

# Chapter 13

## Operators



In this chapter, we assemble some basic properties of the most important types of operators in quantum mechanics.

As we have seen, the states of quantum mechanics are defined on an (extended) Hilbert space  $\mathcal{H}$ . Changes of these states are caused by operators: This can be, for example, the time evolution of the system itself, or the filtering of certain states out of a general state. We have already met up with the zoo of operators of quantum mechanics (Hermitian, unitary and projection operators). But given the central role of operators in quantum mechanics, we want to discuss in this chapter some of their properties in more detail, taking the abstract formulation as a basis.<sup>1</sup>

With one exception, the operators considered in this book are linear. An operator  $A$  is called *linear* if for any two states and any two numbers  $\alpha, \beta \in \mathbb{C}$ , it holds that:

$$A(\alpha|\varphi\rangle + \beta|\psi\rangle) = \alpha A|\varphi\rangle + \beta A|\psi\rangle. \tag{13.1}$$

For the exception, namely an *antilinear* operator  $B$ , it holds that:

$$B(\alpha|\varphi\rangle + \beta|\psi\rangle) = \alpha^* B|\varphi\rangle + \beta^* B|\psi\rangle. \tag{13.2}$$

An anti-linear map is for example the complex conjugation, and thus also the scalar product with respect to the first component, since then  $\langle \lambda a | b \rangle = \lambda^* \langle a | b \rangle$ . Furthermore, the time-reversal operator is anti-linear (see Chap. 21, Vol. 2).

An operator is called *bounded* if there is a constant  $C$  which does not depend on the states  $|\varphi\rangle \in \mathcal{H}$ , so that for all states, it holds that

$$\|A|\varphi\rangle\| \leq C \|\varphi\rangle\|. \tag{13.3}$$

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<sup>1</sup>Further material on operators is found in Appendix I, Vol. 1.

The *domain of definition* (or briefly the domain) of an operator  $A$  is the set of all vectors  $|\varphi\rangle \in \mathcal{H}$ , such that  $A|\varphi\rangle$  also belongs to  $\mathcal{H}$ . One can show that the domain of definition of  $A$  is the whole Hilbert space, if and only if  $A$  is bounded.

If two operators  $A$  and  $B$  commute, one says that they are *simultaneously* measurable. However, this notion is not defined by any sort of time consideration, but is simply a short form for the fact that the measurement result is independent of the chronological order in which we measure  $A$  and  $B$ .

### 13.1 Hermitian Operators, Observables

We can distinguish three levels: First, there is the measurable physical variable  $A_{\text{phys}}$ , which is modelled in quantum mechanics by a Hermitian operator  $A_{op} = A_{op}^\dagger$ . This abstract operator can be expressed, if necessary, in a concrete representation as  $A_{\text{repr}}$ . As an example, we consider the angular momentum. The measurable physical variable is  $\mathbf{l}_{\text{phys}}$ , the corresponding operator  $\mathbf{l}_{op} = \mathbf{r} \times \mathbf{p}$ , and in the position representation, it is  $\mathbf{l}_{\text{repr}} = \frac{\hbar}{i} \mathbf{r} \times \nabla$ , as is well known. As mentioned above, often the same notation is used for all three objects (in the example  $\mathbf{l}$ ), since usually the context makes clear what is meant. We will proceed essentially in this way.

We start from the eigenvalue equation (the spectrum is assumed to be discrete and not degenerate):

$$A|\varphi_n\rangle = a_n|\varphi_n\rangle; \quad n = 1, 2, \dots; \quad A = A^\dagger. \quad (13.4)$$

The possible result of a measurement of the measurable physical variable  $A$  is one of the eigenvalues of the operator  $A$ . Because of the importance of this fact there is a special name, namely *observable*.<sup>2</sup> We mean by this a Hermitian operator that represents a consistently measurable physical quantity. Some remarks on the concept ‘observable’ are found in Appendix I, Vol. 1.

We point out that we use ‘self-adjoint’ and ‘Hermitian’ as equivalents, which applies for all of the systems we consider. In fact, under certain conditions the two terms are not identical; in infinite-dimensional vector spaces, Hermiticity does not necessarily imply self-adjoint. More on this topic may be found in Appendix I, Vol. 1.

Two remarks are appropriate here:

1. An operator  $A$  is called *anti-Hermitian* if  $A^\dagger = -A$ . Each operator  $C$  can be broken into a Hermitian and an anti-Hermitian part<sup>3</sup>:

<sup>2</sup>The term is not defined in the same way everywhere, and is sometimes rather avoided. The reason for this rejection stems in part from the fact that the name ‘observable’ suggests that without an observer (perhaps even a human), physical quantities cannot become real. We explicitly point out that for us, the term observable does not imply this problem, but is simply a technical term in the above sense.

<sup>3</sup>Much in the way that each function can be decomposed into a mirror-symmetric and a point-symmetric part.

$$C = C_{\text{Hermitian}} + C_{\text{anti-Hermitian}} = \frac{C + C^\dagger}{2} + \frac{C - C^\dagger}{2}. \quad (13.5)$$

2. The product of an operator with its adjoint is a Hermitian operator:  $(AA^\dagger)^\dagger = A^{\dagger\dagger}A^\dagger = AA^\dagger$ . In addition,  $AA^\dagger$  is a *positive operator*; that is, for all  $|\varphi\rangle$ , it holds that  $\langle\varphi|AA^\dagger|\varphi\rangle \geq 0$ . This follows from the fact that  $\langle\varphi|AA^\dagger|\varphi\rangle$  is the square of a norm, since we have  $\langle\varphi|AA^\dagger|\varphi\rangle = \|A^\dagger|\varphi\rangle\|^2$ .<sup>4</sup>

Finally, a word about the symmetrization discussed in Chap. 3. For example, in classical mechanics we have  $xp_x = p_x x$ , but for the corresponding quantum-mechanical quantities,  $xp_x \neq p_x x$ . For this reason, we introduced the symmetrized form  $\frac{1}{2}(xp_x + p_x x)$ . We can now deliver the reasoning: Given two Hermitian operators  $A$  and  $B$  with  $[A, B] \neq 0$ . The product  $AB$  is not Hermitian (so it cannot correspond to a measurable variable), for  $(AB)^\dagger = BA \neq AB$ . But we can construct a Hermitian operator by taking the symmetrized form  $C = \frac{1}{2}(AB + BA)$ , because it is  $C^\dagger = \frac{1}{2}(AB + BA)^\dagger = C$ . According to the above considerations, it cannot be guaranteed offhand that this symmetrized operator represents an observable.

### 13.1.1 Three Important Properties of Hermitian Operators

In the following, we want to prove three important properties of Hermitian operators using the bra-ket formalism. We know already two of them, namely that the eigenvalues are real and that the eigenfunctions are pairwise orthogonal (we assume that the spectrum is not degenerate). In addition, we will show that commuting Hermitian operators have a common CONS.

#### 13.1.1.1 Eigenvalues Are Real

Since measurements of physical quantities always mean measurements of real numbers (lengths, angles, arc degrees etc.), we require that the eigenvalues of the modelling operators also be real. This is indeed the case for Hermitian operators, as we now show (again).

The operator  $A$  is Hermitian,  $A^\dagger = A$ ; its eigenvalue equation is

$$A|\varphi_n\rangle = a_n|\varphi_n\rangle; \quad n = 1, 2, \dots \quad (13.6)$$

with eigenvectors  $|\varphi_n\rangle$ . We multiply from the left by a bra:

$$\langle\varphi_n|A|\varphi_n\rangle = a_n\langle\varphi_n|\varphi_n\rangle = a_n. \quad (13.7)$$

<sup>4</sup>We note that the term ‘positive operator’ is common but *not negative or positive-semidefinite* would be more correct. However, one can make the distinction between positive ( $\geq 0$ ) and strictly positive ( $> 0$ ).

We then have:

$$a_n^\dagger = a_n^* = \langle \varphi_n | A | \varphi_n \rangle^\dagger = \langle \varphi_n | A^\dagger | \varphi_n \rangle = \langle \varphi_n | A | \varphi_n \rangle = a_n. \quad (13.8)$$

Thus, the eigenvalues of a Hermitian operator are real.

### 13.1.1.2 Eigenvectors Are Orthogonal

Next, we want to show that we have  $\langle \varphi_m | \varphi_n \rangle = 0$  for  $n \neq m$ , provided that the spectrum is not degenerate (degenerate spectra are discussed further below). We start with

$$A | \varphi_n \rangle = a_n | \varphi_n \rangle \text{ and } \langle \varphi_m | A = a_m \langle \varphi_m |, \quad (13.9)$$

since  $A$  is Hermitian and hence has real eigenvalues. It follows that

$$\langle \varphi_m | A | \varphi_n \rangle = a_n \langle \varphi_m | \varphi_n \rangle \text{ and } \langle \varphi_m | A | \varphi_n \rangle = a_m \langle \varphi_m | \varphi_n \rangle. \quad (13.10)$$

Subtracting the two equations leads to

$$(a_m - a_n) \langle \varphi_m | \varphi_n \rangle = 0. \quad (13.11)$$

Therefore, it must hold (since we have assumed non-degeneracy) that  $\langle \varphi_m | \varphi_n \rangle = 0$  for  $n \neq m$ . If we take into account also the normalization of the eigenfunctions, we find, as expected:

$$\langle \varphi_m | \varphi_n \rangle = \delta_{nm}. \quad (13.12)$$

Thus, the eigenfunctions of a (nondegenerate) Hermitian operator always form an orthonormal system.

### 13.1.1.3 Commuting Hermitian Operators Have a Common CONS

Given two Hermitian operators  $A$  and  $B$  (with nondegenerate spectra). They commute if and only if they have a common CONS of eigenvectors. To prove the claim, two steps are necessary: Step 1:  $[A, B] = 0 \rightarrow$  common system; Step 2: common system  $\rightarrow [A, B] = 0$ .

Step 1. We start with

$$A | \varphi_i \rangle = a_i | \varphi_i \rangle \quad (13.13)$$

where  $\{|\varphi_i\rangle\}$  is a CONS. It follows that

$$BA | \varphi_i \rangle = \begin{cases} Ba_i | \varphi_i \rangle = a_i B | \varphi_i \rangle \\ AB | \varphi_i \rangle, \text{ since } [A, B] = 0 \end{cases} \quad (13.14)$$

or, in summary,

$$AB |\varphi_i\rangle = a_i B |\varphi_i\rangle. \quad (13.15)$$

Comparing this equation with (13.13) shows (because in both cases the same eigenvalue  $a_i$  appears) that  $B |\varphi_i\rangle$  must be a multiple of the eigenfunction  $|\varphi_i\rangle$ :

$$B |\varphi_i\rangle \sim |\varphi_i\rangle. \quad (13.16)$$

We call the proportionality constant  $b_i$ . It follows that

$$B |\varphi_i\rangle = b_i |\varphi_i\rangle, \quad (13.17)$$

i.e. the operator  $B$  has the CONS  $\{\varphi_i\}$ , also. But as the roles of  $A$  and  $B$  can be interchanged in this argument; it follows that both operators have exactly the same CONS. Thus step 1 is completed.

Step 2. On condition that a common CONS exists, it will be shown that the commutator  $[A, B]$  vanishes. Thus we assume:

$$A |\varphi_i\rangle = a_i |\varphi_i\rangle \text{ and } B |\varphi_i\rangle = b_i |\varphi_i\rangle. \quad (13.18)$$

It follows that

$$BA |\varphi_i\rangle = a_i B |\varphi_i\rangle = a_i b_i |\varphi_i\rangle \text{ and } AB |\varphi_i\rangle = b_i A |\varphi_i\rangle = b_i a_i |\varphi_i\rangle. \quad (13.19)$$

The right-hand sides of these equations are equal, hence also the left-hand sides must be equal, so we find

$$(AB - BA) |\varphi_i\rangle = [A, B] |\varphi_i\rangle = 0. \quad (13.20)$$

This equation does not tell us that the commutator vanishes, but only that its application to an *eigenvector* gives zero. On the other hand, we know that the system  $\{\varphi_i\}$  is complete, meaning that *any* vector can be represented as

$$|\Psi\rangle = \sum_i d_i |\varphi_i\rangle. \quad (13.21)$$

With this, we have for any vector  $|\Psi\rangle$

$$[A, B] |\Psi\rangle = \sum_i d_i [A, B] |\varphi_i\rangle = 0 \quad (13.22)$$

and hence the statement  $[A, B] = 0$  is true in the *entire* Hilbert space.

Commuting observables thus have a common system of eigenvectors. A remark: time-independent observables which commute with the Hamiltonian are *conserved quantities*, see Chap. 9.

### 13.1.2 Uncertainty Relations

#### 13.1.2.1 For Two Hermitian Operators

In Chap. 9, we defined the standard deviation or uncertainty  $\Delta A$  by

$$(\Delta A) = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}. \quad (13.23)$$

Starting from this, one can derive the uncertainty relation (or uncertainty principle) for Hermitian operators  $A$  and  $B$ . This is carried out in Appendix I, Vol. 1; we note here only the result:

$$\Delta A \cdot \Delta B \geq \frac{1}{2} |\langle [A, B] \rangle|. \quad (13.24)$$

This general uncertainty relation for two Hermitian operators is particularly popular for the pair  $x$  and  $p_x$ . Because of  $[x, p_x] = i\hbar$ , we have

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}. \quad (13.25)$$

This is sketched in Fig. 13.1.<sup>5</sup>

#### 13.1.2.2 When Does the Uncertainty Relation Hold and What Does It Mean?

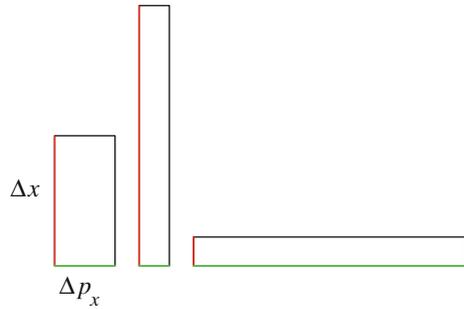
We emphasize that the derivation of the uncertainty relation assumes ideal (error-free) measuring instruments. In fact, the experimental errors of measuring instruments in real experiments are usually much larger than the quantum uncertainties. Accordingly, the uncertainty relation is *not* a statement about the accuracy of measuring instruments, but rather the description of a pure quantum effect.

We have seen in Chap. 9 that expressions such as  $\Delta x$  are *state-dependent* averaging processes. If one does not take this into account, one can deduce everything possible and impossible, and this is also true for the uncertainty relation. The notation  $(\Delta x)_\psi$  or  $\Delta_{\psi}x$  is less common, but its use would prevent this kind of misunderstanding.

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<sup>5</sup>One can show that violating the uncertainty principle implies that it is also possible to violate the second law of thermodynamics; see Esther Hänggi & Stephanie Wehner, 'A violation of the

**Fig. 13.1** Different realizations of the uncertainty relation (13.25). It is like pressing a balloon—pressed in one direction, the balloon evades the pressure and expands in the other direction



In addition, the uncertainty relation (13.24) makes sense only for those states which are in the domain of definition of  $A$  and  $B$  as well as in those of the products of the operators occurring in the derivation. For all other states, the uncertainty principle is irrelevant. For example, there are functions which are in the Hilbert space of square integrable functions, but outside the domains of definition of the (unbounded) operators  $x$  and  $p$ . For these functions, one cannot establish the inequality (13.25). Examples can be found in the exercises and in Appendix I, Vol. 1. Operator equations, and generally statements about operators, do not apply to all states, but only to those that are in the domain of definition of the operators.<sup>6</sup>

Regarding the meaning of the uncertainty relation (13.24), we encounter a typical situation in quantum mechanics. The theoretical formulations and derivations are quite ‘straightforward’ and uncontroversial. Problems occur only when one asks what all this ‘really’ means. We illustrate the situation with the example of the two positions that we have already briefly mentioned in Chap. 2.

1. The first position assumes that the relation (13.24) applies only to an *ensemble*. It is, therefore, about the statistical distribution in the measurement results, if one measures both  $A$  and  $B$  in a large number of identically-prepared systems (i.e. in each system, either  $A$  or  $B$ ). For  $[A, B] \neq 0$ , the measurements are indeed incompatible, but because they are carried out on *different* systems or ensemble members, these measurements can in no way mutually interfere. In this case, the uncertainty principle has nothing to do with the possibility of performing simultaneous measurements of two quantities. It can be interpreted at best as a fundamental limitation in preparing a state (or the corresponding ensemble) as accurately as possible. In this case, the standard deviation  $\Delta A$  is a straightforward concept.
2. The second position assumes that the relation (13.24) applies to *single* events. Of course,  $\Delta A$  has nothing to do in this case with a statistical distribution as in the ensemble position just mentioned. As we have seen and will develop further, a central position of this view of quantum mechanics is that it does not make sense

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uncertainty principle implies a violation of the second law of thermodynamics’, Nature Communications 4, Article number 1670 (2013), <https://doi.org/10.1038/ncomms2665>.

<sup>6</sup>It is not just about the comb, so to speak, but also about the hair that is combed.

for a typical quantum state to say that  $A$  has any value at all (which does not mean that  $A$  has a value which we do not know). Under this assumption,  $\Delta A$  can be interpreted, as we have seen in Chap. 9, as a numerical measure of the extent to which the property  $A$  is *not* owned by the system, since e.g.  $\Delta_\psi A = 0$  means that  $|\psi\rangle$  is an eigenstate of  $A$ . The same applies to  $\Delta_\psi B$ . The uncertainty relation is then a statement as to what extent a system can have or cannot have the properties  $A$  and  $B$  at the same time.

In addition to these two positions or interpretations of quantum mechanics, there are several more, as we shall see in later chapters.<sup>7</sup> Which of these is the ‘correct’ one is not (yet) clear at present. We can just say at this point that the formalism of quantum mechanics is unique, but its interpretation is anything but uncontroversial. In Chap. 14, and Chap. 27, Vol. 2, and especially in Chap. 28, Vol. 2, we will address these questions again.

### 13.1.2.3 Uncertainty Relation for Time and Energy

In the uncertainty relation (13.24), we cannot insert the time directly into  $A$  or  $B$ , since it is not an operator in quantum mechanics, but a simple *parameter* (one cannot say e.g. that “a quantum object has a well-defined time”). Nevertheless, one can formulate a statement that links time and energy. For this we consider a not explicitly time-dependent Hermitian operator  $A$ . As described in Sect. 9.3, we have

$$i\hbar \frac{d}{dt} \langle A \rangle = \langle [A, H] \rangle. \quad (13.26)$$

Together with the uncertainty relation, it follows that

$$\Delta A \cdot \Delta H \geq \frac{1}{2} |\langle [A, H] \rangle| = \frac{\hbar}{2} \left| \frac{d}{dt} \langle A \rangle \right|. \quad (13.27)$$

We define a time interval  $\Delta\tau$  by

$$\Delta\tau = \frac{\Delta A}{\left| \frac{d}{dt} \langle A \rangle \right|}. \quad (13.28)$$

This is a measure of the time during which the value of  $A$  changes by  $\Delta A$ . For example, we have for a conserved quantity  $\frac{d}{dt} \langle A \rangle = 0$ , hence  $\Delta\tau = \infty$ . With these concepts, we find

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<sup>7</sup>Quite apart from the literary process, such as with David Foster Wallace in *Infinite jest*: “The mind says, a box-and-forest-meadows-mind can move with quantum-speed and be anytime anywhere and hear in symphonic sum of the thoughts of the living ... The mind says: It does not really matter whether Gately knows what the term *quanta* means. By and large, it says there are ghosts ... in a completely different Heisenberg dimension of exchange rates and time courses.”

$$\Delta H \cdot \Delta \tau \geq \frac{\hbar}{2} \quad (13.29)$$

which often is written as

$$\Delta E \cdot \Delta t \gtrsim \frac{\hbar}{2} \quad (13.30)$$

This can be interpreted as a correlation between lifetime and variation in energy.

### 13.1.3 Degenerate Spectra

We have essentially confined ourselves to observables with nondegenerate spectra. In the discrete case, the eigenvalue equation is given by

$$A |\varphi_n\rangle = a_n |\varphi_n\rangle, \quad n = 1, 2, \dots \quad (13.31)$$

Since  $A$  is an observable, the set  $\{|\varphi_n\rangle\}$  of the eigenvectors is a basis for  $\mathcal{H}$ , in terms of which any state can be represented by an expansion:

$$|\psi\rangle = \sum_n c_n |\varphi_n\rangle. \quad (13.32)$$

We can express this also by saying that every eigenvector spans a *one-dimensional* subspace.

Let us now turn to the case of a *degenerate discrete spectrum*. The eigenvalue equation is

$$A |\varphi_{n,r}\rangle = a_n |\varphi_{n,r}\rangle, \quad n = 1, 2, \dots; \quad r = 1, 2, \dots, g_n. \quad (13.33)$$

Here,  $g_n$  is the *degree of degeneracy* of the eigenvalue  $a_n$ ; for  $g_n = 1$ ,  $a_n$  is not degenerate. The  $|\varphi_{n,r}\rangle$  are  $g_n$  linearly independent eigenvectors (for given  $n$ ); they span the subspace (eigenspace)  $\mathcal{H}_n$  of dimension  $g_n$  of the eigenvalue  $a_n$ . The eigenvectors  $|\varphi_{n,r}\rangle$  with the same index  $n$  are not necessarily orthogonal to each other (we can always assume, however, that they are normalized), but with the usual methods of orthogonalization one can construct an orthogonal system in terms of them. The subspaces of *different* indices  $n$  are mutually orthogonal,  $\mathcal{H}_n \perp \mathcal{H}_m$  for  $n \neq m$ .<sup>8</sup>

Finally, the expansion of a state is given by:

$$|\psi\rangle = \sum_n \sum_{r=1}^{g_n} c_{n,r} |\varphi_{n,r}\rangle, \quad n = 1, 2, \dots; \quad r = 1, 2, \dots, g_n \quad (13.34)$$

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<sup>8</sup>Two subspaces  $\mathcal{H}_n$  and  $\mathcal{H}_m$  are mutually orthogonal if any vector in  $\mathcal{H}_n$  is orthogonal to any vector in  $\mathcal{H}_m$ .

In the case of a continuous spectrum, we obtain the corresponding statements and formulations by the usual replacements: discrete index  $\rightarrow$  continuous variable; summation  $\rightarrow$  integration; Kronecker symbol  $\rightarrow$  Delta function; cf. Chap. 12. See also the chapter ‘Discrete-continuous’ in Appendix T, Vol. 1.

## 13.2 Unitary Operators

Before we repeat the definition of a unitary operator, we consider the definition of an inverse operator. Thus, we assume that an operator  $A$  with  $Af = g$  exists. If the inverse of this mapping also exists,  $f = A^{-1}g$ , then  $A^{-1}$  is the inverse operator of  $A$ . We have  $AA^{-1} = A^{-1}A$ . A *unitary operator*  $U$  is defined by<sup>9</sup>

$$U^\dagger = U^{-1} \iff U^\dagger U = UU^\dagger = 1. \quad (13.35)$$

For the eigenvalues of a unitary operator, with  $U|u\rangle = u|u\rangle$  and  $\langle u|U^\dagger = u^*\langle u|$ , the equation  $|u|^2 = 1$  applies. Hence, the eigenvalues of a unitary operator are on the unit circle.

### 13.2.1 Unitary Transformations

With unitary operators we can define *unitary transformations* of states and operators. Common notations are

$$U|\Psi\rangle = |\Psi'\rangle \quad \text{and} \quad UAU^\dagger = A'. \quad (13.36)$$

The interesting thing about unitary transformations is that they leave important properties and quantities unchanged, namely the lengths of vectors and the ‘angle’ between them, and thus scalar products, as well as matrix elements and eigenvalues (see exercises). In this respect, a unitary transformation is an analogue of the rotation in elementary vector calculus. We can visualize it as a transition from one basis to another basis or coordinate system. Suppose that there two CONS  $\{|\varphi_n\rangle\}$  and  $\{|\psi_n\rangle\}$ . Then we have

$$|\psi_n\rangle = \sum_m |\varphi_m\rangle \langle \varphi_m | \psi_n \rangle = \sum_m U_{mn} |\varphi_m\rangle, \quad (13.37)$$

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<sup>9</sup>To be exact, there is the second requirement,  $U\alpha|\varphi\rangle = \alpha U|\varphi\rangle$ . For *antiunitary* operators  $T$ , it holds also that  $TT^\dagger = T^\dagger T = 1$ , but in contrast to the unitary operators,  $T\alpha|\varphi\rangle = \alpha^*T|\varphi\rangle$ . Anti-unitary operators appear, apart from the complex conjugation, in quantum mechanics only in connection with time reversal (see Chap. 21, Vol. 2). So the equation  $UU^\dagger = U^\dagger U = 1$  almost always refers to unitary operators.

and it follows that

$$\delta_{n'n} = \langle \psi_{n'} | \psi_n \rangle = \sum_{m'm} U_{m'n'}^* \langle \varphi_{m'} | \varphi_m \rangle U_{mn} = \sum_m U_{m'n'}^* U_{mn} = (U^\dagger U)_{n'n}, \quad (13.38)$$

which is just another notation for  $U^\dagger U = 1$ .

### 13.2.2 Functions of Operators, the Time-Evolution Operator

For a given general operator  $A$ , we can define powers of  $A$ , or construct other expressions such as power series of the form

$$\sum_{n=0}^{\infty} a_n A^n \quad (13.39)$$

as we have already done several times in previous chapters. An example is  $\sum_{n=0}^{\infty} a_n \frac{d^n}{dx^n}$ .

Of course, in view of such expressions there is generally the question whether a series converges at all (i.e. whether it makes sense to write it). The answer depends on the coefficients  $a_n$  and the functions to which we apply the operator.

We want to examine an example in more detail. Consider a time-independent Hamiltonian  $H$

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle. \quad (13.40)$$

We wish to show that the *time-evolution operator*

$$U(t) = \sum_{n=0}^{\infty} \left(-i \frac{t}{\hbar}\right)^n \frac{H^n}{n!} \equiv e^{-i \frac{Ht}{\hbar}} \quad (13.41)$$

is unitary and transforms the initial state  $|\Psi(0)\rangle$  into the state  $|\Psi(t)\rangle$ .<sup>10</sup> To that end, we assume that the state vector can be expanded in a power series about  $t = 0$ :

$$\begin{aligned} |\Psi(t)\rangle &= |\Psi(0)\rangle + \frac{t}{1!} \left(\frac{d}{dt} |\Psi(t)\rangle\right)_{t=0} + \frac{t^2}{2!} \left(\frac{d^2}{dt^2} |\Psi(t)\rangle\right)_{t=0} + \cdots \\ &= \sum_n \frac{t^n}{n!} \left(\frac{d^n}{dt^n} |\Psi(t)\rangle\right)_{t=0}. \end{aligned} \quad (13.42)$$

<sup>10</sup>Since it, so to say, impels or propagates the state  $|\Psi\rangle$  through time, it is also called *propagator*.

The time derivatives can be expressed with the help of the SEq as powers of  $H$ <sup>11</sup>:

$$\begin{aligned} i\hbar \frac{d}{dt} |\Psi(t)\rangle &= H |\Psi(t)\rangle \\ (i\hbar \frac{d}{dt})^2 |\Psi(t)\rangle &= i\hbar \frac{d}{dt} H |\Psi(t)\rangle = H^2 |\Psi(t)\rangle \dots \\ (i\hbar \frac{d}{dt})^n |\Psi(t)\rangle &= i\hbar \frac{d}{dt} H^{n-1} |\Psi(t)\rangle = H^n |\Psi(t)\rangle. \end{aligned} \quad (13.43)$$

We replace the time derivatives in (13.42) by these expressions and find

$$|\Psi(t)\rangle = \sum_n \frac{t^n}{n!} \left( \frac{d^n}{dt^n} |\Psi(t)\rangle \right)_{t=0} = \sum_{n=0}^{\infty} \left( -i \frac{t}{\hbar} \right)^n \frac{H^n}{n!} |\Psi(0)\rangle. \quad (13.44)$$

On the right-hand side, we have an operator which acts on the initial state  $|\Psi(0)\rangle$ :

$$U(t) = \sum_{n=0}^{\infty} \left( -i \frac{t}{\hbar} \right)^n \frac{H^n}{n!} = e^{-i \frac{Ht}{\hbar}}, \quad (13.45)$$

and can thus write the time evolution compactly as

$$|\Psi(t)\rangle = U(t) |\Psi(0)\rangle \quad (13.46)$$

or more generally,  $|\Psi(t_2)\rangle = U(t_2 - t_1) |\Psi(t_1)\rangle$ .

We note that (13.45) and (13.46) are equivalent to the SEq in the form (13.40). Ultimately, it is just a matter of personal preference or habit, which one of the two formulations one uses. In any case, we can see very clearly in (13.46) the deterministic nature of the SEq: specifying an initial condition determines uniquely its solution for all times, as we have already derived in an example in Chap. 5.

Finally, we want to show that the time evolution operator  $U$  is unitary. We extend the proof and show that in general, the following relation holds:

$$\text{For } \hat{U} = e^{iA} \text{ with } A = A^\dagger \text{ follows } \hat{U}^{-1} = \hat{U}^\dagger. \quad (13.47)$$

For the proof, we use the power series of the exponential function:

$$\begin{aligned} \hat{U}^\dagger &= (e^{iA})^\dagger = \sum \left( \frac{i^n}{n!} A^n \right)^\dagger = \sum \frac{(-i)^n}{n!} (A^n)^\dagger \\ &= \sum \frac{(-i)^n}{n!} (A^\dagger)^n = \sum \frac{(-i)^n}{n!} A^n = e^{-iA} = U^{-1}. \end{aligned} \quad (13.48)$$

---

<sup>11</sup>Note that  $H$  does not depend on time, which is why we obtain such simple formulations. Propagators for time-dependent Hamiltonians can also be formulated, but this is somewhat more complicated.

It follows  $\hat{U}^\dagger \hat{U} = e^{iA} e^{-iA} = 1$ ; hence, the operator is unitary and  $U^{-1} = e^{-iA}$ . The general formulation of this fact is found in the theorem of Stone, see Appendix I, Vol. 1.

We finally mention in passing that the propagator can be written as an integral operator, which is advantageous in some contexts. More on this topic in Appendix I, Vol. 1. Note that the propagator plays a dominant role in quantum field theory.

### 13.3 Projection Operators

An expression of the form  $P = |\varphi_1\rangle \langle \varphi_1|$  is the simplest *projection operator*. Applying it to a vector, the operator projects it (as the name suggests) onto a subspace; in this example, that subspace which is spanned by  $|\varphi_1\rangle$ .

Generally, an *idempotent* operator is defined by

$$P^2 = P. \quad (13.49)$$

If  $P$  is Hermitian in addition, it is called a projection operator. In a Hilbert space of dimension  $N$ , we can define, for example, the projection operator

$$P = \sum_{n \leq N'} |\varphi_n\rangle \langle \varphi_n|, \quad (13.50)$$

where  $\{\varphi_n\}$  is an *ON* system of dimension  $N' \leq N$ . That this is indeed a projection operator can be seen from

$$P^2 = \sum_n |\varphi_n\rangle \langle \varphi_n| \sum_m |\varphi_m\rangle \langle \varphi_m| = \sum_n \sum_m |\varphi_n\rangle \delta_{mn} \langle \varphi_m| = \sum_n |\varphi_n\rangle \langle \varphi_n| = P. \quad (13.51)$$

The eigenvalue equation for a projection operator  $P$  reads

$$P |p\rangle = p |p\rangle \quad (13.52)$$

with the eigenvectors  $|p\rangle$  and the eigenvalues  $p$ .<sup>12</sup> Multiplication by  $P$  yields

$$P^2 |p\rangle = P p |p\rangle = p P |p\rangle = p^2 |p\rangle. \quad (13.53)$$

On the other hand, because of  $P^2 = P$ , it follows that

$$P^2 |p\rangle = P |p\rangle = p |p\rangle, \quad (13.54)$$

and therefore,

---

<sup>12</sup>Here the notation  $p$  has, of course, nothing to do with the momentum, but with  $p$  as projection.

$$p^2 = p \text{ or } p = 0 \text{ and } 1. \quad (13.55)$$

As we well know, the completeness relation of a CONS provides us with a special projection operator, namely, a projection onto ‘everything’.

$$P_{\text{whole space}} = \sum_n |\varphi_n\rangle \langle \varphi_n| = 1. \quad (13.56)$$

In words: this projection operator projects onto the whole space.<sup>13</sup> As we have seen, the completeness relation is not only often a very useful tool in conversions, but is also very simple to handle—because we insert just an identity (and this, by the way, gives the procedure its name). A simple example:

$$|\Psi\rangle = 1 \cdot |\Psi\rangle = \sum_n |\varphi_n\rangle \langle \varphi_n | \Psi\rangle = \sum_n |\varphi_n\rangle c_n. \quad (13.57)$$

We see that  $c_n = \langle \varphi_n | \Psi\rangle$  is the projection of  $\Psi$  onto  $\varphi_n$ .

Note: Two projection operators are called (mutually) orthogonal if  $P_1 P_2 = 0$  (this also holds for the corresponding subspaces).

### 13.3.1 Spectral Representation

Suppose that in a Hilbert space  $\mathcal{H}$ , the eigenfunctions of an operator  $A$  form a CONS  $\{|a_n\rangle, n = 1, 2, \dots\}$ . Then we can express the operator using the projection operators  $P_n = |a_n\rangle \langle a_n|$  built with the eigenfunctions. For with

$$A |a_n\rangle = a_n |a_n\rangle, \quad (13.58)$$

and

$$\sum_n |a_n\rangle \langle a_n| = \sum_n P_n = 1, \quad (13.59)$$

it follows that

$$A |a_n\rangle \langle a_n| = a_n |a_n\rangle \langle a_n| \leftrightarrow \sum_n A |a_n\rangle \langle a_n| = \sum_n a_n |a_n\rangle \langle a_n| \quad (13.60)$$

and therefore

$$A = \sum_n a_n |a_n\rangle \langle a_n| = \sum_n a_n P_n. \quad (13.61)$$

---

<sup>13</sup>To avoid misunderstandings, we repeat the remark that the last equation is an *operator equation*, i.e. simply two different representations of one operator.

This is called the *spectral representation* of an operator.<sup>14</sup> The spectral representation in the degenerate case is treated in the exercises.

An operator  $C$  whose eigenfunctions are not  $|a_n\rangle$  can be expressed similarly. It is

$$C = \sum_n |a_n\rangle \langle a_n| C \sum_m |a_m\rangle \langle a_m| = \sum_{n,m} c_{nm} |a_n\rangle \langle a_m|, \quad (13.62)$$

with  $c_{nm} = \langle a_n| C |a_m\rangle$ .

### 13.3.2 Projection and Properties

Using projectors, we can make a connection to the term *property* of a system. We again start from an operator  $A$  with the CONS  $\{|a_n\rangle, n = 1, 2, \dots\}$ , with a non-degenerate spectrum, and from the projection operators  $P_n = |a_n\rangle \langle a_n|$ . For these operators, the eigenvalue equation holds:

$$P_n |a_m\rangle = |a_n\rangle \langle a_n |a_m\rangle = \delta_{nm} \cdot |a_m\rangle. \quad (13.63)$$

That means that  $|a_n\rangle$  is an eigenvector of  $P_n$  with eigenvalue 1; all other states  $|a_m\rangle$  with  $n \neq m$  are eigenvectors of  $P_n$  with the eigenvalue 0. In other words:  $P_n$  projects onto a *one-dimensional* subspace of  $\mathcal{H}$ .

We now consider a system in the normalized state  $|\psi\rangle = \sum_n c_n |a_n\rangle$  and the projection operator  $P_k = |a_k\rangle \langle a_k|$ . We have

$$P_k |\psi\rangle = \sum_n c_n P_k |a_n\rangle = \sum_n c_n |a_k\rangle \langle a_k |a_n\rangle = c_k |a_k\rangle. \quad (13.64)$$

This means that the state  $|\psi\rangle$  is an eigenstate of  $P_k$  with the eigenvalue 1 iff  $c_n = \delta_{kn}$  ( $c_k = 1$ , because of the normalization of the state), and with the eigenvalue 0 iff  $c_k = 0$ :

$$\begin{aligned} P_k |\psi\rangle = 1 \cdot |\psi\rangle &\Leftrightarrow |\psi\rangle = c_k |a_k\rangle ; c_k = 1 \\ P_k |\psi\rangle = 0 \cdot |\psi\rangle &\Leftrightarrow |\psi\rangle = \sum_n c_n |a_n\rangle ; c_k = 0. \end{aligned} \quad (13.65)$$

So we can draw the following conclusion:  $P_k = 1$  means ‘if the system is in the state  $|\psi\rangle$  and  $A$  is measured, then the result is  $a_k$ ’ or (in a slightly more casual formulation) ‘ $A$  has a value of  $a_k$ ’ or ‘the system has the property  $a_k$ ’. In this sense, we can understand projection operators as representing yes-no observables, i.e. as a response to the question of whether the value of a physical quantity  $A$  is given by  $a_k$  (1: Yes, the quantum system has the property  $a_k$ ) or not (0: No, the quantum system does not have the property  $a_k$ ).<sup>15</sup>

<sup>14</sup>We have found it already as an example in an exercise of Chap. 11.

<sup>15</sup>We have here a connection to logic (via ‘1  $\hat{=}$  true’ and ‘0  $\hat{=}$  false’). In classical physics, such a statement (the quantity  $A$  has the value  $a_k$ ) is either true or false; in quantum mechanics or quantum logic, the situation may be more complex.

For if a state has a property  $a_k$  (in the sense that it had it before the measurement and the measurement makes us aware of this previously unknown value, e.g. ‘horizontally linear-polarized’), then  $P_k = 1$  and all other projections equal zero,  $P_{n \neq k} = 0$ .<sup>16</sup>

### 13.3.3 Measurements

We have formulated the measurement process already in previous chapters with the help of projection operators—a measurement corresponds to the projection of a state onto a particular subspace, which is one- or multidimensional, as the case may be. Also, the ‘production’ of an initial state at time  $t = 0$  can be regarded as a kind of measurement, because here a superposition state is projected onto a certain subspace. However, this is generally not called ‘measurement’ but rather *preparation* of a state.<sup>17</sup> We want to set down in this section once again the essential terms in the case of degeneracy.

We start at the initial time with a state that evolves unitarily according to the Schrödinger equation until the time of measurement. We assume that this state is a superposition of basis states, as is described by the expansion theorem. Immediately before the measurement, we can for example write

$$|\Psi\rangle = \sum_n \sum_{r=1}^{g_n} c_{n,r} |\varphi_{n,r}\rangle, \quad (13.66)$$

with

$$\langle \varphi_{m,s} | \varphi_{n,r} \rangle = \delta_{m,n} \delta_{r,s}. \quad (13.67)$$

Through the measurement, the state vector is changed; if we measure the system in the state  $m$  (with or without degeneracy; the denominators are due to the normalization), we obtain

$$|\Psi\rangle \xrightarrow{\text{measurement}} \frac{c_m |\varphi_m\rangle}{|c_m|} \text{ or } |\Psi\rangle \xrightarrow{\text{measurement}} \frac{1}{\sqrt{\sum_{r=1}^{g_m} |c_{m,r}|^2}} \sum_{r=1}^{g_m} c_{m,r} |\varphi_{m,r}\rangle \quad (13.68)$$

(reduction of the wave packet, collapse of the wave function). The vector  $\sum_{r=1}^{g_m} c_{m,r} |\varphi_{m,r}\rangle$  is none other than the projection of  $|\Psi\rangle$  onto the subspace belonging to  $m$ ; the projection operator is

<sup>16</sup>More on this topic in Chap. 27, Vol. 2.

<sup>17</sup>Some remarks on terms that arise in connection with ‘measurements’ are given in Appendix S, Vol. 1.

$$P_m = |\varphi_m\rangle \langle \varphi_m| \text{ or } P_m = \sum_{r=1}^{g_m} |\varphi_{m,r}\rangle \langle \varphi_{m,r}|, \tag{13.69}$$

so that we can write (13.68) compactly (i.e. irrespective of whether or not there is degeneracy) as

$$|\Psi\rangle \xrightarrow{\text{measurement}} \frac{P_m |\Psi\rangle}{\sqrt{\langle \Psi | P_m | \Psi \rangle}} = \frac{P_m |\Psi\rangle}{\sqrt{\langle P_m \rangle}}. \tag{13.70}$$

Therefore, a measurement can be understood in this sense as a projection onto a corresponding subspace.<sup>18</sup>

### 13.4 Systematics of the Operators

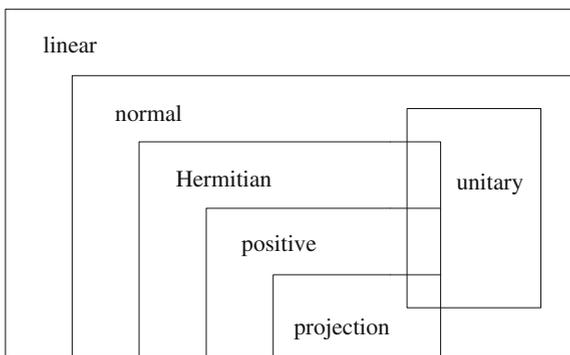
For greater clarity, we want to discuss briefly the ‘family tree’ of the operators used here (see Fig. 13.2); a similar pedigree for matrices can be found in Appendix F, Vol. 1). They are all linear (with the aforementioned exception of the complex conjugation and time reversal operations) and *normal*. An operator  $A$  is called normal if it fulfills  $AA^\dagger = A^\dagger A$ .

We can easily convince ourselves that the operators which are important for quantum mechanics (Hermitian, positive, projection, unitary operators) are all normal:

$$\begin{aligned} A \text{ Hermitian: } A &= A^\dagger \rightarrow AA^\dagger = A^\dagger A \\ U \text{ unitary: } U^{-1} &= U^\dagger \rightarrow UU^\dagger = 1 = U^\dagger U. \end{aligned} \tag{13.71}$$

The interest in normal operators is, among other things, that they can be diagonalized. Actually, we find more generally: An operator can be diagonalized by a

**Fig. 13.2** The family tree of linear operators



<sup>18</sup>We use here the fact that all states  $e^{i\alpha} |\Psi\rangle$  are physically equivalent for arbitrary real  $\alpha$ . See also Chap. 14.

unitary transformation iff it is normal.<sup>19</sup> Non-normal operators can also be diagonalized under some circumstances—but not by a unitary (i.e. length-conserving) transformation. An example is given in the exercises.

Because of the diagonalizability of the operators or matrices occurring in quantum mechanics, we can always expand in terms of eigenfunctions without having to worry about Jordan normal forms or the like. This contributes significantly to the well-behaved character of quantum mechanics.

## 13.5 Exercises

1. Let  $A$  be a linear and  $B$  an anti-linear operator;  $|\varphi\rangle$  is a state. Compute or simplify  $A(i|\varphi\rangle)$  and  $B(i|\varphi\rangle)$ .
2. Show that the complex conjugation  $\mathcal{K}$  is an anti-linear operator.
3. Show that the commutator  $C = [A, B]$  of two Hermitian operators  $A$  and  $B$  is anti-Hermitian.
4. The Hermitian operators  $A$  and  $B$  fulfill  $[A, B] \neq 0$ . Consider the operator  $Q = c[A, B]$ . For which  $c$  is  $Q$  a Hermitian operator?
5. Consider the operator  $Q = AB$ , where  $A$  and  $B$  are Hermitian matrices. Under what conditions is  $Q$  a Hermitian operator?
6. Show in the bra-ket representation that:
  - (a) Hermitian operators have real eigenvalues.
  - (b) The eigenfunctions of Hermitian operators are pairwise orthogonal (assuming the spectrum is not degenerate).
7. Show that the mean value of a Hermitian operator  $A$  is real, and the mean value of an anti-Hermitian operator  $B$  is imaginary.
8. What is the quantum-mechanical operator for the classical term  $\mathbf{p} \times \mathbf{l}$ ?
9. Calculate the mean value of  $\sigma_z$  for the normalized state  $\begin{pmatrix} a \\ b \end{pmatrix}$ .
10. Given the time-independent Hamiltonian  $H$ ; what is the associated time evolution operator  $U(t)$ ?
11. Let  $U$  be the operator  $U = e^{iA}$ , where  $A$  is a Hermitian operator. Show that  $U$  is unitary.
12. What are the eigenvalues that a unitary operator can have?
13. Show that the time evolution operator  $e^{-i\frac{Ht}{\hbar}}$  is unitary.
14. Show that scalar products, matrix elements, eigenvalues and expectation values are invariant under unitary transformations.
15.  $P_1$  and  $P_2$  are projection operators. Under which conditions are  $P = P_1 + P_2$  and  $P = P_1 P_2$  projection operators?
16. Formulate the matrix representation of the operator  $P = |e_1\rangle\langle e_1|$  in  $\mathbb{R}^3$ .
17. What is the general definition of a projection operator?

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<sup>19</sup>The proof is found in Appendix I, Vol. 1.

18. Given the CONS  $\{|\varphi_n\rangle\}$ ; for which  $c_n$  is the operator  $A = \sum c_n |\varphi_n\rangle \langle \varphi_n|$  a projection operator?
19. Which eigenvalues can a projection operator have?
20. Given the CONS  $\{|\varphi_n\rangle\}$  in a Hilbert space of dimension  $N$ . Consider the operator

$$P = \sum_{n \leq N} |\varphi_n\rangle \langle \varphi_n| \quad (13.72)$$

with  $N' \leq N$ . Show that  $P$  is a projection operator.

21. Given the operator  $A$  with degenerate spectrum:

$$A |\varphi_{n,r}\rangle = a_n |\varphi_{n,r}\rangle; \quad r = 1, \dots, g_n. \quad (13.73)$$

- (a) Formulate the projection operator onto the states with subscript  $n$ .
- (b) Formulate the spectral representation of  $A$ .
22. Given the operators  $A = |\varphi\rangle \langle \varphi|$  and  $B = |\psi\rangle \langle \psi|$ . Let  $\langle \varphi | \psi \rangle = \alpha \in \mathbb{C}$ ,  $\alpha \neq 0$ . For which  $\alpha$  is the operator  $C = AB$  a projection operator?
23. Given the operator  $Q = B^\dagger B$ , where  $B$  is unitary. How can  $Q$  be more simply written?
24. Given the operator  $Q = B^\dagger B$ , where  $B$  is not unitary. Show that the eigenvalues of  $Q$  are real and that they are not negative.
25. Given the operator  $A = \beta |\varphi\rangle \langle \psi|$ . Let  $\langle \psi | \varphi \rangle = \alpha \neq 0$ ;  $\alpha$  and  $\beta$  are complex constants. The states  $|\varphi\rangle$  and  $|\psi\rangle$  are normalized. Which conditions must  $|\varphi\rangle$ ,  $|\psi\rangle$ ,  $\alpha$  and  $\beta$  fulfill to ensure that  $A$  is a Hermitian, a unitary, or a projection operator?
26. Given a CONS  $\{|\varphi_n\rangle\}$  and an operator

$$A = \sum_{n,m} c_{nm} |\varphi_n\rangle \langle \varphi_m|; \quad c_{nm} \in \mathbb{C}. \quad (13.74)$$

How must the coefficients  $c_{nm}$  be chosen in order that  $A$  be a Hermitian, a unitary, or a projection operator?

27. A CONS  $\{|\varphi_n\rangle, n = 1, 2, \dots, N\}$  spans a vector space  $\mathcal{V}$ .

(a) Show that each operator  $A$  acting in  $\mathcal{V}$  can be represented as

$$A = \sum_{n,m} c_{nm} |\varphi_n\rangle \langle \varphi_m|. \quad (13.75)$$

(b) Consider the special case  $N = 3$ :

$$A |\varphi_1\rangle = -|\varphi_2\rangle; \quad A |\varphi_2\rangle = -|\varphi_3\rangle; \quad A |\varphi_3\rangle = -|\varphi_1\rangle + |\varphi_2\rangle. \quad (13.76)$$

What is the operator  $A$ ? (Determine the coefficients  $c_{nm}$ , i.e. formulate  $A$  as a linear combination of products  $|\varphi_i\rangle\langle\varphi_j|$ .)

28. How is the generalized Heisenberg uncertainty relation formulated for each of the pairs  $(x, l_x)$ ,  $(x, l_y)$ ,  $(x, l_z)$ ?
29. For the Pauli matrices, the following uncertainty relation holds:

$$\Delta\sigma_x\Delta\sigma_y \geq |\langle\sigma_z\rangle|. \quad (13.77)$$

For which normalized states  $\psi = \begin{pmatrix} a \\ b \end{pmatrix}$  is the right-hand side a minimum/maximum?

30. What is the generalized uncertainty relation for  $H$  and  $\mathbf{p}$ ?
31. The position operator in the Heisenberg picture,<sup>20</sup>  $x_H$ , is given by

$$x_H = e^{i\frac{Ht}{\hbar}} x e^{-i\frac{Ht}{\hbar}}. \quad (13.78)$$

How does this operator depend explicitly on time? The potential is assumed to be constant,  $\frac{dV}{dx} = 0$ . Hint: Use the equation

$$e^{iA} B e^{-iA} = B + i [A, B] + \frac{i^2}{2!} [A, [A, B]] + \frac{i^3}{3!} [A, [A, [A, B]]] + \dots \quad (13.79)$$

or

$$i\hbar \frac{d}{dt} x_H = [x_H, H] \quad (13.80)$$

(or both for practice).

32. A Hamiltonian  $H$  depends on a parameter  $q$ ,  $H = H(q)$ . In addition,  $E(q)$  is a nondegenerate eigenvalue and  $|\varphi(q)\rangle$  the corresponding eigenvector:

$$H(q) |\varphi(q)\rangle = E(q) |\varphi(q)\rangle. \quad (13.81)$$

Show that

$$\frac{\partial E(q)}{\partial q} = \langle\varphi(q)| \frac{\partial H(q)}{\partial q} |\varphi(q)\rangle. \quad (13.82)$$

(This equation is also called the Feynman-Hellmann theorem.)

33.  $\{|n\rangle\}$  is a CONS. Every solution of the SEq may be written as

$$|\psi\rangle = \sum_l a_l |l\rangle \quad (13.83)$$

<sup>20</sup>See also Appendix Q, Vol. 1, ‘Schrödinger picture, Heisenberg picture and interaction picture’.

and every operator  $A$  as

$$A = \sum_{mn} c_{mn} |n\rangle \langle m|. \quad (13.84)$$

Can the non-Hermitian operator  $A$  (i.e.  $c_{mn} \neq c_{mn}^*$  for at least one pair  $n, m$ ) have a real expectation value (for arbitrary states  $|\psi\rangle$ ) under these conditions?

34. We consider the Hamiltonian  $H = 1 + a\sigma_y$ , already introduced in the exercises for Chap. 8.

(a) What is the expected result of the measurement of the  $x$ -component of the spin in the state  $|\psi_t\rangle$  with  $|\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ ?

(b) What is the uncertainty  $\Delta s_x$  in this state?

(c) Calculate the commutator  $[s_x, s_y]$  and formulate the uncertainty relation for the observables  $s_x$  and  $s_y$  for arbitrary times  $t$ .

35. Given an eigenvalue problem  $A |a_m\rangle = a_m |a_m\rangle$  ( $\{|a_m\rangle\}$  is a CONS); we can define a function of the operator by

$$F(A) |a_m\rangle := F(a_m) |a_m\rangle. \quad (13.85)$$

(a) Show that:

$$F(A) = \sum_m F(a_m) P_m \quad (13.86)$$

with  $P_m = |a_m\rangle \langle a_m|$ .

(b) Show that if  $F(a)$  is real for all eigenvalues  $a_m$ , then  $F(A)$  is self-adjoint.

36. What are the conditions which the elements of a two-dimensional normal matrix have to fulfill?

37. Given the matrix

$$A = \begin{pmatrix} 0 & \gamma^2 \\ 1 & 0 \end{pmatrix}; \quad \gamma \neq 0. \quad (13.87)$$

(a) Is  $A$  normal?

(b) Show that  $A$  is diagonalizable for almost all  $\gamma$ , but not by a unitary transformation.

38. In the derivation of the uncertainty relation, the functions must be in the domains of definition of the operators and of the operator products involved. If they are not, we do not obtain meaningful statements. As an example, we consider the function:

$$f(x) = \frac{\sin x^2}{x}. \quad (13.88)$$

(a) Is  $f(x)$  square-integrable?

(b) Is  $f(x)$  within the domains of definition of the operator  $x$ ?

- (c) Can a meaningful uncertainty relation be derived for  $f(x)$ ?  
 (d) Can similar statements be made for the function  $g(x) = \frac{\sin x}{x}$ ?  
 39. Given two operators  $A$  and  $B$  which commute with their commutator,  $[A, [A, B]] = [B, [A, B]] = 0$ . Show that:

$$[B, A^n] = n [B, A] A^{n-1}. \quad (13.89)$$

40. Show that the momentum operator is given in the coordinate representation by  $p = \frac{\hbar}{i} \frac{d}{dx}$ . Make use only of the commutator  $[x, p] = i\hbar$  and derive, making use of the previous exercise, the result:

$$[p, f(x)] = \frac{\hbar}{i} \frac{df(x)}{dx}. \quad (13.90)$$

41. Given two operators  $A$  and  $B$  which commute with their commutator,  $[A, [A, B]] = [B, [A, B]] = 0$ . Show that

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A, B]}. \quad (13.91)$$

This is a special case of the *Baker-Campbell-Hausdorff formula* (relation, theorem). The general case considers  $e^{A+B}$  for two operators, which do not have to commute with their commutator (this is used e.g. in (13.79)). By the way, these authors published their work in 1900, well before the birth of quantum mechanics.

- (a) First, prove the equation

$$[B, e^{xA}] = e^{xA} [B, A] x. \quad (13.92)$$

- (b) Define

$$G(x) = e^{xA} e^{xB} \quad (13.93)$$

and show that the following equation holds:

$$\frac{dG}{dx} = (A + B + [A, B] x) G. \quad (13.94)$$

Integrate this equation.