \quad \varphi_\mathrm{r}(q) = \alpha_-\,e^{-ik_1 q}\,; \quad \varphi_\mathrm{d}(q) = \gamma_+\,e^{ik_3 q}\ .$$

Current densities:

$$j_1 = \frac{\hbar\,k_1}{m}\,; \quad j_\mathrm{r} = -\frac{\hbar\,k_1}{m}\,|\alpha_-|^2\,; \quad j_\mathrm{d} = \frac{\hbar\,k_3}{m}\,|\gamma_+|^2$$
$$\Longrightarrow\ R = \left|\frac{j_\mathrm{r}}{j_1}\right| = |\alpha_-|^2\ ,$$
$$T = \left|\frac{j_\mathrm{d}}{j_1}\right| = \frac{k_3}{k_1}|\gamma_+|^2 = \frac{y}{x}|\gamma_+|^2\ .$$

Fitting conditions at $-q_0$:

$$e^{-ik_1q_0} + \alpha_- e^{ik_1q_0} = \beta_+ e^{-ikq_0} + \beta_- e^{ikq_0} ,$$
$$i k_1 (e^{-ik_1q_0} - \alpha_- e^{ik_1q_0}) = i k (\beta_+ e^{-ikq_0} - \beta_- e^{ikq_0}) .$$

These can be reformulated:

$$(1+x) e^{-ik_1q_0} + \alpha_- (1-x) e^{ik_1q_0} = 2\beta_+ e^{-ikq_0} ,$$
$$(1-x) e^{-ik_1q_0} + \alpha_- (1+x) e^{ik_1q_0} = 2\beta_- e^{ikq_0} .$$

Fitting conditions at $+q_0$:

$$\beta_+ e^{ikq_0} + \beta_- e^{-ikq_0} = \gamma_+ e^{ik_3q_0} ,$$
$$i k (\beta_+ e^{ikq_0} - \beta_- e^{-ikq_0}) = i k_3 \gamma_+ e^{ik_3q_0} .$$

These can be combined as follows:

$$2\beta_+ e^{ikq_0} = (1+y) \gamma_+ e^{ik_3q_0} ,$$
$$2\beta_- e^{-ikq_0} = (1-y) \gamma_+ e^{ik_3q_0} .$$

By insertion we get from the four conditional equations a system of two equations for the two unknowns γ_+ and α_-:

$$(1+x) e^{-ik_1q_0} = -\alpha_- (1-x) e^{ik_1q_0} + (1+y) \gamma_+ e^{i(k_3-2k)q_0} ,$$
$$(1-x) e^{-ik_1q_0} = -\alpha_- (1+x) e^{ik_1q_0} + (1-y) \gamma_+ e^{i(k_3+2k)q_0} .$$

The determinant of the coefficients

$$\det A = \det \begin{pmatrix} -(1-x) e^{ik_1q_0} & (1+y) e^{i(k_3-2k)q_0} \\ -(1+x) e^{ik_1q_0} & (1-y) e^{i(k_3+2k)q_0} \end{pmatrix}$$
$$= e^{i(k_1+k_3)q_0} \left\{ -(1-x)(1-y) e^{2ikq_0} + (1+x)(1+y) e^{-2ikq_0} \right\}$$

is always unequal zero. There does exist therefore for **all** $E > V_3$ a solution.
$\Longrightarrow$ continuous spectrum.

We need later:

$$|\det A|^2 = 4(x+y)^2 \cos^2 2kq_0 + 4(1+xy)^2 \sin^2 2kq_0$$
$$= 4(x+y)^2 + 4(1-x^2)(1-y^2) \sin^2 2kq_0 .$$

We determine the coefficients α_- and γ_+ by the use of Cramer's rule:

$$\begin{aligned}
\alpha_- \det A &= \det \begin{pmatrix} (1+x)\, e^{-ik_1 q_0} & (1+y)\, e^{i(k_3-2k)q_0} \\ (1-x)\, e^{-ik_1 q_0} & (1-y)\, e^{i(k_3+2k)q_0} \end{pmatrix} \\
&= e^{i(k_3-k_1)q_0} \left\{ (1+x)(1-y)\, e^{2ikq_0} - (1-x)(1+y)\, e^{-2ikq_0} \right\} , \\
\gamma_+ \det A &= \det \begin{pmatrix} -(1-x)\, e^{ik_1 q_0} & (1+x)\, e^{-ik_1 q_0} \\ -(1+x)\, e^{ik_1 q_0} & (1-x)\, e^{-ik_1 q_0} \end{pmatrix} \\
&= -(1-x)^2 + (1+x)^2 = 4x \, .
\end{aligned}$$

Reflection coefficient:

$$R = |\alpha_-|^2 = \frac{4(x-y)^2 + 4(1-x^2)(1-y^2)\sin^2 2kq_0}{|\det A|^2} \, .$$

Transmission coefficient:

$$T = \frac{y}{x} |\gamma_+|^2 = \frac{16\, x\, y}{|\det A|^2} \, .$$

The condition $T + R = 1$ is obviously fulfilled. In the case of $k_1 = k_3 \iff y = x$ the results (4.63) and (4.64) of the potential well are reproduced.

Solution 4.2.10

1.

$$\begin{aligned}
1 = A^2 \int_{-q_0}^{+q_0} dq \, \left(q^2 - q_0^2\right)^2 &= A^2 \int_{-q_0}^{+q_0} dq \, \left(q^4 - 2q_0^2 q^2 + q_0^4\right) = \\
= A^2 \left(\frac{2}{5} q_0^5 - \frac{4}{3} q_0^5 + 2\, q_0^5 \right) & \\
\Longrightarrow \quad A = \frac{1}{4} \sqrt{\frac{15}{q_0^5}} \, . &
\end{aligned}$$

2.

$$\psi(q) = \sum_m c_m \, \varphi_m(q) \, .$$

Probability amplitude:

$$c_n = \int\limits_{-q_0}^{+q_0} dq\, \varphi_n^*(q)\, \psi(q) = \frac{\sqrt{15}}{4q_0^3} \int\limits_{-q_0}^{+q_0} dq \sin\left(\frac{\pi}{q_0}\, n\, q\right) (q^2 - q_0^2) = 0\ ,$$

since the integrand is an odd function of q!

3.

$$c_n = \frac{\sqrt{15}}{4q_0^3} \int\limits_{-q_0}^{+q_0} dq \cos\left(\frac{\pi}{2q_0}\,(2n+1)\, q\right) (q^2 - q_0^2)\ .$$

Substitution:

$$y = \frac{\pi}{2q_0}\,(2n+1)\, q \implies dq = \frac{2q_0}{\pi(2n+1)}\, dy\ ,$$

$$q^2 = \frac{4q_0^2}{\pi^2(2n+1)^2}\, y^2\ ,$$

$$c_n = \frac{\sqrt{15}}{4q_0^3}\, \frac{2q_0}{\pi(2n+1)} \int\limits_{-\frac{\pi}{2}(2n+1)}^{\frac{\pi}{2}(2n+1)} dy\, \cos y \left(\frac{4q_0^2}{\pi^2(2n+1)^2}\, y^2 - q_0^2\right)\ ,$$

$$\int\limits_{-\frac{\pi}{2}(2n+1)}^{+\frac{\pi}{2}(2n+1)} dy \cos y\, y^2 = \left[2y\cos y + (y^2-2)\sin y\right]\Big|_{-\frac{\pi}{2}(2n+1)}^{\frac{\pi}{2}(2n+1)}$$

$$= \left[\frac{\pi^2}{4}\,(2n+1)^2 - 2\right] 2(-1)^n$$

$$\int\limits_{-\frac{\pi}{2}(2n+1)}^{+\frac{\pi}{2}(2n+1)} dy \cos y = 2(-1)^n$$

$$\implies c_n = \frac{\sqrt{15}}{2\pi(2n+1)} \left\{ \frac{4}{\pi^2(2n+1)^2} \left[\frac{\pi^2}{4}(2n+1)^2 - 2\right] - 1 \right\} 2(-1)^n$$

$$= -8(-1)^n\, \frac{\sqrt{15}}{\pi^3(2n+1)^3} \implies w_n = |c_n|^2 = \frac{960}{\pi^6(2n+1)^6}\ .$$

Section 4.3.6

Solution 4.3.1 Because of $E > V_0$ the whole region is *classically allowed*. The wave function therefore exhibits everywhere oscillatory behavior. Ansatz for the solution:

$$\begin{array}{lll} q \le 0: & \varphi = e^{ik_0 q} + \alpha\, e^{-ik_0 q}: & k_0^2 = \frac{2m}{\hbar^2} E\,, \\ 0 < q < q_0: & \varphi = \beta_+\, e^{ik_\mathrm{b} q} + \beta_-\, e^{-ik_\mathrm{b} q}: & k_\mathrm{b}^2 = \frac{2m}{\hbar^2}\left(E - \frac{V_0}{2}\right)\,, \\ q_0 \le q: & \varphi = \gamma\, e^{ikq}: & k^2 = \frac{2m}{\hbar^2}\,(E - V_0)\,. \end{array}$$

Current densities:

$$\begin{aligned} &\text{incident wave:} \quad j_0 = \frac{\hbar\, k_0}{m}\,, \\ &\text{reflected wave:} \quad j_\mathrm{r} = -\frac{\hbar\, k_0}{m}|\alpha|^2\,. \end{aligned}$$

Reflection coefficient:

$$R = \left|\frac{j_\mathrm{r}}{j_0}\right| = |\alpha|^2\,.$$

We write for abbreviation:

$$y = \frac{k_\mathrm{b}}{k_0}\,; \quad x = \frac{k}{k_\mathrm{b}}$$

and formulate the continuity-conditions:

$\underline{q = 0}$

$$\begin{aligned} 1 + \alpha &= \beta_+ + \beta_-\,, \\ 1 - \alpha &= y(\beta_+ - \beta_-)\,. \end{aligned}$$

$\underline{q = q_0}$

$$\begin{aligned} \beta_+\, e^{ik_\mathrm{b} q_0} + \beta_-\, e^{-ik_\mathrm{b} q_0} &= \gamma\, e^{ikq_0}\,, \\ \beta_+\, e^{ik_\mathrm{b} q_0} - \beta_-\, e^{-ik_\mathrm{b} q_0} &= x\,\gamma\, e^{ikq_0}\,. \end{aligned}$$

The last two equations yield:

$$2\beta_\pm\, e^{\pm ik_\mathrm{b} q_0} = (1 \pm x)\,\gamma\, e^{ikq_0}\,.$$

The first two equations can be remodeled

$$\alpha = \frac{1}{2}(1-y)\,\beta_+ + \frac{1}{2}(1+y)\,\beta_- ,$$
$$1 = \frac{1}{2}(1+y)\,\beta_+ + \frac{1}{2}(1-y)\,\beta_- .$$

By insertion of β_+ and β_- into the last equation one gets for γ:

$$1 = \frac{1}{2}(1+y)\,\frac{1}{2}(1+x)\,\gamma\, e^{i(k-k_\mathrm{b})q_0} + \frac{1}{2}(1-y)\,\frac{1}{2}(1-x)\,\gamma\, e^{i(k+k_\mathrm{b})q_0}$$
$$\Longrightarrow\ \gamma = \frac{2e^{-ikq_0}}{(1+xy)\cos k_\mathrm{b}q_0 - i(x+y)\sin k_\mathrm{b}q_0}$$
$$\Longrightarrow\ |\gamma|^2 = \frac{4}{(1+xy)^2 - (1-x^2)(1-y^2)\sin^2 k_\mathrm{b}q_0} .$$

Analogously we get for α by insertion of $\beta_\pm$ into the above relation:

$$\frac{\alpha}{\gamma} = \frac{1}{2}(1-y)\,\frac{1}{2}(1+x)\,e^{i(k-k_\mathrm{b})q_0} + \frac{1}{2}(1+y)\,\frac{1}{2}(1-x)\,e^{i(k+k_\mathrm{b})q_0}$$
$$\Longrightarrow\ \left|\frac{\alpha}{\gamma}\right|^2 = \frac{1}{4}\left\{(1-xy)^2\cos^2 k_\mathrm{b}\,q_0 + (x-y)^2\sin^2 k_\mathrm{b}\,q_0\right\} .$$

Finally it follows therewith:

$$R = |\alpha|^2 = \frac{(1-xy)^2 - (1-x^2)(1-y^2)\sin^2 k_\mathrm{b}q_0}{(1+xy)^2 - (1-x^2)(1-y^2)\sin^2 k_\mathrm{b}q_0} .$$

For the simple-step potential we had found in Sect. 4.3.1:

$$R_1 = \frac{(1-xy)^2}{(1+xy)^2} .$$

Because of $0 \le x \le 1,\ 0 \le y \le 1,\ 0 \le \sin^2 k_\mathrm{b}q_0 \le 1$ it can be estimated:

$$a^2 = (1+xy)^2 \ge b^2 = (1-xy)^2 \ge (1-x^2)(1-y^2)\sin^2 k_\mathrm{b}q_0 = d^2$$
$$\Longleftrightarrow a^2 \ge b^2$$
$$\Longleftrightarrow\ -d^2a^2 \le -d^2b^2 \ \Longleftrightarrow\ a^2b^2 - d^2a^2 \le a^2b^2 - d^2b^2$$
$$\Longleftrightarrow\ \frac{b^2-d^2}{a^2-d^2}\,\frac{a^2}{b^2} \le 1 \ \Longleftrightarrow\ \frac{R}{R_1} \le 1 .$$

The reflection coefficient is therefore for the double-step potential smaller than for the simple-step potential. Only for $E = V_0$, i.e. $k = x = 0$, both are equal to one.

Solution 4.3.2 The problem is formally identical to that of the potential well discussed in Sect. 4.2.2. With the replacements

$$k \to i\kappa\,; \quad \kappa = \sqrt{\frac{2m}{\hbar^2}\,(V_0 - E)}\,,$$

$$y \to i\,x\,; \quad x = \frac{\kappa}{k_0} = \sqrt{\frac{V_0 - E}{E}}$$

the results from Sect. 4.2.2 can be, to a great extent, taken over.

1. $\underline{q \geq q_0}$

$$|\varphi(q)|^2 = |\gamma_+|^2 = T(E)\,.$$

$T\,(E)$ has already been calculated with (4.89).

2. $\underline{-q_0 \leq q \leq +q_0}$

$$\varphi(q) = \beta_+\, e^{-\kappa q} + \beta_-\, e^{\kappa q}\,.$$

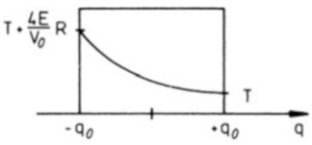
With the equations before (4.60):

$$\begin{aligned}
\beta_+ &= \frac{1}{\det A}\, 2(1 + i\,x)\, e^{\kappa q_0}\, e^{-ik_0 q_0}\,, \\
\beta_- &= \frac{-1}{\det A}\, 2(1 - i\,x)\, e^{-\kappa q_0}\, e^{-ik_0 q_0}\,, \\
|\det A|^2 &= 4\big[4x^2 + (1 + x^2)^2 \sinh^2 2\kappa q_0\big] = \\
&\overset{(4.89)}{=} \frac{16\,x^2}{T(E)} \overset{(4.89)}{=} \frac{4(1 + x^2)^2 \sinh^2 2\kappa q_0}{R(E)}\,.
\end{aligned}$$

It follows therewith:

$$\begin{aligned}
|\varphi(q)|^2 &= |\beta_+|^2\, e^{-2\kappa q} + |\beta_-|^2\, e^{2\kappa q} + (\beta_+\, \beta_-^* + \beta_+^*\, \beta_-) \\
&= \frac{1}{|\det A|^2}\, [4|1 + i\,x|^2\, e^{2\kappa(q_0 - q)} + 4|1 - i\,x|^2\, e^{-2\kappa(q_0 - q)} - 8(1 - x^2)] \\
&= \frac{1}{|\det A|^2}\, [16(1 + x^2) \sinh^2 \kappa(q_0 - q) + 16\,x^2] \\
\Longrightarrow\ |\varphi(q)|^2 &= T\,(E) + \frac{4E}{V_0}\, R(E)\, \frac{\sinh^2 \kappa(q_0 - q)}{\sinh^2 2\kappa q_0}\,.
\end{aligned}$$

Fig. A.14



Inside the potential wall, $|\varphi(q)|^2$ decreases monotonously from (Fig. A.14)

$$T(E) + \frac{4E}{V_0} R(E) = |\varphi(-q_0)|^2$$

to

$$T(E) = |\varphi(q_0)|^2 ,$$

where $T(E)$ and $R(E)$ are the transmission and the reflection coefficients known from (4.89) and (4.90).

3. $\underline{-\infty < q \leq -q_0}$

$$\varphi(q) = e^{ik_0 q} + \alpha_- e^{-ik_0 q} ,$$

$$(4.61) \implies \alpha_- = 2 \sinh 2\kappa q_0 \frac{1 + x^2}{\det A} e^{-2ik_0 q_0} ,$$

$$(4.59) \implies \det A = (1 + ix)^2 e^{2\kappa q_0} - (1 - ix)^2 e^{-2\kappa q_0} ,$$

$$(4.90) \implies |\alpha_-|^2 = R(E) .$$

It follows therewith at first:

$$|\varphi(q)|^2 = 1 + R(E) + 2 \,\mathrm{Re}\, \left(\alpha_-^* e^{2ik_0 q}\right) =$$

$$= 1 + R(E) + 4 \sinh 2\kappa q_0 \frac{(1 + x^2)}{|\det A|^2} \,\mathrm{Re}\, \left(\det A \, e^{2ik_0(q_0 + q)}\right) =$$

$$= 1 + R(E) + \frac{R(E)}{(1 + x^2) \sinh 2\kappa q_0} \left[2\left(1 - x^2\right) \sinh 2\kappa q_0 \cos 2k_0(q_0 + q) - \right.$$

$$\left. - 4x \cosh 2\kappa q_0 \sin 2k_0(q_0 + q)\right]$$

$$\implies |\varphi(q)|^2 =$$

$$= 1 + R(E) + \frac{2R(E)}{1 + x^2} \left[(1 - x^2) \cos 2k_0(q_0 + q) - 2x \coth 2\kappa q_0 \sin 2k_0(q_0 + q)\right] .$$

The interference of incident and reflected wave takes care for an oscillatory behavior of the position-probability:

$$|\varphi(-q_0)|^2 = 1 + R(E) + 2R(E)\,\frac{1-x^2}{1+x^2} = T\,(E) + \frac{4E}{V_0}\,R(E) \quad \text{(see 2.)}\ .$$

Solution 4.3.3 We define:

$$k_0^2 = \frac{2m}{\hbar^2}E\ ;\ \ k_d^2 = \frac{2m}{\hbar^2}\left(E - \frac{1}{2}V_0\right)\ ;\ \ k_i^2 = \frac{2m}{\hbar^2}\,(E - V_0) = -\kappa^2\ .$$

Ansatz for the solution:

$$\varphi(q) = \begin{cases} \varphi_0(q) + \varphi_r(q) & \text{for } -\infty < q \le -q_0 \\ b_+ e^{\kappa q} + b_- e^{-\kappa q} & \text{for } -q_0 \le q \le +q_0 \\ \varphi_d(q) & \text{for } +q_0 \le q < +\infty\ . \end{cases}$$

Obviously we must have:

$$\varphi_0(q) = e^{ik_0 q}\ ;\ \ \varphi_r(q) = a_- e^{-ik_0 q}\ ;\ \ \varphi_d(q) = c_+ e^{ik_d q}\ .$$

The ansatz for φ_d exploits the fact that from $+\infty$ nothing can be reflected.
Current densities:

$$j_\alpha = \frac{\hbar}{2mi}\left(\varphi_\alpha^\star \frac{d}{dq}\varphi_\alpha - \varphi_\alpha \frac{d}{dq}\varphi_\alpha^\star\right)\ ;\ \ \alpha = 0, r, d\ .$$

One easily calculates:

$$j_0 = \frac{\hbar k_0}{m}\ ;\ \ j_r = -\frac{\hbar k_0}{m}|a_-|^2\ ;\ \ j_d = \frac{\hbar k_d}{m}|c_+|^2\ .$$

Reflection and transmission coefficients:

$$R(E) = \left|\frac{j_r}{j_0}\right| = |a_-|^2\ ;\ \ T(E) = \left|\frac{j_d}{j_0}\right| = \frac{k_d}{k_0}|c_+|^2\ .$$

We thus need the coefficients a_- and c_+. That is achieved by successive fitting of the wave function and its first derivative at $\pm q_0$.

- $\underline{q = -q_0}$

$$e^{-ik_0 q_0} + a_- e^{ik_0 q_0} = b_+ e^{-\kappa q_0} + b_- e^{\kappa q_0} \tag{A.12}$$

$$ik_0\left(e^{-ik_0 q_0} - a_- e^{ik_0 q_0}\right) = \kappa\left(b_+ e^{-\kappa q_0} - b_- e^{\kappa q_0}\right)\ . \tag{A.13}$$

- $\underline{q = +q_0}$

$$b_+ e^{\kappa q_0} + b_- e^{-\kappa q_0} = c_+ e^{ik_d q_0} \tag{A.14}$$

$$\kappa \left(b_+ e^{\kappa q_0} - b_- e^{-\kappa q_0}\right) = ik_d c_+ e^{ik_d q_0} \; . \tag{A.15}$$

We write for abbreviation:

$$x = \frac{\kappa}{k_0} = \sqrt{\frac{V_0 - E}{E}} \; ; \quad y = \frac{\kappa}{k_d} = \sqrt{\frac{V_0 - E}{E - \frac{1}{2}V_0}} \; .$$

Divide(A.13) by ik_0 and add it to (A.12):

$$2e^{-ik_0 q_0} = b_+(1 - ix)e^{-\kappa q_0} + b_-(1 + ix)e^{\kappa q_0} \; . \tag{A.16}$$

Divide (A.15) by ik_d and subtract it from (A.14):

$$0 = b_+(1 + iy)e^{\kappa q_0} + b_-(1 - iy)e^{-\kappa q_0} \; . \tag{A.17}$$

(A.16) and (A.17) build an inhomogeneous system of equations for the coefficients b_+, b_-. Secular determinant:

$$\begin{aligned} \Delta &= (1 - ix)(1 - iy)e^{-2\kappa q_0} - (1 + ix)(1 + iy)e^{2\kappa q_0} \\ &= (1 - xy)\left(e^{-2\kappa q_0} - e^{2\kappa q_0}\right) - i(x + y)\left(e^{-2\kappa q_0} + e^{2\kappa q_0}\right) \; . \end{aligned}$$

The secular determinant

$$\Delta = 2(xy - 1)\sinh 2\kappa q_0 - 2i(x + y)\cosh 2\kappa q_0 \tag{A.18}$$

is for all energies E unequal zero. The inhomogeneous system of equations (A.16) and (A.17) has therefore a solution for all energies E. Hence, we expect a continuous spectrum! For later purposes we need $|\Delta|^2$:

$$\begin{aligned} |\Delta|^2 &= 4(xy - 1)^2 \sinh^2 2\kappa q_0 + 4(x + y)^2 \cosh^2 2\kappa q_0 \\ &= 4(x + y)^2 + 4(1 + x^2)(1 + y^2)\sinh^2 2\kappa q_0 \; . \end{aligned} \tag{A.19}$$

In the last step, $\cosh^2 x - \sinh^2 x = 1$ was used.
Cramer's rule:

$$b_+ \Delta = \det \begin{pmatrix} 2e^{-ik_0 q_0} & (1 + ix)\, e^{\kappa q_0} \\ 0 & (1 - iy)\, e^{-\kappa q_0} \end{pmatrix}$$

$$b_- \Delta = \det \begin{pmatrix} (1 - ix)\, e^{-\kappa q_0} & 2e^{-ik_0 q_0} \\ (1 + iy)\, e^{\kappa q_0} & 0 \end{pmatrix} \; .$$

The coefficients $b_\pm$ are now determined with (A.18):

$$b_+ = \frac{2}{\Delta}(1 - iy)\, e^{-(ik_0+\kappa)q_0} \tag{A.20}$$

$$b_- = -\frac{2}{\Delta}(1 + iy)\, e^{-(ik_0-\kappa)q_0} \ . \tag{A.21}$$

Continuity at $q = +q_0$:

$$\begin{aligned} b_+ e^{\kappa q_0} + b_- e^{-\kappa q_0} &= \frac{2}{\Delta}\, e^{-ik_0 q_0}(1 - iy - 1 - iy) \\ &= -4i\frac{y}{\Delta}\, e^{-ik_0 q_0} \stackrel{!}{=} c_+\, e^{ik_d q_0} \\ \curvearrowright \quad c_+ &= -i\frac{4y}{delta}\, e^{-i(k_0+k_d)q_0} \ . \end{aligned} \tag{A.22}$$

Continuity at $q = -q_0$:

$$\begin{aligned} 2a_-\, e^{ik_0 q_0} &= b_+(1 + ix)\, e^{-\kappa q_0} + b_-(1 - ix)\, e^{\kappa q_0} \\ &= \frac{2}{\Delta}\, e^{-ik_0 q_0}\left((1 - iy)(1 + ix)\, e^{-2\kappa q_0} - (1 + iy)(1 - ix)\, e^{2\kappa q_0}\right) \\ &= \frac{2}{\Delta}\, e^{-ik_0 q_0}\left((1 - iy + xy + ix)\, e^{-2\kappa q_0} - (1 + iy + xy - ix)\, e^{2\kappa q_0}\right) \\ &= \frac{2}{\Delta}\, e^{-ik_0 q_0}\left(2i(x - y)\cosh 2\kappa q_0 - 2(1 + xy)\sinh 2\kappa q_0\right) \ . \end{aligned}$$

It follows:

$$a_- = -\frac{2}{\Delta}\, e^{-2ik_0 q_0}\left((1 + xy)\sinh 2\kappa q_0 - i(x - y)\cosh 2\kappa q_0\right) . \tag{A.23}$$

With (A.20)–(A.23), the solution is complete. We are now able to calculate the coefficients of transmission and reflection. For that we need:

$$\begin{aligned} |a_-|^2 &= \frac{4}{|\Delta|^2}\left((1 + xy)^2 \sinh^2 2\kappa q_0 + (x - y)^2 \cosh^2 2\kappa q_0\right) \\ &= \frac{4}{|\Delta|^2}\left((x - y)^2 + (1 + x^2)(1 + y^2)\sinh^2 2\kappa q_0\right) \\ \frac{k_d}{k_0}|c_+|^2 &= \frac{x}{y}\frac{16y^2}{|\Delta|^2} = \frac{16xy}{|\Delta|^2} \ . \end{aligned}$$

It finally follows with (A.19) for transmission and reflection:

$$R(E) = \frac{(x-y)^2 + (1+x^2)(1+y^2)\sinh^2 2\kappa q_0}{(x+y)^2 + (1+x^2)(1+y^2)\sinh^2 2\kappa q_0}$$
$$T(E) = \frac{4xy}{(x+y)^2 + (1+x^2)(1+y^2)\sinh^2 2\kappa q_0} \; .$$

'Particle conservation' is obviously guaranteed:

$$R(E) + T(E) = 1 \; .$$

For $x = y$ we get the results (4.89) and (4.90) for the symmetric potential wall.

Solution 4.3.4

1. Oscillatory behavior of the wave function in the *classically allowed region A*:

$$\varphi(q) = e^{ik_0 q} + \alpha_- \, e^{-ik_0 q} = \varphi_0(q) + \varphi_r(q) \qquad \text{for } -\infty < q < -q_0 \; .$$

Region B is also *classically allowed*:

$$\varphi(q) = \beta_+ \, e^{ik_0 q} + \beta_- \, e^{-ik_0 q} \qquad \text{for } -q_0 < q \leq 0 \; .$$

Region C:

$$\varphi(q) \equiv 0 \qquad \text{for } q \geq 0.$$

2. Fitting conditions:
$\underline{q = 0}$

$$\varphi(0) = 0 = \beta_+ + \beta_- \implies \beta_+ = -\beta_- = \beta \; .$$

$\underline{q = -q_0}$

$$\varphi(-q_0) = e^{-ik_0 q_0} + \alpha_- \, e^{ik_0 q_0} = 2i\,\beta \sin(-k_0 q_0) \; .$$

The derivative is, because of the δ-potential, not continuous at $-q_0$. Like in the solution of Exercise 4.2.5, we integrate the Schrödinger equation over a small interval around the point $q = -q_0$:

$\eta = 0^+ :$

$$\int_{-q_0-\eta}^{-q_0+\eta} dq\, \varphi''(q) - v_0 \int_{-q_0-\eta}^{-q_0+\eta} \delta(q+q_0)\, \varphi(q)\, dq = -\frac{2m}{\hbar^2} E \int_{-q_0-\eta}^{-q_0+\eta} \varphi(q)\, dq \; .$$

Continuity of the wave function:

$$\Longrightarrow \varphi'(-q_0+\eta)-\varphi'(-q_0-\eta)=v_0\,\varphi(-q_0)\ .$$

This means in the present case:

$$i\,k_0(\beta_+\,e^{-i\,k_0q_0}-\beta_-\,e^{ik_0q_0}-e^{-ik_0q_0}+\alpha_-\,e^{ik_0q_0})=-2i\,\beta\,v_0\sin k_0q_0\ .$$

We thus have to solve, finally, the following system of equations:

$$\begin{aligned}&\alpha_-\,e^{ik_0q_0}+\beta(2i\sin k_0q_0)=-e^{-ik_0q_0}\ ,\\ &\alpha_-\,k_0\,e^{ik_0q_0}+\beta\,(2k_0\cos k_0q_0+2v_0\sin k_0q_0)=k_0\,e^{-ik_0q_0}\ .\end{aligned}$$

Determinant of the coefficients:

$$\begin{aligned}\det A\ &=\ 2\,e^{ik_0q_0}\,\Delta(q_0)\ ,\\ \Delta(q_0)\ &=\ k_0\cos k_0q_0+(v_0-i\,k_0)\sin k_0q_0\ .\end{aligned}$$

Cramer's rule:

$$\begin{aligned}\alpha_-\ &=\ -e^{-2ik_0q_0}\,\frac{delta^*(q_0)}{\Delta(q_0)}\ ,\\ \beta\ &=\ \frac{k_0\,e^{-ik_0q_0}}{\Delta(q_0)}\ .\end{aligned}$$

The wave function $\varphi(q)$ is therewith completely determined!

3. Partial current densities $[j=\hbar/2m_i\,(\varphi^*\varphi'-\varphi\,\varphi^{*\prime})]$:

$$j_0=\frac{\hbar\,k_0}{m}\ ;\quad j_{\rm r}=-\frac{\hbar\,k_0}{m}\,|\alpha_-|^2$$

$$\Longrightarrow\ \textit{reflection coefficient: } R(E)=\left|\frac{j_{\rm r}}{j_0}\right|=|\alpha_-|^2\equiv 1\ .$$

It is physically clear that $R=1$, since otherwise particles would accumulate in region B. A penetration into region C is namely impossible because of the infinitely high potential.

4. In the region B we have for the wave function:

$$\begin{aligned}&\varphi(q)=2\,i\,\beta\sin k_0q\ ;\quad -q_0<q\le 0\\ &\Longrightarrow\qquad |\varphi(q)|^2=4|\beta|^2\sin^2 k_0q\ ,\\ &|\beta|^2=\left[\left(\cos k_0q_0+\frac{v_0}{k_0}\sin k_0q_0\right)^2+\sin^2 k_0q_0\right]^{-1}\ .\end{aligned}$$

a) $|\beta|^2$ is independent of v_0 and q_0, if

$$k_0^{(n)} = \frac{\pi}{q_0}\, n\,; \qquad n = \pm 1,\, \pm 2, \ldots$$

because then it follows:

$$\sin k_0 q_0 = 0; \quad \cos k_0 q_0 = (-1)^n\,; \quad |\beta|^2 = 1\,.$$

The $k_0^{(n)}$ are just the wave numbers, which lead to the bound, stationary states in the infinitely high potential well of the width q_0 (see Exercise 4.2.1).

b) There is another possibility. For the case

$$\frac{v_0}{k_0} \sin k_0 q_0 = -2 \cos k_0 q_0$$

it is, because of $\sin^2 x + \cos^2 x = 1$, also $|\beta|^2 = 1$, i.e., in particular independent of v_0 and q_0.

Condition:

$$\tan k_0 q_0 = -\frac{2k_0}{v_0}\,.$$

Solution 4.3.5 Tunnel current:

$$j_\mathrm{d} = j_0\, T(E = \varepsilon_\mathrm{F})\,.$$

Tunnel probability according to (4.95):

$$T(\varepsilon_\mathrm{F}) = \exp\left[-\frac{2}{\hbar}\int\limits_0^{q_\mathrm{F}} \sqrt{2m(V(q) - \varepsilon_\mathrm{F})}\, dq\right]\,.$$

Essentially, it remains to be calculated:

$$I = \int\limits_0^{q_\mathrm{F}} \sqrt{2m(V_0 - e\,E\,q - \varepsilon_\mathrm{F})}\, dq\,.$$

q_F is determined by the requirement:

$$\varepsilon_\mathrm{F} \stackrel{!}{=} V_0 - e\,E\,q_\mathrm{F} \implies q_\mathrm{F} = \frac{V_0 - \varepsilon_\mathrm{F}}{e\,E}\,.$$

With the substitution

$$x = \frac{e\,E}{V_0 - \varepsilon_\mathrm{F}}\,q \implies dq = \frac{V_0 - \varepsilon_\mathrm{F}}{e\,E}\,dx\,,$$
$$x(q_\mathrm{F}) = 1\,, \quad x(0) = 0$$

it follows:

$$I = \sqrt{2m}\,\frac{(V_0 - \varepsilon_\mathrm{F})^{3/2}}{e\,E} \underbrace{\int_0^1 \sqrt{1-x}\,dx}_{-\frac{2}{3}\,(1-x)^{3/2}\big|_0^1 = \frac{2}{3}}$$

$$\implies I = \frac{2}{3}\,\sqrt{2m}\,\frac{(V_0 - \varepsilon_\mathrm{F})^{3/2}}{e\,E}\,.$$

Tunnel current:

$$j_\mathrm{d} = j_0\,\exp\left(-\frac{4\sqrt{2m}}{3\hbar}\,\frac{W^{3/2}}{eE}\right)\,.$$

Solution 4.3.6

1. The regions B_n are *classically allowed*, while the regions C_n are *classically forbidden*:

$$k^2 = \frac{2m}{\hbar^2}\,E\,; \quad \kappa^2 = \frac{2m}{\hbar^2}\,(V_0 - E)\,; \quad 0 < E < V_0\,.$$

   Ansatz:

$$\varphi(q) = a_n\,e^{ik(q-n\,l)} + b_n\,e^{-ik(q-n\,l)} \quad \text{in } B_n\,,$$
$$\varphi(q) = \overline{a}_n\,e^{\kappa(q-n\,l+b)} + \overline{b}_n\,e^{-\kappa(q-n\,l+b)} \quad \text{in } C_n\,.$$

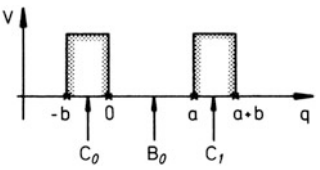
2. Bloch theorem (4.110):

$$\varphi_K(q + n\,l) = e^{iKnl}\,\varphi_K(q), \quad -\pi < K\,l \leq +\pi\,.$$

   This means:

$$\begin{Bmatrix} a_n\,e^{ikq} + b_n\,e^{-ikq} \\ \overline{a}_n\,e^{\kappa(q+b)} + \overline{b}_n\,e^{-\kappa(q+b)} \end{Bmatrix} \overset{!}{=} e^{iKn\,l} \begin{Bmatrix} a_0\,e^{ikq} + b_0\,e^{-ikq} \\ \overline{a}_0\,e^{\kappa(q+b)} + \overline{b}_0\,e^{-\kappa(q+b)} \end{Bmatrix}\,.$$

Fig. A.15



With $a_0, b_0, \overline{a}_0, \overline{b}_0$ all the others coefficients are fixed:

$$a_n\,(b_n,\,\overline{a}_n,\,\overline{b}_n) = e^{iKnl}\,a_0\,(b_0,\,\overline{a}_0,\,\overline{b}_0)\ .$$

3. Periodic boundary conditions:

$$\begin{aligned}&\varphi_K(q + N\,l) \stackrel{!}{=} \varphi_K(q)\\ \Longleftrightarrow\ e^{iKNl} \stackrel{!}{=} 1 \ &\Longleftrightarrow\ K = \frac{2\pi}{N\,l}\,m\,; \quad m = 0, \pm 1, \ldots \pm\left(\frac{N}{2} - 1\right), +\frac{N}{2}\ .\end{aligned}$$

4. Fitting conditions at $q = 0$ and $q = a$ (Fig. A.15):

$$\begin{aligned}\varphi_K\,(q = 0) &= \overline{a}_0\,e^{\kappa b} + \overline{b}_0\,e^{-\kappa b} = a_0 + b_0\ ,\\ \varphi'_K\,(q = 0) &= \kappa\,(\overline{a}_0\,e^{\kappa b} - \overline{b}_0\,e^{-\kappa b}) = i\,k\,(a_0 - b_0)\ ,\\ \varphi_K\,(q = a) &= 6a_0\,e^{ika} + b_0\,e^{-ika} = \overline{a}_1 + \overline{b}_1 = e^{iKl}\,(\overline{a}_0 + \overline{b}_0)\ ,\\ \varphi'_K\,(q = a) &= i\,k\,(a_0\,e^{ika} - b_0\,e^{-ika}) = \kappa\,(\overline{a}_1 - \overline{b}_1) = \kappa\,e^{iKl}\,(\overline{a}_0 - \overline{b}_0)\ .\end{aligned}$$

We therefore have to solve the following homogeneous system of equations:

$$\begin{pmatrix} 1 & 1 & -e^{\kappa b} & -e^{-\kappa b} \\ i\,k & -i\,k & -\kappa\,e^{\kappa b} & \kappa\,e^{-\kappa b} \\ e^{ika} & e^{-ika} & -e^{iKl} & -e^{iKl} \\ i\,k\,e^{ika} & -i\,ke^{-ika} & -\kappa\,e^{iKl} & \kappa\,e^{iKl} \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \\ \overline{a}_0 \\ \overline{b}_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}\ .$$

Determinant of the coefficients:

$$\det A = 8i\,e^{iKl}\left[k\,\kappa\,(\cos K\,l - \cos k\,a\,\cosh\kappa b) + \frac{1}{2}\,(k^2 - \kappa^2)\sin k\,a\,\sinh\kappa b\right]\ .$$

Condition for the solvability:

$$\begin{aligned}&\det A = 0 \implies \cos K\,l \stackrel{!}{=} f(E)\ ,\\ &f(E) = \cos k\,a\,\cosh\kappa b + \frac{\kappa^2 - k^2}{2k\,\kappa}\sin k\,a\,\sinh\kappa b\ .\end{aligned}$$

5.

$$l \to a\,; \quad \kappa^2 \approx \frac{2m}{\hbar^2} V_0 \to \infty\,,$$
$$\kappa b \sim \sqrt{V_0}\, b \to 0\,,$$
$$\kappa^2 b \to \frac{2m}{\hbar^2} D\,.$$

We have therewith:

$$\cosh(\kappa b) \to 1\,,$$
$$\frac{\kappa^2 - k^2}{2k\kappa} \sin\kappa b \approx \frac{\kappa^2}{2k} b \longrightarrow \frac{m D}{\hbar^2 k}\,.$$

The conditional equation for the eigen-values then reads:

$$\cos K a = \cos k a + \frac{m D}{\hbar^2 k} \sin k a\,.$$

That is exactly the conditional equation (4.114) of the Kronig-Penney model.

6. Because of $-1 \le \cos K l \le +1$, the conditional equation is solvable only for

$$|f(E)| \le 1\,.$$

$f(E)$ performs similar oscillations as those, which we have discussed in Sect. 4.3.5 for the Kronig-Penney model.
If one takes $k a = n\pi$, then $\sin k a = 0$ and $\cos k a = (-1)^n$. The above requirement

$$|f(E)| = |\cosh\kappa b| \le 1$$

is for $\kappa b \neq 0$ not satisfiable. The energy values

$$E_n = \frac{\hbar^2 \pi^2}{2m a^2} n^2$$

are thus forbidden, including their immediate neighborhood, since $f(E)$ is a continuous function. In the Kronig-Penney model ($\kappa b \to 0$), these energies represent, according to (4.115), just the lower edges of the forbidden zones.

7. For lower lying energy levels between high potential hills ($E \ll V_0$), it will be $\kappa b \gg 1$. Then it can be estimated:

$$\sinh\kappa b \approx \cosh\kappa b \approx \frac{1}{2} e^{\kappa b}\,.$$

It then comes out of the conditional equation in 4.:

$$\cos K\,l\,e^{-\kappa b} \approx \frac{1}{2}\cos k\,a + \frac{\kappa^2 - k^2}{4k\,\kappa}\sin k\,a\ .$$

The condition $|f(E)| \leq 1$ in 6. transfers to:

$$\left|\frac{1}{2}\cos k\,a + \frac{\kappa^2 - k^2}{4k\,\kappa}\sin k\,a\right| < e^{-\kappa b}\ .$$

This inequality is fulfilled, because of $e^{-\kappa b} \ll 1$, only in very narrow zones around the zeros on the left-hand side. The resulting energy bands are therefore very narrow. κ becomes, for given V_0, larger with decreasing E. The bands are therefore the smaller the deeper in energy.
The zeros of the left-hand side are therefore interesting, because they lie in any case within the allowed energy bands. They are determined by

$$2\kappa\,k\cot k\,a + \kappa^2 - k^2 \stackrel{!}{=} 0\ .$$

If we take $a = 2q_0$ and exploit

$$\cot 2kq_0 = \frac{1}{2}\left(\cot kq_0 - \frac{1}{\cot kq_0}\right)$$

then the conditional equation for the zeros

$$\kappa\,k\left(\cot kq_0 - \frac{1}{\cot kq_0}\right) = k^2 - \kappa^2$$

is solved by

$$k\,\tan kq_0 = \kappa$$

as well as by

$$k\cot kq_0 = -\kappa\ .$$

But these are just the conditional equations (4.40) and (4.43) for the energies of the bound states in the potential well of the width $a = 2q_0$. With increasing energetic distance $V_0 - E$, but also with larger lattice distance b, the potential wells become more and more decoupled. There does obviously exist a unique relationship between the energy bands and the energy levels in the potential well (atom $\rightarrow$ solid).

Solution 4.3.7 With some substitutions we can adopt the solution in part 4. of the preceding exercise:

$$E > V_0 \implies \varepsilon = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} > 0 \; ; \quad \kappa = i\,\varepsilon \; .$$

This we insert into the conditional equation

$$\cos K\,l \stackrel{!}{=} f(E) \; .$$

With

$$\cosh(i\,x) = \cos x \; ; \quad \sinh i\,x = i \sin x$$

it is:

$$f(E) = \cos k\,a\, \cos \varepsilon\, b - \frac{\varepsilon^2 + k^2}{2k\,\varepsilon} \sin k\,a\, \sin \varepsilon\, b \; .$$

Addition theorem:

$$\begin{aligned} &\cos(x + y) = \cos x \cos y - \sin x \sin y \\ \implies &f(E) = \cos(k\,a + \varepsilon\, b) - \frac{(\varepsilon - k)^2}{2k\,\varepsilon} \sin k\,a\, \sin \varepsilon\, b \; . \end{aligned}$$

Case A:

$$k\,a + \varepsilon\, b = 2m\,\pi \; ; \qquad m = 0, 1, \ldots$$

In this case $\cos(k\,a + \varepsilon\, b) = 1$. Furthermore, we write:

$$\begin{aligned} &\varepsilon\, b = m\,\pi + \varphi \; ; \qquad k\,a = m\,\pi - \varphi \\ \implies &\sin \varepsilon\, b = \sin(m\,\pi + \varphi) = \sin m\,\pi\, \cos\varphi + \cos m\,\pi\, \sin\varphi = (-1)^m \sin\varphi \; , \\ &\sin k\,a = \sin(m\,\pi - \varphi) = -(-1)^m \sin\varphi \; . \end{aligned}$$

It follows therewith:

$$f(E) = 1 + \frac{(\varepsilon - k)^2}{2k\,\varepsilon} \sin^2\varphi > 1 \; .$$

The condition $f(E) = \cos K\,l$ can therefore not be fulfilled. Energies with

$$k\,a + \varepsilon\, b = 2m\,\pi$$

are forbidden!

Case B:

$$k\,a + \varepsilon\,b = (2m+1)\,\pi\;; \qquad m = 0, 1, \ldots$$

Now $\cos(k\,a + \varepsilon\,b) = -1$. We define, similarly as in case A:

$$\varepsilon\,b = \left(m + \frac{1}{2}\right)\pi + \overline{\varphi}\;; \quad k\,a = \left(m + \frac{1}{2}\right)\pi - \overline{\varphi}$$

$$\Longrightarrow \quad \sin\varepsilon\,b = \sin\left[\left(m + \frac{1}{2}\right)\pi\right]\cos\overline{\varphi} + \cos\left[\left(m + \frac{1}{2}\right)\pi\right]\sin\overline{\varphi} = (-1)^m\cos\overline{\varphi}\;,$$

$$\sin k\,a = (-1)^m\cos\overline{\varphi}\;.$$

It follows therewith:

$$f(E) = -1 - \frac{(\varepsilon - k)^2}{2k\,\varepsilon}\cos^2\overline{\varphi} < -1\;.$$

The condition $f(E) = \cos K\,l$, even in this case, can not be fulfilled. Energies, for which $k\,a + \varepsilon\,b = (2m+1)\,\pi$, are forbidden! Because of the continuity of $f(E)$ it can even be concluded that there are **finite** forbidden regions around the above discussed energies. There are therefore even for $E > V_0$ energy gaps!

Section 4.4.7.

Solution 4.4.1

1. Proof by complete induction:

   $\underline{m = 1}$

   $$[a, a^+]_- = 1 \quad \text{known,}$$

   $\underline{m \;\Longrightarrow\; m+1}$

   $$[a^{m+1}, a^+]_- = a[a^m, a^+]_- + [a, a^+]_-\,a^m = a\,m\,a^{m-1} + 1\,a^m = (m+1)\,a^m \quad \text{q.e.d.}$$

2. $\underline{m = 1}$

   $$[a, a^+]_- = 1 \quad \text{known,}$$

   $\underline{m \;\Longrightarrow\; m+1}$

   $$\left[a, (a^+)^{m+1}\right]_- = a^+\,[a, a^{+m}]_- + [a, a^+]_-\,a^{+m}$$
   $$= a^+\,m\,(a^+)^{m-1} + 1\,a^{+m} = (m+1)\,a^{+m} \quad \text{q.e.d.}$$

3.

$$[\widehat{n}, a^m]_- = [a^+ a, a^m]_- = a^+ [a, a^m]_- + [a^+, a^m]_- \, a \overset{1.}{=} 0 - m\, a^{m-1}\, a = -m\, a^m$$

4.

$$[\widehat{n}, a^{+m}]_- = a^+ [a, a^{+m}]_- \; + [a^+, a^{+m}]_- \, a \overset{2.}{=} m\, a^{+m} \; .$$

Solution 4.4.2 W.l.o.g.: $n > m$:

$$\begin{aligned} \langle n|m\rangle &\overset{(4.143)}{=} \frac{1}{\sqrt{n!}} \langle 0|\, a^n |\, m\rangle = \frac{1}{\sqrt{n!}} \langle 0|a^{n-m}\, a^m|m\rangle \\ &\overset{(4.140)}{=} \sqrt{\frac{m!}{n!}}\, \langle 0|a^{n-m}|0\rangle = 0 \\ \langle n|\, n\rangle \;\; &= \;\; \langle 0|\, 0\rangle = 1 \end{aligned}$$

Solution 4.4.3

$$\begin{aligned} \langle n|T|n\rangle &= \frac{1}{2m} \langle n|p^2|n\rangle \\ &= -\frac{1}{2m} \frac{\hbar\, m\omega}{2} \langle n|(a^2 - a\, a^+ - a^+ a + a^{+2})|n\rangle \\ &= \frac{\hbar\, \omega}{4} \langle n|(2a^+ a + 1)|n\rangle = \frac{\hbar\, \omega}{4} (2n+1) = \frac{1}{2} \hbar\, \omega \left(n + \frac{1}{2}\right) , \\ \langle n|V|n\rangle &= \frac{1}{2} m\omega^2 \langle n|q^2|n\rangle \\ &= \frac{1}{2} m\omega^2 \frac{\hbar}{2m\omega} \langle n|(a^2 + a\, a^+ \; + a^+ a + a^{+2})|n\rangle \\ &= \frac{1}{4} \hbar\, \omega \langle n|(2a^+ a + 1)|n\rangle = \frac{1}{4} \hbar\, \omega (2n+1) = \frac{1}{2} \hbar\, \omega \left(n + \frac{1}{2}\right) , \\ \Longleftrightarrow \;\; \langle n|T|n\rangle &= \langle n|V|n\rangle \; . \end{aligned}$$

Solution 4.4.4

1. Momentum-representation:

$$\widehat{p} \to p \; ; \quad \widehat{q} \to -\frac{\hbar}{i} \frac{d}{dp} \; .$$

Creation and annihilation operators in momentum-representation:

$$a = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}\left(-\frac{\hbar}{i}\frac{d}{dp}\right) + \frac{i}{\sqrt{m\omega}}p\right)$$
$$a^+ = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}\left(-\frac{\hbar}{i}\frac{d}{dp}\right) - \frac{i}{\sqrt{m\omega}}p\right) .$$

It follows with

$$y = \frac{p}{\sqrt{\hbar m\omega}} \quad \curvearrowright \quad \frac{d}{dp} = \frac{1}{\sqrt{\hbar m\omega}}\frac{d}{dy}$$

in the y-representation:

$$a = \frac{i}{\sqrt{2}}\left(\frac{d}{dy} + y\right) ; \quad a^+ = \frac{i}{\sqrt{2}}\left(\frac{d}{dy} - y\right) .$$

2. Let $|0\rangle$ be the vacuum state:

$$a|0\rangle = 0$$

and $\varphi_0(p) \equiv \langle p\,|0\rangle$ and $\varphi_0(y) \equiv \langle y\,|0\rangle$, respectively, the corresponding wave functions in the momentum and y-representation. From

$$\langle y\,|a\,|0\rangle = 0$$

we then have (principle of correspondence (3.252)):

$$\frac{i}{\sqrt{2}}\left(\frac{d}{dy} + y\right)\varphi_0(y) = 0 \quad \curvearrowright \quad \varphi_0(y) = c_0 \exp\left(-\frac{y^2}{2}\right) .$$

3. n-th energy-eigen state:

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(a^+\right)^n |0\rangle .$$

It follows therewith:

$$\varphi_n(y) = \langle y\,|n\rangle = \frac{1}{\sqrt{n!}}\langle y\,|\left(a^+\right)^n |0\rangle$$
$$= \frac{i^n}{\sqrt{2^n n!}}\left(\frac{d}{dy} - y\right)^n \varphi_0(y)$$

$$= \frac{c_0(-i)^n}{\sqrt{2^n n!}} \left(y - \frac{d}{dy}\right)^n \exp\left(-\frac{1}{2}y^2\right)$$
$$= c_0 \frac{(-i)^n}{\sqrt{2^n n!}} \exp\left(-\frac{1}{2}y^2\right) H_n(y) \; .$$

4.

$$a^+ |n\rangle = \sqrt{n+1}\, |n+1\rangle \; ; \quad a\, |n\rangle = \sqrt{n}\, |n-1\rangle \; .$$

Translation code:

$$\frac{i}{\sqrt{2}} \left(\frac{d}{dy} - y\right) \varphi_n(y) = \sqrt{n+1}\, \varphi_{n+1}(y)$$
$$\frac{i}{\sqrt{2}} \left(\frac{d}{dy} + y\right) \varphi_n(y) = \sqrt{n}\, \varphi_{n-1}(y) \; .$$

Subtraction:

$$-i\sqrt{2}\, y\, \varphi_n(y) = \sqrt{n+1}\, \varphi_{n+1}(y) - \sqrt{n}\, \varphi_{n-1}(y) \; .$$

Solution 4.4.5

1.

$$\left(\frac{1}{f(x)} \frac{d}{dx} f(x)\right) \varphi(x) = \varphi'(x) + \frac{f'(x)}{f(x)} \varphi(x) = \left(\frac{d}{dx} + \frac{f'(x)}{f(x)}\right) \varphi(x) \; ,$$
$\varphi(x)$ arbitrary $\implies$ q.e.d.

2.

$$\left(\frac{1}{f} \frac{d}{dx} f\right)^n = \frac{1}{f} \frac{d}{dx} f \frac{1}{f} \frac{d}{dx} f \cdots \frac{1}{f} \frac{d}{dx} f = \frac{1}{f} \frac{d^n}{dx^n} f \; .$$

3.

$$H_n(x) \overset{(4.163)}{=} (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \overset{2.}{=} (-1)^n \left[e^{x^2} \frac{d}{dx} e^{-x^2}\right]^n =$$
$$= (-1)^n \left[e^{\frac{x^2}{2}} e^{\frac{x^2}{2}} \frac{d}{dx} e^{-\frac{x^2}{2}} e^{-\frac{x^2}{2}}\right]^n$$
$$\overset{1.}{=} (-1)^n \left[e^{\frac{x^2}{2}} \left(\frac{d}{dx} - x\right) e^{-\frac{x^2}{2}}\right]^n$$

$$
\begin{aligned}
&= e^{\frac{x^2}{2}} \left(x - \frac{d}{dx}\right) e^{-\frac{x^2}{2}} e^{\frac{x^2}{2}} \left(x - \frac{d}{dx}\right) e^{-\frac{x^2}{2}} \dots e^{\frac{x^2}{2}} \left(x - \frac{d}{dx}\right) e^{-\frac{x^2}{2}} \\
&= e^{\frac{x^2}{2}} \left(x - \frac{d}{dx}\right)^n e^{-\frac{x^2}{2}} \overset{(4.160)}{=} H_n(x) \, .
\end{aligned}
$$

Solution 4.4.6 Hamilton operator:

$$
\begin{aligned}
H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 &= -\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \frac{1}{2} m\omega^2 q^2 \, , \\
\frac{d^2}{dq^2} &= \frac{m\omega}{\hbar} \frac{d^2}{dx^2} \\
\Longrightarrow \quad H &= \frac{1}{2} \hbar\, \omega \left(-\frac{d^2}{dx^2} + x^2\right) \, , \\
\frac{d}{dx} \varphi(x) &= \alpha \left(4x - 2x^3 + x\right) e^{-x^2/2} \, , \\
\frac{d^2}{dx^2} \varphi(x) &= \alpha \left(5 - 6x^2 - 5x^2 + 2x^4\right) e^{-x^2/2}
\end{aligned}
$$

$$
\begin{aligned}
\Longrightarrow \quad \left(-\frac{d^2}{dx^2} + x^2\right) \varphi(x) &= \alpha \left(-5 + 11x^2 - 2x^4 + 2x^4 - x^2\right) e^{-x^2/2} \\
&= 5\alpha \left(2x^2 - 1\right) e^{-x^2/2} = 5\varphi(x) \\
\Longrightarrow \quad H\, \varphi(x) &= \frac{5}{2} \hbar\, \omega\, \varphi(x) \, .
\end{aligned}
$$

$\varphi(x)$ is thus eigen-function with the eigen-value $(5/2)\, \hbar\, \omega$!

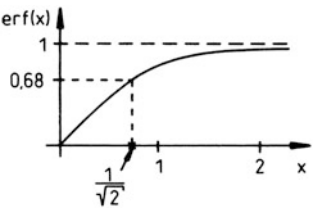
Solution 4.4.7 Ground state:

$$
\begin{aligned}
\varphi_0(x) &= c_0\, e^{-x^2/2} \, , \quad c_0 = \left(\frac{m\omega}{\hbar\, \pi}\right)^{1/4} \, , \\
E_0 &= \frac{1}{2} \hbar\, \omega \, .
\end{aligned}
$$

Classical turning points:

$$
\begin{aligned}
V(q_\pm) &\overset{!}{=} E_0 = \frac{1}{2} \hbar\, \omega \\
\Longleftrightarrow \quad \frac{1}{2} m\omega^2 q_\pm^2 = \frac{1}{2} \hbar\, \omega \quad &\Longleftrightarrow \quad q_\pm = \pm \sqrt{\frac{\hbar}{m\omega}} \quad \Longleftrightarrow \quad x_\pm = \pm 1 \, .
\end{aligned}
$$

Fig. A.16



Probability to find the particle in the *allowed region*:

$$w\,(\text{allowed}) = \int_{q-}^{q+} dq|\varphi_0(q)|^2 = \sqrt{\frac{\hbar}{m\omega}} \int_{-1}^{+1} dx|\varphi_0(x)|^2$$

$$= \frac{1}{\sqrt{\pi}} \int_{-1}^{+1} dx\, e^{-x^2} = \text{erf}\,(1) = 0.8427\,.$$

Error function (Fig. A.16):

$$\text{erf}\,(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt\,.$$

Not elementarily calculable, but available in tabulated form:

$$\text{erf}\,(0) = 0\,,$$
$$\text{erf}\,(\infty) = 1\,,$$
$$\text{erf}\,(-x) = -\,\text{erf}\,(x)\,.$$

Probability to find the particle outside the classical boundaries:

$$w\,(\text{forbidden}) = 1 - w\,(\text{allowed}) = 1 - \text{erf}\,(1) = 0.1573\,.$$

Probability **not at all** negligible!

Solution 4.4.8

1.

$$E_1 = \frac{3}{2}\hbar\,\omega\,; \quad E_0 = \frac{1}{2}\hbar\,\omega$$
$$\Longrightarrow \Delta E = E_1 - E_0 = 2\varepsilon = 7.2\,eV\,.$$

The amplitude A corresponds classically to the turning point, at which the total energy consists only of potential energy. It therefore holds classically:

$$E_0 = \frac{1}{2} m\omega^2 A^2 \stackrel{!}{=} \frac{1}{2} \hbar\,\omega$$

$$\Longrightarrow\ A = \sqrt{\frac{\hbar}{m\omega}} = \frac{\hbar}{\sqrt{2m\varepsilon}}\ .$$

One finds with the given numerical values:

$$A = 4.45 \cdot 10^{-3}\,\mathring{\mathrm{A}}\ .$$

2. The problem corresponds exactly to that of Exercise 4.4.7. We can therefore use:

$$\text{Normalized probability}\ \approx\ 0.1573\ .$$

Solution 4.4.9

1.

$$H_0(x) = \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{+\infty} dy\, e^{-y^2} = 1\ ,$$

$$H_1(x) = \frac{2}{\sqrt{\pi}} \int\limits_{-\infty}^{+\infty} dy\,(x + i\,y)\, e^{-y^2}$$

$$= \frac{2}{\sqrt{\pi}}\, x \int\limits_{-\infty}^{+\infty} dy\, e^{-y^2} = \qquad \text{(second integrand is odd as function of } y\text{)},$$

$$= 2x\ ,$$

$$H_2(x) = \frac{4}{\sqrt{\pi}} \int\limits_{-\infty}^{+\infty} dy\,(x + i\,y)^2\, e^{-y^2}$$

$$= \frac{4}{\sqrt{\pi}}\, x^2 \int\limits_{-\infty}^{+\infty} dy\, e^{-y^2} - \frac{4}{\sqrt{\pi}} \int\limits_{-\infty}^{+\infty} dy\, y^2\, e^{-y^2}\ .$$

After integration by parts:

$$\int\limits_{-\infty}^{+\infty} dy\, e^{-y^2} = \underbrace{y\, e^{-y^2}}_{=\,0}\Big|_{-\infty}^{+\infty} + 2 \int\limits_{-\infty}^{+\infty} dy\, y^2\, e^{-y^2}\ .$$

We use this for $H_2(x)$:

$$H_2(x) = \frac{4}{\sqrt{\pi}} \left(x^2 - \frac{1}{2}\right) \int_{-\infty}^{+\infty} dy\, e^{-y^2} = (2x)^2 - 2 \,.$$

2.

$$\begin{aligned}
\sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x) &= \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dy\, (x + i\,y)^n\, e^{-y^2} \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dy\, e^{-y^2} \sum_{n=0}^{\infty} \frac{(2tx + i\,2t\,y)^n}{n!} \\
&= \frac{e^{2tx}}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dy\, e^{-(y^2 - 2ity)} = \frac{e^{-t^2+2tx}}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dy\, e^{-(y-it)^2} \\
&= \frac{1}{\sqrt{\pi}}\, e^{-t^2+2tx} \int_{-\infty - it}^{+\infty - it} dz\, e^{-z^2} \,.
\end{aligned}$$

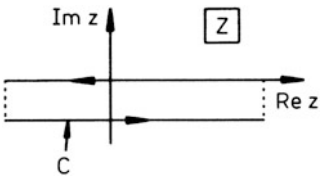
$\int_C dz\, e^{-z^2} = 0$, since no pole in the region enclosed by the path C (Fig. A.17).
The branches to the left and to the right are located at infinity, and therefore do not contribute! It remains:

$$0 = \int_{-\infty - it}^{+\infty - it} dz\, e^{-z^2} + \int_{+\infty}^{-\infty} dz\, e^{-z^2} \implies \int_{-\infty - it}^{+\infty - it} dz\, e^{-z^2} = \sqrt{\pi} \,.$$

It follows therewith what was to be proven:

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x) = e^{-t^2+2tx} \,.$$

Fig. A.17



Solution 4.4.10

$$\varphi_n(x) \overset{(4.174)}{=} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} (n!\,2^n)^{-\frac{1}{2}}\; e^{-\frac{x^2}{2}} H_n(x) \overset{!}{=} v_n(x)\, e^{-\frac{x^2}{2}}$$

$$\curvearrowright \quad v_n(x) \quad = \quad \alpha_n \cdot H_n(x) = \sum_{\mu=0,1}^{n} \gamma_\mu x^\mu \ .$$

It follows with $\eta = 2n + 1$ and the recursion formula (4.177):

$$\gamma_{\mu+2} = \frac{2\mu - 2n}{(\mu+2)\,(\mu+1)} \gamma_\mu \ . \tag{A.24}$$

It must therefore be:

$$H_n(x) = \alpha_n^{-1} \sum_{\mu=0,1}^{n} \gamma_\mu x^\mu$$

$$= \sum_{\mu=0,1}^{n} \widehat{\gamma}_\mu x^\mu \ .$$

Ansatz:

$$H_n(x) = \sum_{\nu=0}^{\langle \frac{n}{2} \rangle} \frac{(-1)^\nu n!}{\nu!\,(n-2\nu)!} (2x)^{n-2\nu}$$

$$k = n - 2\nu \ \curvearrowright \ \nu = \frac{n-k}{2}$$

$$n \text{ even } \curvearrowright \ k \text{ even } \curvearrowright \left\langle \frac{n}{2} \right\rangle = \frac{n}{2}$$

$$n \text{ odd } \curvearrowright \ k \text{ odd } \curvearrowright \left\langle \frac{n}{2} \right\rangle = \frac{n-1}{2}$$

$$\curvearrowright \ k_{\max} = n$$

$$k_{\min} = \begin{cases} 0, & \text{if } n \text{ even} \\ 1, & \text{if } n \text{ odd} \end{cases}$$

$$\curvearrowright \ H_n(x) = \sum_{k=0,1}^{n} \beta_k x^k$$

$$\begin{aligned}
\beta_k &= \frac{(-1)^{\frac{n-k}{2}}\, n!\, 2^k}{\left(\frac{n-k}{2}\right)!\, k!} \\
\beta_{k+2} &= \frac{(-1)^{\frac{n-k}{2}}\, n!\, 2^k}{\left(\frac{n-k}{2}\right)!\, k!} \cdot \frac{(-1)^1 \cdot 2^2 \cdot \frac{n-k}{2}}{(k+2)\,(k+1)} \\
&= \beta_k \frac{-2\,(n-k)}{(k+1)\,(k+2)} \\
&= \frac{2\,(k-n)}{(k+1)\,(k+2)} \beta_k \ .
\end{aligned}$$

That corresponds to the recursion formula (A.24). The above ansatz is thus correct.

Solution 4.4.11 The required eigen-functions $\overline{\varphi}_n(q)$ should vanish for $q < 0$, and for $q > 0$ should agree with the oscillator-eigen functions (4.159). The continuity condition at $q = 0$ is, however, satisfied only for the eigen-functions with odd parity, i.e., with odd indexes n. We already know therewith the complete solution:

Eigen-values:

$$\overline{E}_m = \hbar\,\omega \left(2m + 1 + \frac{1}{2}\right) = \hbar\,\omega \left(2m + \frac{3}{2}\right) \ ; \quad m = 0, 1, 2, \ldots$$

Eigen-functions:

$$\overline{\varphi}_m(q) = \begin{cases} 0 & \text{for } q < 0, \\ \sqrt{2}\,\varphi_{2m+1}(q) & \text{for } q > 0. \end{cases} \ ; \quad m = 0, 1, 2, \ldots$$

$\varphi_{2m+1}(q)$ as in (4.159) with $x = \sqrt{\frac{m\omega}{\hbar}}\, q$, and with the factor $\sqrt{2}$, to bring the normalization *'in order'*.

Solution 4.4.12

1.

$$q_{mn} \equiv \int_{-\infty}^{+\infty} dq\, \varphi_m(q)\, q\, \varphi_n(q) \ ; \qquad q_0 = \sqrt{\frac{\hbar}{m\omega}} \ , \qquad x = \frac{q}{q_0} \ .$$

Equation before (4.168):

$$\sqrt{2}\, x\, \varphi_n(x) = \sqrt{n+1}\, \varphi_{n+1}(x) + \sqrt{n}\, \varphi_{n-1}(x) \ ,$$

$$q_{mn} = q_0^2 \int_{-\infty}^{+\infty} dx\, \varphi_m(x)\, x\, \varphi_n(x) =$$

$$= \frac{q_0^2}{\sqrt{2}} \left[\sqrt{n+1} \int dx\, \varphi_m(x)\, \varphi_{n+1}(x) + \sqrt{n} \int dx\, \varphi_m(x)\, \varphi_{n-1}(x) \right]$$
$$= \frac{q_0}{\sqrt{2}} \left[\sqrt{n+1} \int dq\, \varphi_m(q)\, \varphi_{n+1}(q) + \sqrt{n} \int dq\, \varphi_m(q)\, \varphi_{n-1}(q) \right] .$$

The orthonormality relation for the eigen-functions $\varphi_n(q)$ (4.164) then yields:

$$q_{mn} = \sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n+1}\, \delta_{m\,n+1} + \sqrt{n}\, \delta_{m\,n-1} \right] .$$

We apply the above recursion formula twice in a row:

$$x^2 \varphi_n = \frac{1}{\sqrt{2}} \left[\sqrt{n+1}\, x\, \varphi_{n+1} + \sqrt{n}\, x\, \varphi_{n-1} \right] =$$
$$= \frac{1}{2} \left[\sqrt{(n+1)\,(n+2)}\, \varphi_{n+2} + (2n+1)\, \varphi_n + \sqrt{n(n-1)}\, \varphi_{n-2} \right] .$$

Analogously as above, we now calculate:

$$q_{mn}^2 =$$
$$= \int_{-\infty}^{+\infty} dq\, \varphi_m(q)\, q^2 \varphi_n(q)$$
$$= q_0^3 \frac{1}{2} \left[\sqrt{(n+1)\,(n+2)} \int_{-\infty}^{+\infty} dx\, \varphi_m(x)\, \varphi_{n+2}(x) \; + \right.$$
$$\left. + \; (2n+1) \int_{-\infty}^{+\infty} dx\, \varphi_m(x)\, \varphi_n(x) + \sqrt{n(n-1)} \int_{-\infty}^{+\infty} dx\, \varphi_m(x)\, \varphi_{n-2}(x) \right] ,$$
$$q_{mn}^2 = \frac{\hbar}{2m\omega} \left[\sqrt{(n+1)\,(n+2)}\, \delta_{m\,n+2} + (2n+1)\, \delta_{mn} + \sqrt{n(n-1)}\, \delta_{m\,n-2} \right] .$$

2. For the calculation of the matrix elements of the momentum we use the recursion formula before (4.169):

$$\frac{d}{dx} \varphi_n(x) = \sqrt{2n}\, \varphi_{n-1}(x) - x\, \varphi_n(x)$$
$$= \sqrt{2n}\, \varphi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\, \varphi_{n+1}(x) - \sqrt{\frac{n}{2}}\, \varphi_{n-1}(x)$$
$$= \frac{1}{\sqrt{2}} \left[\sqrt{n}\, \varphi_{n-1}(x) - \sqrt{n+1}\, \varphi_{n+1}(x) \right] .$$

It follows therewith:

$$\begin{aligned} p_{mn} &= \int dq\, \varphi_m(q)\, p\, \varphi_n(q) = \frac{\hbar}{i} \int dq\, \varphi_m(q)\, \frac{d}{dq}\, \varphi_n(q) \\ &= \frac{\hbar}{i} \int dx\, \varphi_m(x)\, \frac{d}{dx}\, \varphi_n(x) \\ &= \frac{\hbar}{i\sqrt{2}} \left[\sqrt{n} \int dx\, \varphi_m(x)\, \varphi_{n-1}(x) - \sqrt{n+1} \int dx\, \varphi_m(x)\, \varphi_{n+1}(x) \right] \\ \Longrightarrow\ p_{mn} &= -i \sqrt{\frac{1}{2}\, \hbar\, m\omega} \left[\sqrt{n}\, \delta_{m\,n-1} - \sqrt{n+1}\, \delta_{m\,n+1} \right] . \end{aligned}$$

We differentiate the above recursion formula once more:

$$\begin{aligned} &\frac{d^2}{dx^2}\, \varphi_n(x) = \\ &= \frac{1}{\sqrt{2}} \left[\sqrt{n}\, \frac{d}{dx}\, \varphi_{n-1}(x) - \sqrt{n+1}\, \frac{d}{dx}\, \varphi_{n+1}(x) \right] = \\ &= \frac{1}{2} \left[\sqrt{n(n-1)}\, \varphi_{n-2}(x) - (2n+1)\, \varphi_n(x) + \sqrt{(n+1)\,(n+2)}\, \varphi_{n+2}(x) \right] . \end{aligned}$$

We calculate therewith the following matrix elements:

$$\begin{aligned} p_{mn}^2 &= \int dq\, \varphi_m(q)\, p^2\, \varphi_n(q) = -\hbar^2 \int dq\, \varphi_m(q)\, \frac{d^2}{dq^2}\, \varphi_n(q) \\ &= -\frac{\hbar^2}{q_0} \int dx\, \varphi_m(x)\, \frac{d^2}{dx^2}\, \varphi_n(x) \\ &= -\frac{\hbar^2}{2q_0} \left[\sqrt{n(n-1)} \int dx\, \varphi_m(x)\, \varphi_{n-2}(x) - (2n+1) \int dx\, \varphi_m(x)\, \varphi_n(x) + \right. \\ &\qquad \left. + \sqrt{(n+1)\,(n+2)} \int dx\, \varphi_m(x)\, \varphi_{n+2}(x) \right] . \end{aligned}$$

It follows:

$$p_{mn}^2 = \frac{1}{2}\, \hbar\, m\omega \left[-\sqrt{n(n-1)}\, \delta_{m\,n-2} + (2n+1)\, \delta_{mn} - \sqrt{(n+1)\,(n+2)}\, \delta_{m\,n+2} \right] .$$

We further verify the matrix elements of the Hamilton operator:

$$H_{mn} = \frac{1}{2m}\, p_{mn}^2 + \frac{1}{2}\, m\omega^2\, q_{mn}^2 = \frac{1}{2}\, \hbar\, \omega\, (2n+1)\, \delta_{mn} \quad \text{q.e.d.}$$

Solution 4.4.13 According to (4.127) and (4.128) we can use:

$$q = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+)\,; \quad p = -i\sqrt{\frac{1}{2}\,\hbar\, m\omega}\;(a - a^+)\,.$$

This means:

$$q_{mn} = \sqrt{\frac{\hbar}{2m\omega}}\,\left(\langle m|a|n\rangle + \langle m|a^+|n\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\,\left(\sqrt{n}\,\delta_{m\,n-1} + \sqrt{n+1}\,\delta_{m\,n+1}\right)\,.$$

This is of course identical to the result of the preceding exercise; the derivation, though, is essentially simpler.

$$\hat{q} \equiv \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \\ & & & & 0 \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \ddots \\ & 0 & & \ddots & \ddots \end{pmatrix}\,.$$

Analogously, we find the matrix representation for the momentum operator:

$$p_{mn} = -i\sqrt{\frac{1}{2}\,\hbar\, m\omega}\,\left(\sqrt{n}\,\delta_{m\,n-1} - \sqrt{n+1}\,\delta_{m\,n+1}\right)\,,$$

$$\hat{p} = -i\sqrt{\frac{1}{2}\,\hbar\, m\omega}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \\ & & & & 0 \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & -\sqrt{3} & 0 & \ddots \\ & 0 & & & \end{pmatrix}\,,$$

$$\hat{q}\,\hat{p} = -i\,\frac{\hbar}{2}\begin{pmatrix} -1 & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & -1 & 0 & \sqrt{6} & 0 & \dots \\ -\sqrt{2} & 0 & -1 & 0 & \sqrt{12} & \dots \\ 0 & -\sqrt{6} & 0 & -1 & 0 & \dots \\ 0 & 0 & -\sqrt{12} & 0 & -1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}\,,$$

$$\hat{p}\,\hat{q} = -i\,\frac{\hbar}{2}\begin{pmatrix} 1 & 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 1 & 0 & \sqrt{6} & 0 & \dots \\ -\sqrt{2} & 0 & 1 & 0 & \sqrt{12} & \dots \\ 0 & -\sqrt{6} & 0 & 1 & 0 & \dots \\ 0 & 0 & -\sqrt{12} & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} .$$

One recognizes:

$$[\hat{q},\,\hat{p}]_- = i\,\hbar\begin{pmatrix} 1 & & & & \\ & 1 & & 0 & \\ & & \ddots & & \\ & & & 1 & \\ & 0 & & & \ddots \end{pmatrix} \quad \text{q.e.d.}$$

Solution 4.4.14 Contribution to the potential by the constant electric field:

$$V_1(q) = -\hat{q}\,E\,q \qquad (E\text{: electric field strength}) .$$

Hamilton operator:

$$H = \frac{p^2}{2m} + \frac{1}{2}\,m\omega^2 q^2 - \hat{q}\,E\,q .$$

Transformation:

$$\begin{aligned} H &= \frac{p^2}{2m} + \frac{1}{2}\,m\omega^2\left(q^2 - 2\frac{\hat{q}\,E}{m\omega^2}\,q\right) \\ &= \frac{p^2}{2m} + \frac{1}{2}\,m\omega^2\left(q - \frac{\hat{q}\,E}{m\omega^2}\right)^2 - \frac{\hat{q}^2E^2}{2m\omega^2} . \end{aligned}$$

Substitution of the variable:

$$y = q - \frac{\hat{q}\,E}{m\omega^2} \equiv q - y_0 .$$

Because of

$$\frac{\hbar}{i}\,\frac{d}{dq} = \frac{\hbar}{i}\,\frac{d}{dy}$$

also p and the *new* variable y are canonically conjugate!

Hamilton operator:

$$H = \widehat{H} - \frac{\hat{q}^2 E^2}{2m\omega^2} \ ,$$
$$\widehat{H} = \frac{p^2}{2m} + \frac{1}{2}\, m\omega^2 y^2 \ .$$

Eigen-value problem for $\widehat{H}$ is known:

$$\widehat{H}\,\varphi_n(y) = \widehat{E}_n\,\varphi_n(y) \ ,$$
$$\widehat{E}_n = \hbar\,\omega\,\left(n + \frac{1}{2}\right); \quad n = 0, 1, 2, \dots \ ,$$
$$\varphi_n(y) = \left(\frac{m\omega}{\hbar\,\pi}\right)^{1/4} (n!\,2^n)^{-1/2}\, e^{-y^2/2q_0^2}\, H_n\left(\frac{y}{q_0}\right) \ ; \quad q_0 = \sqrt{\frac{\hbar}{m\omega}} \ .$$

Solution to H:

$$H\,\varphi_n(y) = E_n\,\varphi_n(y)$$
$$\iff \widehat{H}\,\varphi_n(y) = \left(E_n + \frac{\hat{q}^2 E^2}{2m\omega^2}\right)\varphi_n(y) \stackrel{!}{=} \widehat{E}_n\,\varphi_n(y) \ .$$

$\Longrightarrow$ Eigen-values:

$$E_n = \hbar\,\omega\,\left(n + \frac{1}{2}\right) - \frac{\hat{q}^2 E^2}{2m\omega^2} \ .$$

Eigen-functions:

$$\varphi_n(q) = \left(\frac{m\omega}{\hbar\,\pi}\right)^{\frac{1}{4}} (n!\,2^n)^{-\frac{1}{2}}\, \exp\left(-\frac{(q-y_0)^2}{2q_0^2}\right) H_n\left(\frac{q-y_0}{q_0}\right) \ .$$

Solution 4.4.15

1. We have already derived in Exercise 3.5.6:

$$T\,q\,T^+ = q - y_0\,\mathbb{1} \qquad \text{(translation!)}.$$

From that it follows, if one applies from the right T:

$$T\,q\,T^+\,T = T\,q = q\,T - y_0\,T \implies [q, T]_- = y_0\,T \ .$$

2.

$$\overline{H} = T\,H\,T^+ = H\,T\,T^+ - [H, T]_-\,T^+ = H - [H, T]_-\,T^+ \ .$$

We calculate the commutator:

$$[H,T]_- = \frac{1}{2m}\,[p^2,T]_- + \frac{1}{2}\,m\omega^2[q^2,T]_- - \hat{q}\,E[q,T]_- \ .$$

The first commutator vanishes because T is a function of p. It thus remains:

$$\begin{aligned}[H,T]_- &= \frac{1}{2}\,m\omega^2\left(q[q,T]_- + [q,T]_-\,q\right) - \hat{q}\,E[q,T]_- \\ &\overset{1.}{=} \frac{1}{2}\,m\omega^2\,y_0\,(q\,T + T\,q) - \hat{q}\,E\,y_0 T \ .\end{aligned}$$

From that it follows after multiplication by T^+:

$$\begin{aligned}[H,T]_-\,T^+ &= \frac{1}{2}\,m\omega^2\,y_0\,(q + T\,q\,T^+) - \hat{q}\,E\,y_0 \\ &= -\frac{1}{2}\,m\omega^2\,y_0^2 - \hat{q}\,E\,y_0 + m\omega^2\,y_0\,q \\ &= -\frac{1}{2}\,\frac{\hat{q}^2\,E^2}{m\omega^2} + \frac{\hat{q}^2\,E^2}{m\omega^2} - \hat{q}\,E\,q = \frac{1}{2}\,\frac{\hat{q}^2\,E^2}{m\omega^2} - \hat{q}\,E\,q \\ \Longrightarrow\ \overline{H} &= \frac{p^2}{2m} + \frac{1}{2}\,m\omega^2\,q^2 - \frac{1}{2}\,\frac{\hat{q}^2\,E^2}{m\omega^2} \ .\end{aligned}$$

The unitary transformation of the Hamilton operator, mediated by $T\,(y_0)$, achieves the same as the substitution of the position operator ($q \to y = q - y_0$) in the solution to Exercise 4.4.14. The substitution is therefore in any case justified, since unitary transformations *do not change the physics*. One comes to completely equivalent statements!

Solution 4.4.16 We write

$$\Pi = \exp\left[i\,\pi\left(\widehat{A} - \frac{1}{2}\right)\right]$$

with

$$\widehat{A} \equiv \frac{\hat{p}^2}{2\alpha} + \frac{\alpha}{2\hbar^2}\,\hat{q}^2 \ .$$

We set

$$\omega = \frac{1}{\hbar}$$

having then formally the Hamiltonian of the linear harmonic oscillator (*'mass'* $= \alpha$):

$$\widehat{A} = \frac{\hat{p}^2}{2\alpha} + \frac{1}{2}\,\alpha\,\omega^2\,\hat{q}^2\ .$$

We have already solved the corresponding eigen-value problem :

$$\widehat{A}\,\varphi_n(q) = \hbar\,\omega\,\left(n + \frac{1}{2}\right)\,\varphi_n(q) = \left(n + \frac{1}{2}\right)\,\varphi_n(q)\ .$$

$\varphi_n(q)$ as in (4.159), only m replaced by α!

The eigen-functions of the harmonic oscillator represent a complete system of functions. Any arbitrary wave function $\psi(q)$ can therefore expanded in them:

$$\begin{aligned}
\psi(q) &= \sum_n a_n\,\varphi_n(q) \\
\Longrightarrow\quad \Pi\,\psi(q) &= \sum_n a_n\,\exp\left[i\,\pi\,\left(\widehat{A} - \frac{1}{2}\right)\right]\,\varphi_n(q) \\
&= \sum_n a_n\,\exp\left[i\,\pi\,\left(n + \frac{1}{2} - \frac{1}{2}\right)\right]\,\varphi_n(q) \\
&= \sum_n a_n\,(-1)^n\,\varphi_n(q) \overset{(4.161)}{=} \sum_n a_n\,\varphi_n(-q) = \psi(-q)\ .
\end{aligned}$$

Since ψ was chosen arbitrarily, Π must be the parity operator, if it can still be shown that $\Pi = \Pi^+ = \Pi^{-1}$ (4.16). $\widehat{A}$ is Hermitian and therefore Π unitary, i.e., $\Pi^+ = \Pi^{-1}$. – Because of $e^{i\pi n} = e^{-i\pi n}$ Π^+ has, in addition, for all $\psi(q)$ of the Hilbert space the same impact as Π:

$$\Pi^+\,\psi(q) = \psi(-q)\ .$$

We can conclude therewith that Π is also Hermitian: $\Pi = \Pi^+ = \Pi^{-1}$.

Solution 4.4.17

1. According to Eq. (2.39) in Vol. 2:

$$H = \frac{1}{2m}\,\left(\mathbf{p} + e\,\mathbf{A}(\mathbf{r})\right)^2\ .$$

2. With

$$\mathbf{A}(\mathbf{r}) = (0,\,Bx,\,0)$$

we obviously have simultaneously:

$$\operatorname{div}\mathbf{A} = 0 \;\text{ and }\; \operatorname{curl}\mathbf{A} = B\,\mathbf{e}_z \;.$$

3.

$$\widehat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} + e\,\widehat{\mathbf{A}}\right)^2 = \frac{1}{2m}\left(\hat{\mathbf{p}}^2 + e^2\,\widehat{\mathbf{A}}^2 + e\;\hat{\mathbf{p}}\cdot\widehat{\mathbf{A}} + e\;\widehat{\mathbf{A}}\cdot\hat{\mathbf{p}}\right) \;.$$

Position representation:

$$\hat{\mathbf{p}}\cdot\widehat{\mathbf{A}}\,\psi(\mathbf{r}) = \frac{\hbar}{i}\,(\operatorname{div}\mathbf{A})\,\psi + \frac{\hbar}{i}\,(\nabla\psi)\cdot\mathbf{A} = \frac{\hbar}{i}\,\mathbf{A}\cdot(\nabla\psi) = \widehat{\mathbf{A}}\cdot\hat{\mathbf{p}}\,\psi(\mathbf{r}) \;.$$

Only because of the Coulomb gauge, the operators $\hat{\mathbf{p}}$ and $\widehat{\mathbf{A}}$ commute:

$$H = \frac{1}{2m}\left(\hat{\mathbf{p}}^2 + e^2\,\widehat{\mathbf{A}}^2 + 2e\,\widehat{\mathbf{A}}\cdot\hat{\mathbf{p}}\right) = \frac{1}{2m}\left[\hat{p}_x^2 + \hat{p}_z^2 + (\hat{p}_y + e\,B\,\widehat{x})^2\right] \;.$$

Position representation:

$$p_x = \frac{\hbar}{i}\,\frac{d}{dx}\;;\quad p_y = \frac{\hbar}{i}\,\frac{d}{dy}\;;\quad p_z = \frac{\hbar}{i}\,\frac{d}{dz}\;.$$

Ansatz:

$$\begin{aligned}
&\psi(x,y,z) = e^{ik_z z}\,e^{ik_y y}\,\varphi(x)\;,\\
&H\,\psi = E\,\psi\\
\Longrightarrow\;\; &\frac{1}{2m}\left[-\hbar^2\,\frac{d^2}{dx^2} + \hbar^2\,k_z^2 + (\hbar\,k_y + e\,Bx)^2\right]\psi = E\,\psi\;.
\end{aligned}$$

This is equivalent to:

$$\left[-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2} + \frac{1}{2m}\,(\hbar\,k_y + e\,Bx)^2\right]\varphi(x) = \left(E - \frac{\hbar^2\,k_z^2}{2m}\right)\varphi(x)\;.$$

Substitution:

$$\begin{aligned}
\omega_{\mathrm{c}} &= \frac{e\,B}{m} \qquad \textit{cyclotron frequency}\,,\\
q &= x + \frac{\hbar\,k_y}{m\omega_{\mathrm{c}}} \;\Longrightarrow\; \frac{d^2}{dx^2} = \frac{d^2}{dq^2}\;.
\end{aligned}$$

It remains to be solved:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}+\frac{1}{2}m\omega_c^2 q^2\right)\varphi(q)=\widehat{E}\,\varphi(q)\;;\quad \widehat{E}=E-\frac{\hbar^2 k_z^2}{2m}\;.$$

This is the eigen-value equation of the linear harmonic oscillator!

4. Eigen-energies:

$$E_n(k_z)=\hbar\,\omega_c\left(n+\frac{1}{2}\right)+\frac{\hbar^2 k_z^2}{2m}\;.$$

The motion of the electron is therefore quantized in the plane perpendicular to the field (*'Landau levels'*), but undisturbed in the direction parallel to the field.

Eigen functions:

$$\psi_n(\mathbf{r})=e^{ik_z z}\,e^{k_y y}\,\varphi_n(q)$$

($\varphi_n(q)$ as in (4.159)).

Solution 4.4.18

1. According to Eq. (2.39) in Vol. 2:

$$H=\frac{1}{2m}\left(\mathbf{p}+e\,\mathbf{A}(\mathbf{r})\right)^2+\frac{1}{2}m\omega^2 z^2\;.$$

Coulomb gauge:

$$\begin{aligned}&\operatorname{div}\mathbf{A}=0\quad;\qquad \operatorname{curl}\mathbf{A}=\mathbf{B}=B\,\mathbf{e}_z\\ &\Longrightarrow\;\mathbf{A}(\mathbf{r})=(0,Bx,0)\;.\end{aligned}$$

It follows therewith, analogously to solution 4.4.17:

$$H=\frac{1}{2m}\left[p_x^2+p_z^2+(p_y+e\,Bx)^2\right]+\frac{1}{2}m\omega^2 z^2\;.$$

2.

$$H\,\psi=E\,\psi\;.$$

Convenient separation ansatz:

$$\psi(x,y,z)=e^{ik_y y}\,\lambda(x)\,\varphi(z)\;.$$

After insertion, it is left:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)+(\hbar\,k_y+e\,Bx)^2+\frac{1}{2}\,m\omega^2 z^2\right]\psi(x,y,z)=E\,\psi(x,y,z)\;.$$

We still rearrange a bit:

$$\left[-\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial x^2}+(\hbar\,k_y+e\,Bx)^2\right]\lambda(x)\,\varphi(z)+\left[-\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial z^2}+\frac{1}{2}\,m\omega^2 z^2\right]\lambda(x)\,\varphi(z)$$
$$=E\,\lambda(x)\,\varphi(z)\;.$$

After division by $\lambda\,\varphi$,

$$\frac{1}{\lambda(x)}\left[-\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial x^2}+(\hbar\,k_y+e\,Bx)^2\right]\lambda(x)+$$
$$+\frac{1}{\varphi(z)}\left[-\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial z^2}+\frac{1}{2}\,m\omega^2 z^2\right]\varphi(z)=E\;,$$

The first summand on the left-hand side of the equation depends only on x, and the second only on z. The sum of these two terms can then be constant, only if each summand by itself is constant:

$$\left[-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2}+(\hbar\,k_y+e\,Bx)^2\right]\lambda(x)=D\,\lambda(x)\;,$$
$$\left[-\frac{\hbar^2}{2m}\,\frac{d^2}{dz^2}+\frac{1}{2}\,m\omega^2 z^2\right]\varphi(z)=\widehat{E}\,\varphi(z)\;;\quad\widehat{E}=E-D\;.$$

In the first differential equation we make the substitution, already used in the solution of Exercise 4.4.17,

$$\omega_c=\frac{e\,B}{m}\;;\quad q=x+\frac{\hbar\,k_y}{m\omega_c}\;.$$

and have then, in both cases, to solve the eigen-value-problem of the linear harmonic oscillator:

$$\left[-\frac{\hbar^2}{2m}\,\frac{d^2}{dq^2}+\frac{1}{2}\,m\omega_c^2\,q^2\right]\lambda(q)=D\,\lambda(q)\;.$$

3. Solutions are known:

$$D_n = \hbar\,\omega_c\left(n+\frac{1}{2}\right)\;; \qquad n = 0,1,2,\ldots$$

$$\widehat{E}_p = \hbar\,\omega\left(p+\frac{1}{2}\right)\;; \qquad p = 0,1,2,\ldots$$

$\Longrightarrow$ Eigen-values:

$$E_{p,n} = \hbar\,\omega\left(p+\frac{1}{2}\right) + \hbar\,\omega_c\left(n+\frac{1}{2}\right)\;.$$

Eigen-functions:

$$\begin{aligned}
\psi_{p,n}(\mathbf{r}) &= e^{ik_y y}\,\lambda_n(x)\,\varphi_p(z)\;,\\
\lambda_n(x) &= \left(\frac{m\omega_c}{\hbar\,\pi}\right)^{\frac{1}{4}}(n!\,2^n)^{-\frac{1}{2}}\,\exp\left[-\frac{m\omega_c}{2\hbar}\left(x+\frac{\hbar\,k_y}{m\omega_c}\right)^2\right]\cdot\\
&\quad\cdot\; H_n\left[\sqrt{\frac{m\omega_c}{\hbar}}\left(x+\frac{\hbar\,k_y}{m\omega_c}\right)\right]\;,\\
\varphi_p(z) &= \left(\frac{m\omega}{\hbar\,\pi}\right)^{\frac{1}{4}}(p!\,2^p)^{-\frac{1}{2}}\,\exp\left(-\frac{m\omega}{2\hbar}\,z^2\right)H_p\left(\sqrt{\frac{m\omega}{\hbar}}\,z\right)\;.
\end{aligned}$$

Solution 4.4.19

1.

$$\begin{aligned}
&\psi(q,0) = \sum_n \alpha_n\,\varphi_n(q)\\
&\Longrightarrow\quad \alpha_n = \int_{-\infty}^{+\infty} dq\,\varphi_n^*(q)\,\psi(q,0)\;,\\
&\alpha_n = \left(\frac{m\omega}{\hbar\,\pi}\right)^{\frac{1}{2}}(n!\,2^n)^{-1/2}\int_{-\infty}^{+\infty} dq\,e^{-q^2/2q_0^2}\,H_n\left(\frac{q}{q_0}\right)e^{-(q-\overline{q})^2/2q_0^2}\;,\\
&q_0 = \sqrt{\frac{\hbar}{m\omega}}\;;\quad x = \frac{q}{q_0}\\
&\Longrightarrow\quad \alpha_n = \frac{1}{\sqrt{\pi}}(n!\,2^n)^{-1/2}\,e^{-\overline{q}^2/4q_0^2}\int_{-\infty}^{+\infty} dx\,e^{-\left(x-\frac{\overline{q}}{2q_0}\right)^2}H_n(x)\;.
\end{aligned}$$

With the given integral formula we then have:

$$\alpha_n = \frac{\left(\frac{\overline{q}}{q_0}\right)^n \exp\left(-\frac{\overline{q}^2}{4q_0^2}\right)}{\sqrt{n!\,2^n}} \,.$$

2.

$$\psi(q,t) = e^{-\frac{i}{\hbar}Ht}\,\psi(q,0) = \sum_n \alpha_n\, e^{-\frac{i}{\hbar}Ht}\,\varphi_n(q) = \sum_n \alpha_n\, e^{-i\omega\left(n+\frac{1}{2}\right)t}\,\varphi_n(q) \,.$$

Insertion of α_n from part 1.:

$$\begin{aligned}
\psi(q,t) &= \left(\frac{m\omega}{\hbar\,\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{\overline{q}^2}{4q_0^2} - \frac{q^2}{2q_0^2} - \frac{i}{2}\,\omega t\right] X \,, \\
X &= \sum_n e^{-i\omega n t}\, H_n\left(\frac{q}{q_0}\right)\, (n!\,2^n)^{-1} \left(\frac{\overline{q}}{q_0}\right)^n \\
&= \sum_n \frac{H_n\left(\frac{q}{q_0}\right)}{n!} \left(e^{-i\omega t}\,\frac{\overline{q}}{2q_0}\right)^n \,.
\end{aligned}$$

We now apply the generating function from part 2. in Exercise 4.4.9:

$$X = \exp\left[-e^{-2i\omega t}\,\frac{\overline{q}^2}{4q_0^2} + 2\,\frac{q}{q_0}\,e^{-i\omega t}\,\frac{\overline{q}}{2q_0}\right] \,.$$

With Euler's formula

$$\begin{aligned}
e^{-2i\omega t} &= \cos 2\omega t - i \sin 2\omega t \,, \\
e^{-i\omega t} &= \cos \omega t - i \sin \omega t
\end{aligned}$$

it follows then:

$$\begin{aligned}
\psi(q,t) &= \left(\frac{m\omega}{\hbar\,\pi}\right)^{\frac{1}{4}} \exp(B(q,t) - i\,A(q,t)) \,, \\
A(q,t) &= \frac{1}{2}\,\omega t + \frac{q\,\overline{q}}{q_0^2} \sin \omega t - \frac{\overline{q}^2}{4q_0^2} \sin 2\omega t \,, \\
B(q,t) &= -\frac{\overline{q}^2}{4q_0^2} - \frac{q^2}{2q_0^2} - \cos 2\omega t\,\frac{\overline{q}^2}{4q_0^2} + \frac{q\,\overline{q}}{q_0^2} \cos \omega t \,.
\end{aligned}$$

$B(q,t)$ can be shortened by the addition theorem

$$\cos 2\omega t = \cos^2 \omega t - \sin^2 \omega t$$

to

$$B(q,t) = -\frac{1}{2q_0^2}\,(q - \overline{q}\cos\omega t)^2 \ .$$

3.

$$\begin{aligned} |\psi(q,t)|^2 &= \sqrt{\frac{m\omega}{\hbar\pi}}\exp\left[-\frac{m\omega}{\hbar}(q-\overline{q}\cos\omega t)^2\right] \\ &= \frac{1}{\sqrt{\pi}\,\Delta b}\exp\left[-\frac{(q-\overline{q}\cos\omega t)^2}{deltab^2}\right] . \end{aligned}$$

That is the Gaussian wave packet with the time-**in**dependent width

$$\Delta b(t) \equiv \Delta b = \sqrt{\frac{\hbar}{m\omega}} \ .$$

Hence, the wave packet does **not** diffluence. Compare the result with the behavior of the Gaussian wave packet for the free particle in (2.64) and (2.65), respectively!

4. The calculation of $\langle q\rangle_t$ and Δq_t corresponds to that in the solution of Exercise 2.2.7. We can directly adopt:

$$\begin{aligned} \langle q\rangle_t &= \overline{q}\cos\omega t \ , \\ \Delta q_t &= \frac{1}{\sqrt{2}}\,\Delta b = \sqrt{\frac{\hbar}{2m\omega}} \ . \end{aligned}$$

5. Probability:

$$\begin{aligned} w_n &= |\langle n|\psi(q,t)\rangle|^2 = \left|\left\langle n\left|e^{-\frac{i}{\hbar}Ht}\right|\psi(q,0)\right\rangle\right|^2 \\ &= \left|e^{-i\omega\left(n+\frac{1}{2}\right)t}\,\langle n|\psi(q,0)\rangle\right|^2 = \left|\langle n|\psi(q,0)\rangle\right|^2 = |\alpha_n|^2 \\ \Longrightarrow\quad w_n &= \frac{1}{n!}\left(\frac{\overline{q}}{\sqrt{2}q_0}\right)^{2n} e^{-\overline{q}^2/2q_0^2} \ . \end{aligned}$$

Solution 4.4.20

1. According to (3.149):

$$\langle H\rangle = \frac{\mathrm{Tr}(\rho H)}{\mathrm{Tr}\rho} \ .$$

The denominator normalizes the density matrix. The trace is independent of the basis which is used for the evaluation. Here it is recommendable, of course, to use the eigen-states $|n\rangle$ of the linear harmonic oscillator:

$$\langle H\rangle = \frac{\sum_n \langle n\,|e^{-\beta H} H|\,n\rangle}{\sum_n \langle n\,|e^{-\beta H}|\,n\rangle}\ ,$$

$$\beta \equiv \frac{1}{k_B T}\ .$$

It is then to be evaluated:

$$\begin{aligned}
\langle H\rangle &= \frac{\sum_n \hbar\,\omega\left(n+\frac{1}{2}\right)\exp\left[-\beta\,\hbar\,\omega\left(n+\frac{1}{2}\right)\right]}{\sum_n \exp\left[-\beta\,\hbar\,\omega\left(n+\frac{1}{2}\right)\right]} \\
&= -\frac{\partial}{\partial\beta}\ln\left\{\sum_n \exp\left[-\beta\,\hbar\,\omega\left(n+\frac{1}{2}\right)\right]\right\}\ , \\
\sum_{n=0}^{\infty} &\exp\left[-\beta\,\hbar\,\omega\left(n+\frac{1}{2}\right)\right] = \exp\left(-\beta\frac{\hbar\,\omega}{2}\right)\sum_{n=0}^{\infty}[\exp(-\beta\,\hbar\,\omega)]^n \\
&= \exp\left(-\beta\frac{\hbar\,\omega}{2}\right)\frac{1}{1-e^{-\beta\hbar\omega}} \\
\Longrightarrow\quad \langle H\rangle &= \frac{1}{2}\hbar\,\omega + \frac{\frac{\partial}{\partial\beta}\left(1-e^{-\beta\hbar\omega}\right)}{1-e^{-\beta\hbar\omega}} \\
\Longrightarrow\quad \langle H\rangle &= \frac{1}{2}\hbar\,\omega + \frac{\hbar\,\omega}{e^{\beta\hbar\omega}-1}\ .
\end{aligned}$$

One should compare the result with Planck's formula (1.28)! The difference lies only in the zero-point energy!

2. According to (3.151) we have to simply calculate:

$$w(E_n) = \langle n|\frac{\rho}{\mathrm{Tr}\rho}|n\rangle = \frac{\exp\left[-\beta\,\hbar\,\omega\left(n+\frac{1}{2}\right)\right]}{\sum_n \exp\left[-\beta\,\hbar\,\omega\left(n+\frac{1}{2}\right)\right]}\ .$$

With the intermediate result of part 1.:

$$\begin{aligned}
w(E_n) &= \exp(-\beta\,\hbar\,\omega\,n)\,[1-\exp(-\beta\,\hbar\,\omega)]\ , \\
&\qquad T\to 0 \iff \beta\to\infty \\
\Longrightarrow\quad w(E_0) &= 1\ ,\quad w(E_n) = 0 \text{ for } n>0\ .
\end{aligned}$$

Solution 4.4.21

$$I_n \equiv \int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} H_n(x) = \sqrt{\pi}(2x_0)^n \ .$$

Proof by complete induction!

- $\underline{n = 1}$

$$\begin{aligned} I_1 &\overset{(4.164)}{=} -\int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} e^{x^2} \frac{d}{dx} e^{-x^2} \\ &= +2 \int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} e^{x^2} x e^{-x^2} \\ &= +2 \int_{-\infty}^{+\infty} dy\, e^{-y^2} (y + x_0) \\ &= 0 + 2x_0 \int_{-\infty}^{+\infty} dy\, e^{-y^2} \\ &= \sqrt{\pi}(2x_0) \ . \end{aligned}$$

- $\underline{n \implies n+1}$

We have to show:

$$I_{n+1} \overset{!}{=} 2x_0 I_n$$

$$\begin{aligned} I_{n+1} &= \int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} H_{n+1}(x) \\ &\overset{(4.169)}{=} 2 \int_{-\infty}^{+\infty} dx\, x\, e^{-(x-x_0)^2} H_n(x) - 2n \int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} H_{n-1}(x) \\ &= \int_{-\infty}^{+\infty} dx \left(\left(-\frac{d}{dx} + 2x_0 \right) e^{-(x-x_0)^2} \right) H_n(x) - 2n I_{n-1} \end{aligned}$$

$$
\begin{aligned}
&= \underbrace{-e^{-(x-x_0)^2} H_n(x)\Big|_{-\infty}^{+\infty}}_{=0} + \int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} \left(\frac{d}{dx} H_n(x)\right) \\
&\qquad +2x_0 I_n - 2nI_{n-1} \\
&\overset{(4.170)}{=} \int_{-\infty}^{+\infty} dx\, e^{-(x-x_0)^2} \left(2n\, H_{n-1}(x)\right) + 2x_0 I_n - 2nI_{n-1} \\
&= 2nI_{n-1} + +2x_0 I_n - 2nI_{n-1} \\
&= 2x_0 I_n \qquad\qquad \text{q.e.d.}
\end{aligned}
$$

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