

# Chapter 3

## More on the Schrödinger Equation



We first examine some general properties of the Schrödinger equation. Among other topics, the concept of *vector space* emerges—the solutions of the Schrödinger equation form such a space. In the Schrödinger equation, operators occur. We see that the order of the operators plays a role, provided that they do not commute.

In Chap. 1, we introduced the Schrödinger equation (SEq)

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) + V(\mathbf{r}, t) \Psi(\mathbf{r}, t). \quad (3.1)$$

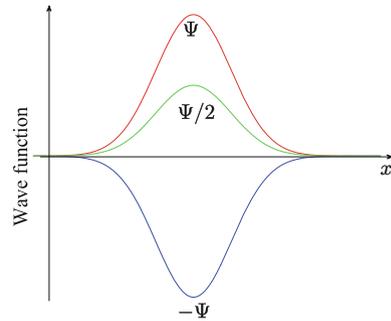
For our considerations it is *the* basic differential equation of quantum mechanics. In view of its central role, we want to examine in the following which properties the SEq has and which consequences follow from those properties. By separating out the time, one can obtain from (3.1) the *stationary Schrödinger equation* (also known as the time-independent Schrödinger equation), which for us is the workhorse of quantum mechanics. Finally, we make a few preliminary comments on operators, which in quantum mechanics are identified with measurable quantities.

### 3.1 Properties of the Schrödinger Equation

The SEq has several immediately recognizable features which model important physical properties and imply certain consequences. For example, one sees immediately that  $\Psi(\mathbf{r}, t)$  *must* be complex if the potential  $V$  is real (we will restrict ourselves to this case; the reason will be discussed later). Certain features are treated here only provisionally, while more detailed treatments follow in subsequent chapters. Some basic facts about differential equations are summarized in Appendix E, Vol. 1.

1. The SEq is *linear* in  $\Psi$ . If one has found two solutions  $\Psi_1$  and  $\Psi_2$ , then any linear combination  $c\Psi_1 + d\Psi_2$  is also a solution (with  $c, d \in \mathbb{C}$ ). This means that one can superimpose the solutions - the *superposition principle* holds. This

**Fig. 3.1** Schematic representation of three physically-equivalent wave functions  $\Psi(x)$ ,  $\frac{1}{2}\Psi(x)$ ,  $-\Psi(x)$



principle, known e.g. from the description of classical waves, has far-reaching consequences in quantum mechanics. Properties of the microscopic world which for our everyday understanding are very ‘bizarre’ are largely due to the seemingly trivial fact of linearity. Incidentally, due to this linearity, the total wave functions  $\Psi$  and  $c\Psi$  are physically equivalent, or to be more precise, they *must* be physically equivalent; see Fig. 3.1.

Being a linear equation, the SEq always has the solution  $\Psi \equiv 0$ , the so-called *trivial solution*. This solution does not describe a physical state, as one can for example add arbitrary multiples of it to any other state without changing anything physically. In other words, if it turns out that the state of a physical system is described by the trivial solution, then we know that this state does not exist.

2. The SEq is a differential equation of *first order in time*. This means that for a given *initial condition*  $\Psi(\mathbf{r}, t = 0)$ , the wave function  $\Psi(\mathbf{r}, t)$  is determined for *all times* (greater and less than zero). In other words, in the time evolution of  $\Psi(\mathbf{r}, t)$ , there are no stochastic or random elements — by specifying  $\Psi(\mathbf{r}, t = 0)$ , one uniquely defines the wave function for all past and future times.
3. The SEq is a differential equation of *second order in space*. To describe a specific given physical situation, the solution must satisfy certain *boundary conditions*.
4. The SEq determines, as we shall see below, which results are generally possible, but not which result will be realized in an actual measurement. This information must therefore come from somewhere else.<sup>1</sup>

The ability to form superpositions is a fundamental property of all elements of a *vector space*  $\mathcal{V}$ . In fact, it can easily be shown that the solutions of the SEq span a vector space over the complex numbers—see the definition in Appendix G, Vol. 1. Thus, we have a similar situation as for the polarization: The states of a system are described by elements of a vector space, in which the superposition principle applies. The dimensions of the spaces may be different—it is 2 in the case of polarization, while the dimension of the solution space of the SEq is unknown to us yet. But at least we have found with  $\mathcal{V}$  a structure which is common to both the approaches of Chaps. 1 and 2.

<sup>1</sup>One can summarize the difference between classical mechanics and quantum mechanics in a bold and simple way as follows: Classical mechanics describes the time evolution of the *factual*, quantum mechanics (i.e. the SEq) describes the time evolution of the *possible*.

Things are different for the pair of concepts ‘determinism—probability’. In this regard, our two approaches to quantum mechanics (still) do not match. Probabilities which we *had* to introduce in the algebraic approach to the transition from classical mechanics  $\rightarrow$  quantum mechanics do not appear in the SEq. On the contrary, the SEq is a deterministic equation whose solutions are uniquely determined for all times, given the initial conditions. Hence, the apparent randomness of quantum mechanics (e.g. in radioactive decay) is *not* hidden in the SEq.

As we will see in the next chapters, chance comes into play through the wavefunction. We emphasize once again that the wavefunction as a solution of the SEq has *no direct, intuitive meaning* in the ‘everyday world’. In this respect, the question of what  $\Psi$  ‘actually is’ cannot be answered in everyday terms. Perhaps the idea mentioned in Chap. 1, of a complex-valued field of possibilities, is the most appropriate.

## 3.2 The Time-Independent Schrödinger Equation

In Chap. 1, we found that the solutions of the *free* Schrödinger equation ((3.1) with  $V \equiv 0$ ) are plane waves with the dispersion relation  $\hbar\omega = \hbar^2 k^2 / 2m$ . But what are the solutions for a non-vanishing potential  $V$ ? The answer is: There are virtually no closed or analytical solutions in this case. Apart from just a handful of special potentials, one always has to deal with approximations or numerical results.

Nevertheless, the approach to the Schrödinger equation may be facilitated by separating out the variable  $t$ . This leads to the so-called *stationary* or time-independent Schrödinger equation which depends on space variables only. The prerequisite is, however, that the potential  $V$  must not depend on time:

$$V(\mathbf{r}, t) = V(\mathbf{r}). \quad (3.2)$$

Of course there are also physically reasonable potentials which do depend on time, but we will restrict ourselves to *time-independent potentials* in the following.

The method of choice is again the separation of variables. We insert the *ansatz*

$$\Psi(\mathbf{r}, t) = f(t) \cdot \varphi(\mathbf{r}) \quad (3.3)$$

into the Schrödinger Equation (3.1) and obtain

$$i\hbar \frac{\dot{f}}{f} = -\frac{\hbar^2}{2m} \frac{1}{\varphi} \nabla^2 \varphi + V. \quad (3.4)$$

The right- and the left-hand sides must be constant (because the independent variables ‘space’ and ‘time’ are separated):

$$i\hbar \frac{\dot{f}}{f} = \text{const.} = E = \hbar\omega. \quad (3.5)$$

$E$  and  $\omega$  are a yet undetermined energy (this follows from its physical units) and frequency. The sign (i.e.  $E$  and not  $-E$ ) is chosen in such a way that it agrees with the usual definition of the energy. A solution of this last equation is

$$f(t) = e^{-iEt/\hbar} = e^{-i\omega t} \quad (3.6)$$

or

$$\Psi(\mathbf{r}, t) = e^{-i\omega t} \varphi(\mathbf{r}). \quad (3.7)$$

$E$  must be a real number, because otherwise the solutions would be unphysical, since they would tend for  $t \rightarrow \infty$  or  $t \rightarrow -\infty$  towards infinity and would not be bounded.

Inserting the wavefunction (3.7) into the *time-dependent* Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) + V(\mathbf{r}) \Psi(\mathbf{r}, t) \quad (3.8)$$

leads to the *time-independent* (= *stationary*) Schrödinger equation:

$$E\varphi(\mathbf{r}) = -\frac{\hbar^2}{2m} \nabla^2 \varphi(\mathbf{r}) + V(\mathbf{r}) \varphi(\mathbf{r}). \quad (3.9)$$

At this point, the possible values of  $E$  are not explicitly defined. We take up this issue again in Chap. 5.

In the last two equations, the expression  $-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})$  occurs. It is called the *Hamiltonian operator*  $H$  (or simply *Hamiltonian* for short) and is a central term in quantum mechanics:

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}). \quad (3.10)$$

With this, the time-dependent Schrödinger equation is written as

$$i\hbar \frac{\partial}{\partial t} \Psi = H\Psi. \quad (3.11)$$

Note that the expression (3.10) is just *one* possible form of the Hamiltonian, and indeed a particularly simple one. Other formulations (which are considered in the Appendix) contain vector potentials or describe relativistic situations.

The properties of the Schrödinger equation which we listed above hold true for *all* SEq (3.11), independently of the special form of the Hamiltonian  $H$ . This applies also to the method used to derive the time-independent SEq from the time-dependent SEq, as long as the otherwise arbitrary operator  $H$  does not depend on time. In that case, the separation *ansatz*  $\psi(\mathbf{r}, t) = e^{-i\omega t} \varphi(\mathbf{r})$  *always* leads to the stationary SEq

$$H\varphi = E\varphi. \quad (3.12)$$

In a certain sense, this *is* quantum mechanics in short form.

### 3.3 Operators

Mathematically, the stationary SEq (3.12) is none other than an eigenvalue problem. You perhaps remember such problems from school days in the following form: Given a matrix  $A$  and a vector  $x$ , for which numbers  $\lambda \neq 0$  do there exist solutions  $x$  of the equation  $Ax = \lambda x$ ? The answer is that the allowed values of  $\lambda$  are given by the solutions of the *secular equation*  $\det(A - \lambda) = 0$ .

In the SEq (3.12), the Hamiltonian operator  $H$  appears on the left side instead of the matrix  $A$ . The concept of an *operator*<sup>2</sup> plays an essential role in quantum mechanics. While in the following chapters we will return repeatedly to this topic, here we give just a brief heuristic consideration or motivation. The term ‘operator’ can be best illustrated by ‘manipulation’ or ‘tool’. To apply an operator  $A$  to a function means to manipulate this function in a prescribed manner.

For example, the operator  $A = \frac{\partial}{\partial x}$  differentiates a function partially with respect to  $x$ . The operator  $B = \frac{\partial}{\partial x}x$  multiplies a function by  $x$  and then differentiates the product. Products of operators are performed from right to left;  $ABf$  means that we first apply  $B$  to  $f$  and then  $A$  to  $Bf$ . In the following, we always take for granted that the functions have the properties which are required for the application of the operator under consideration. For instance, the functions on which  $A = \frac{\partial}{\partial x}$  acts must be differentiable with respect to  $x$ .

The eigenvalue problem can be formulated in a general way. Consider a general operator  $A$  (which can be a matrix or a differential operator, for example). If the equation

$$Af = \alpha f \tag{3.13}$$

can be solved for certain numbers  $\alpha \in \mathbb{C}$  (which means that there are solutions  $f$ ), then  $\alpha$  is called an *eigenvalue* of the operator  $A$  and  $f$  is called the associated *eigenfunction*. If one wants to emphasize that the function  $f$  is an element of a vector space, then  $f$  is called an *eigenvector* instead of an eigenfunction. The set of all eigenvalues is termed the *spectrum*; the spectrum can contain finitely or infinitely many elements. The eigenvalues may be countable (*discrete spectrum*) or uncountable (*continuous spectrum*); spectra can contain both discrete and continuous components.

If there are two or more (e.g.  $n$ ) linearly-independent eigenfunctions corresponding to the same eigenvalue, one speaks of *degeneracy*. The eigenvalue is called  $n$ -fold degenerate, where  $n$  is the *degree of degeneracy*. Degeneracy is the consequence of a symmetry which is intrinsic to the problem; it can in principle be avoided by an arbitrary small, suitable ‘perturbation operator’.

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<sup>2</sup>A mapping between two vector spaces (whose elements can be functions, for example) is usually called an *operator*; a mapping from one vector space to its scalar field a *functional*. Integral transforms such as the Fourier or the Laplace transform can be viewed as integral operators.

In the interest of a unique terminology, we fix the difference between operator and function as follows: The domain of definition and the range of operators are vector spaces, while for functions, they are sets of numbers.

Here are two simple examples of eigenvalue problems:

1. Given the operator  $\frac{\partial}{\partial x}$ , the eigenvalue problem reads

$$\frac{\partial}{\partial x} f(x) = \gamma f(x); \gamma \in \mathbb{C}. \quad (3.14)$$

Obviously, we can solve this equation for all  $\gamma$ . The solution is

$$f(x) = f_0 e^{\gamma x}. \quad (3.15)$$

The spectrum is continuous and not degenerate.

2. Given the operator  $\frac{\partial^2}{\partial x^2}$ , the eigenvalue problem

$$\frac{\partial^2}{\partial x^2} f = \delta^2 f; \delta \in \mathbb{C}. \quad (3.16)$$

is clearly invariant under the exchange  $x \rightarrow -x$ , and its solutions are

$$f = f_{0+} e^{+\delta x} \text{ and } f = f_{0-} e^{-\delta x}. \quad (3.17)$$

The spectrum is continuous and doubly degenerate (for one value of  $\delta^2$  there exist the two linearly-independent eigenfunctions  $e^{+\delta x}$  and  $e^{-\delta x}$ ).

The limitation of the range of allowed functions in these two examples (for instance due to boundary conditions) can lead to a discrete spectrum; examples are found in the exercises. A (classical) example is the vibration of a violin string. The fundamental vibrational mode has the wavelength  $\lambda = 2L$ , where  $L$  is the length of the string (i.e. the position variable  $x$  along the string is bounded,  $0 \leq x \leq L$ ). Other allowed solutions are harmonics of the fundamental mode, i.e. their frequencies are whole-number multiples of the fundamental frequency. The (countable) eigenvalues are these integer multiples, giving a discrete spectrum.

### 3.3.1 *Classical Numbers and Quantum-Mechanical Operators*

The SEq (3.1) formally resembles the expression for the classical energy

$$E = \frac{\mathbf{p}^2}{2m} + V. \quad (3.18)$$

Indeed, one can transform the *numerical* (3.18) into an *operator* equation and *vice versa*, if one identifies<sup>3</sup>:

$$\begin{aligned} x &\leftrightarrow x \quad \text{or} \quad \mathbf{r} \leftrightarrow \mathbf{r} \\ p_x &\leftrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x} \quad \text{or} \quad \mathbf{p} \leftrightarrow \frac{\hbar}{i} \nabla. \\ E &\leftrightarrow i\hbar \frac{\partial}{\partial t} \end{aligned} \quad (3.19)$$

In this way, the expression (3.18) leads to the SEq (3.1) in its representation as an operator equation:

$$i\hbar \frac{\partial}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) = H. \quad (3.20)$$

We can motivate these ‘translations’ from classical to quantum-mechanical quantities as follows: We differentiate a plane wave

$$f = e^{i(kx - \omega t)} \quad (3.21)$$

with respect to  $x$ :

$$\frac{\partial f}{\partial x} = ik e^{i(kx - \omega t)} = ikf. \quad (3.22)$$

In order to find the momentum, we multiply both sides with  $\hbar/i$  and obtain with  $p = \hbar k$

$$\frac{\hbar}{i} \frac{\partial f}{\partial x} = \hbar k f = p f \quad \text{or} \quad \frac{\hbar}{i} \frac{\partial}{\partial x} f = p f \quad \text{or} \quad \left( \frac{\hbar}{i} \frac{\partial}{\partial x} - p \right) f = 0. \quad (3.23)$$

The bracket in the last equation does not depend on the particular wave number  $k$ . Because of its linearity, this equation applies to all functions which we can generate by a superposition of plane waves (i.e. all ‘sufficiently reasonable’ functions), if we understand  $p$  to represent not the momentum of a single wave, but that of the whole new function. It is quite natural to define an *operator*  $p$  (*momentum operator*, usually just called  $p$ , sometimes also  $p_{op}$  or  $\hat{p}$ ):

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x}. \quad (3.24)$$

In this context,  $x$  is also called the *position operator*. This formulation may appear unnecessarily complicated at this point, since the application of the position operator simply means multiplication by  $x$ . But later on we will encounter other contexts where this is no longer the case. Here, we can at least motivate the terminology by the following parallel

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<sup>3</sup>This small table is sometimes (rather jokingly) referred to as the ‘dictionary of quantum mechanics.’

application of the  $\begin{matrix} \text{momentum} \\ \text{position} \end{matrix}$  operator to  $e^{i(kx-\omega t)}$  yields  $\begin{matrix} p \\ x \end{matrix} e^{i(kx-\omega t)}$ . (3.25)

The crucial point of the translations table (3.19), which in more sophisticated language is referred to as the *correspondence principle*,<sup>4</sup> is that it allows the translation of classical expressions into those of quantum mechanics. Some examples: The classical expression  $E = \frac{p_x^2}{2m}$  becomes in quantum mechanics  $i\hbar \frac{\partial}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ , and  $E = \frac{p^2}{2m}$  becomes  $i\hbar \frac{\partial}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2$ . The classical angular momentum  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$  leads to the quantum-mechanical angular momentum operator  $\mathbf{l} = \frac{\hbar}{i} \mathbf{r} \times \nabla$ , and from the relativistic energy-momentum relation  $E^2 = m_0^2 c^4 + p^2 c^2$ , we obtain  $-\hbar^2 \frac{\partial^2}{\partial t^2} = m_0^2 c^4 - c^2 \hbar^2 \nabla^2$ . This last expression is the so-called *Klein-Gordon equation* which describes free relativistic quantum objects with zero spin.

### 3.3.2 Commutation of Operators; Commutators

In this process of translation, however, problems can arise if we translate products of two or more variables. These are due to the fact that numbers commute, but in general operators do not.<sup>5</sup> As an illustrative example, we consider the classical expression  $x p_x$  which obviously equals  $p_x x$ . But this no longer applies to its quantum-mechanical replacement by operators

$$x p_x = x \frac{\hbar}{i} \frac{\partial}{\partial x} \neq p_x x = \frac{\hbar}{i} \frac{\partial}{\partial x} x = \frac{\hbar}{i} \left( 1 + x \frac{\partial}{\partial x} \right). \quad (3.26)$$

Anyone who is not sure about such considerations should transform the operator equations into ‘usual’ equations by applying the operators to a function (the function need not be specified in detail here, but must of course meet the necessary technical requirements). Then, for example, we have for the operator  $\frac{\partial}{\partial x} x$  due to the product rule

$$\frac{\partial}{\partial x} x f = f + x \frac{\partial f}{\partial x} = \frac{\partial}{\partial x} x f = \left( 1 + x \frac{\partial}{\partial x} \right) f \quad (3.27)$$

or briefly, in operator notation,

$$\frac{\partial}{\partial x} x = 1 + x \frac{\partial}{\partial x}. \quad (3.28)$$

<sup>4</sup>In the old quantum theory, the (Bohr) correspondence principle denoted an approximate agreement of quantum-mechanical and classical calculations for large quantum numbers. In modern quantum mechanics, correspondence refers to the assignment of classical observables to corresponding operators. This assignment, however, has mainly a heuristic value and must always be verified or confirmed experimentally. A more consistent procedure is for example the introduction of position and momentum operators by means of symmetry transformations (see Chap. 21 Vol. 2).

<sup>5</sup>It is known for example that for two square matrices  $A$  and  $B$  (= operators acting on vectors), in general  $AB \neq BA$  holds.

The importance of the topic of ‘operators’ in quantum mechanics is based, among other things, on the fact that *measurable variables* (such as the momentum  $p_x$ ) are represented by operators (such as  $-i\hbar\partial_x$ ). If, as in (3.26), the *order* of the operators matters because of  $x\frac{\hbar}{i}\frac{\partial}{\partial x} \neq \frac{\hbar}{i}\frac{\partial}{\partial x}x$ , then this holds true also for the corresponding measurement variables. In other words, it makes a difference in quantum mechanics whether we measure first the position  $x$  and then the momentum  $p_x$ , or *vice versa*.

For the corresponding operators, the equality

$$(xp_x - p_x x) f = \frac{\hbar}{i} \left( x \frac{\partial f}{\partial x} - x \frac{\partial f}{\partial x} - f \right) = i\hbar f \quad (3.29)$$

holds, or

$$xp_x - p_x x = i\hbar. \quad (3.30)$$

Because differences of this kind play a key role in quantum mechanics, there is a special notation, namely a square bracket, called the *commutator*:

$$[x, p_x] = xp_x - p_x x = i\hbar. \quad (3.31)$$

For two operators  $A$  and  $B$ , the commutator<sup>6</sup> is defined as

$$[A, B] = AB - BA. \quad (3.32)$$

If it is equal to zero,  $A$  and  $B$  are called *commuting operators*.<sup>7</sup>

We repeat our remark that the *order is crucial* (of operators as well as of measurements). Of course there are commuting operators, such as for instance  $p_x$  and  $y$  or  $p_x$  and  $z$ , and so on. Position and momentum commute if and only if they do not refer to the same coordinate.

<sup>6</sup>The *anticommutator* is defined as

$$\{A, B\} = AB + BA$$

(despite the use of the same curly brackets, it is of course quite different from the Poisson brackets of classical mechanics).

<sup>7</sup>There is an interesting connection with classical mechanics which we have already mentioned briefly in a footnote in Chap. 1: In classical mechanics, the Poisson bracket for two variables  $U$  and  $V$  is defined as

$$\{U, V\}_{\text{Poisson}} = \sum_i \left( \frac{\partial U}{\partial q_i} \frac{\partial V}{\partial p_i} - \frac{\partial U}{\partial p_i} \frac{\partial V}{\partial q_i} \right),$$

where  $q_i$  and  $p_i$  are the positions and (generalized) momenta of  $n$  particles,  $i = 1, 2, \dots, 3n$ . In order to avoid confusion with the anticommutator, we have added the (otherwise uncommon) index *Poisson*. If  $U$  and  $V$  are defined as quantum-mechanical operators, their commutator is obtained by setting  $[U, V] = i\hbar \{U, V\}_{\text{Poisson}}$ . Example: In classical mechanics, we choose  $U = q_1 \equiv x$  and  $V = p_1 \equiv p_x$ . Then it follows that  $\{q_1, p_1\}_{\text{Poisson}} = 1$ , and we find the quantum-mechanical result  $[q_1, p_1] = [x, p_x] = i\hbar$ . This method, called ‘canonical quantization’, is considered in more detail in the relativistic sections in the Appendix.

A short remark concerning the problem of translation of ‘ambiguous’ terms such as  $xp_x$ : The problem can be resolved by symmetrization. The reason will be discussed in Chap. 13; here, it suffices to say that in this way one gets the correct quantum-mechanical expression. With the two possibilities  $xp_x$  and  $p_x x$ , we construct the symmetrized expression

$$A_{\text{QM}} = \frac{xp_x + p_x x}{2} = \frac{\hbar}{2i} \left( x \frac{\partial}{\partial x} + \frac{\partial}{\partial x} x \right) = \frac{\hbar}{2i} \left( 1 + 2x \frac{\partial}{\partial x} \right). \quad (3.33)$$

However, this trick is hereafter hardly ever needed — quantum mechanics is very good-natured in a certain sense.<sup>8</sup> Consider, for example, the angular momentum  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ . Must it be symmetrized, i.e.  $\mathbf{l} = \frac{\mathbf{r} \times \mathbf{p}}{2} - \frac{\mathbf{p} \times \mathbf{r}}{2}$ , for the translation into quantum mechanics? The answer is ‘no’, because for it we have

$$l_x = (\mathbf{r} \times \mathbf{p})_x = yp_z - zp_y = \frac{\hbar}{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right), \quad (3.34)$$

and we see that we need not symmetrize, since position and momentum commute if they belong to different coordinates:

$$\partial_z y f(y, z) = y \partial_z f(y, z) \quad (3.35)$$

or

$$[x, p_x] = i\hbar; [x, p_y] = [x, p_z] = 0; \text{ analogously for } y, z. \quad (3.36)$$

Actually, for the ‘standard’ operators, one can do without symmetrization.

One of the few counterexamples is the radial momentum  $\mathbf{pr}/r$  which occurs e.g. in the formulation of the kinetic energy in spherical coordinates (see exercises). Another example is the *Lenz vector*  $\mathbf{\Lambda}$ . If a particle with mass  $m$  moves in a potential  $U = -\frac{\alpha}{r}$ , then the vector  $\mathbf{\Lambda}$ , defined by

$$\mathbf{\Lambda} = \frac{1}{m\alpha} (\mathbf{l} \times \mathbf{p}) + \frac{\mathbf{r}}{r}, \quad (3.37)$$

is a conserved quantity. For the translation into quantum mechanics, the term  $\mathbf{l} \times \mathbf{p}$  must be symmetrized. For more on the Lenz vector, see Appendix G, Vol. 2.

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<sup>8</sup>Actually that is good news, because this symmetrization is not without problems. Take for example  $x^2 p$ —is the symmetrized expression  $xpx$ ,  $\frac{1}{2}(x^2 p + px^2)$ ,  $\frac{1}{3}(x^2 p + xpx + px^2)$ ,  $\frac{1}{4}(x^2 p + 2xpx + px^2)$  or a completely different term? Or does everything lead to the same quantum-mechanical expression (as is indeed the case in this example)?

### 3.4 Exercises

1. Show explicitly that the solutions of the Schrödinger (3.1) span a vector space.
2. Calculate  $\left[ x, \frac{\partial^2}{\partial x^2} \right]$ .
3. Given the relativistic energy-momentum relation  $E^2 = m_0^2 c^4 + c^2 p^2$ ; from this dispersion relation, deduce a differential equation.
4. Separation: Deduce the time-independent Schrödinger equation from the time-dependent Schrödinger equation by means of the separation of variables.
5. Given the eigenvalue problem

$$\frac{\partial}{\partial x} f(x) = \gamma f(x); \quad \gamma \in \mathbb{C} \quad (3.38)$$

with  $f(x)$  satisfying the boundary conditions  $f(0) = 1$  and  $f(1) = 2$ , calculate the eigenfunction and eigenvalue.

6. Given the eigenvalue problem

$$\frac{\partial^2}{\partial x^2} f = \delta^2 f; \quad \delta \in \mathbb{C} \quad (3.39)$$

with  $f(x)$  satisfying the boundary conditions  $f(0) = f(L) = 0$  and  $L \neq 0$ ,  $\delta \neq 0$ , calculate eigenfunctions and eigenvalues.

7. Given the nonlinear differential equation

$$y'(x) = \frac{dy(x)}{dx} = y^2(x). \quad (3.40)$$

$y_1(x)$  and  $y_2(x)$  are two different nontrivial solutions of (3.40), i.e.  $y_1 \neq \text{const} \cdot y_2$  and  $y_1 y_2 \neq 0$ .

- (a) Show that a multiple of a solution, i.e.  $f(x) = c y_1(x)$  with  $c \neq 0$ ,  $c \neq 1$ , is not a solution of (3.40).
  - (b) Show that a linear combination of two solutions, i.e.  $g(x) = a y_1(x) + b y_2(x)$  with  $ab \neq 0$ , but otherwise arbitrary, is not a solution of (3.40).
  - (c) Find the general solution of (3.40).
8. Radial momentum

- (a) Show that the classical momentum  $\mathbf{p}$  obeys

$$\mathbf{p}^2 = (\mathbf{p}\hat{r})^2 + (\mathbf{p} \times \hat{r})^2. \quad (3.41)$$

- (b) Deduce the quantum-mechanical expression  $p_r$  for the classical radial momentum  $\hat{r}\mathbf{p}$  ( $= \mathbf{p}\hat{r}$ ).

9. Show explicitly that the classical expression  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$  need not be symmetrized for the translation into quantum mechanics.
10. Given the operators  $A = x \frac{d}{dx}$ ,  $B = \frac{d}{dx}x$  and  $C = \frac{d}{dx}$ :
- Calculate  $Af_i(x)$  for the functions  $f_1(x) = x^2$ ,  $f_2(x) = e^{ikx}$  and  $f_3(x) = \ln x$ .
  - Determine  $A^2 f(x)$  for arbitrary  $f(x)$ .
  - Calculate the commutators  $[A, B]$  and  $[B, C]$ .
  - Compute  $e^{iC}x^2 - (x + i)^2$ . Prove the equation  $e^{iC}e^{ikx} = e^{-k}e^{ikx}$ .