8 Dynamics of Quantum Systems

This chapter is devoted to the study of the dynamics of quantum systems, based on the formalism presented in Chapter 7 and previous chapters. Given the discussion in Section 4.6 we will use the operator notation and its matrix representation without distinction, moving freely from one to the other as convenient. This will allow us to study the system's evolution from different perspectives, depending on the description adopted. The chapter includes a discussion of the statistical information contained in the quantum formalism and a formal derivation of the Heisenberg inequalities, followed by an introduction to quantum canonical transformations. More advanced topics, which provide a valuable complement, include the relationship between the symmetry properties and the conserved dynamical variables of the system.

8.1 Dynamics in the Heisenberg Description

We will start from the Heisenberg equation of evolution for an operator $\hat{F}$ representing a generic dynamical variable F, introduced in Chapter 3, Eq. (3.43),

$$i\hbar\frac{d\hat{F}}{dt} = i\hbar\frac{\partial\hat{F}}{\partial t} + \left[\hat{F},\hat{H}\right]. \tag{8.1}$$

The description in terms of this equation is called the *Heisenberg description*. Multiplying this equation from the left by the bra $\langle m|$ and from the right by the ket $|n\rangle$ we obtain

$$\frac{d}{dt}\langle m|\widehat{F}|n\rangle = \langle m|\frac{\partial\widehat{F}}{\partial t}|n\rangle + \frac{1}{i\hbar}\langle m|[\widehat{F},\widehat{H}]|n\rangle. \tag{8.2}$$

Note that in this description, the matrix elements F_{mn} evolve because the *operator* $\widehat{F}$ evolves in time according to Eq. (8.1), while the state vectors $|m\rangle$ and $|n\rangle$ do not change. Equation (8.2), on the other hand, contains the complete information about the evolution of $\widehat{F}(\boldsymbol{x},\boldsymbol{p},t)$, encoded in its matrix elements in an *unspecified* description.

Exercise E8.1. Heisenberg's elementary oscillators

Using the basis of energy eigenstates, show that the matrix elements of any time-independent dynamical variable oscillate in time.

Solution. We apply Eq. (8.2) to a dynamical variable F that does not explicitly depend on time,

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

$$i\hbar\frac{d}{dt}\langle m|\widehat{F}|n\rangle = \langle m|[\widehat{F},\widehat{H}]|n\rangle, \tag{8.3}$$

and consider that the ket $|n\rangle$ represents an energy eigenstate, with eigenvalue E_n. Then

$$\begin{aligned}\langle m|[\widehat{F},\widehat{H}]|n\rangle &= \langle m|\widehat{F}\widehat{H}|n\rangle - \langle m|\widehat{H}\widehat{F}|n\rangle \\ &= E_n\langle m|\widehat{F}|n\rangle - E_m\langle m|\widehat{F}|n\rangle = -(E_m - E_n)\langle m|\widehat{F}|n\rangle,\end{aligned} \tag{8.4}$$

which when substituted in (8.3) gives

$$\frac{d}{dt}\langle m|\widehat{F}|n\rangle = -\frac{1}{i\hbar}(E_m - E_n)\langle m|\widehat{F}|n\rangle. \tag{8.5}$$

In terms of the Bohr transition frequency

$$\omega_{mn} = \frac{E_m - E_n}{\hbar}, \tag{8.6}$$

Eq. (8.5) reads

$$\frac{d}{dt}\langle m|\widehat{F}|n\rangle = i\omega_{mn}\langle m|\widehat{F}|n\rangle. \tag{8.7}$$

with solution

$$F_{mn}(t) = \langle m|\widehat{F}|n\rangle = F_{mn}e^{i\omega_{mn}t}, \tag{8.8}$$

We see that the matrix $\hat{F}$ in the energy representation has constant elements on the main diagonal and elements oscillating at a Bohr transition frequency outside it. This complements the results obtained for $x_{mn}(t)$ and $p_{mn}(t)$ in Section 3.5.3.

8.2 The Schrödinger Description

To study the quantum dynamics in the Schrödinger description we take into account that in this description the evolution of the (time-independent) variable F is expressed in the state vectors; in other words, we propose that (8.2) holds because the state vectors $|n\rangle$ and $|m\rangle$ evolve in Hilbert space. In this case, for an operator $\widehat{F}$ that does not depend explicitly on time, we can write from (8.2)

$$i\hbar\langle m|\widehat{F}|\frac{d|n\rangle}{dt} + i\hbar\frac{d\langle m|}{dt}\widehat{F}|n\rangle = \langle m|\widehat{F}\widehat{H}|n\rangle - \langle m|\widehat{H}\widehat{F}|n\rangle. \tag{8.9}$$

We observe that this equation is identically satisfied if

$$i\hbar\langle m|\widehat{F}\frac{d|n\rangle}{dt} = \langle m|\widehat{F}\widehat{H}|n\rangle. \tag{8.10}$$

The rest of Eq. (8.9) gives then

$$-i\hbar\frac{d\langle m|}{dt}\widehat{F}|n\rangle = \langle m|\widehat{H}\widehat{F}|n\rangle, \tag{8.11}$$

which is merely the adjoint of the previous one, with the exchange of the indices m and n; so the equation is indeed satisfied. Writing the solution in the form

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

$$\langle m|\widehat{F}\left[i\hbar\frac{d|n\rangle}{dt}-\widehat{H}|n\rangle\right]=0, \tag{8.12}$$

it follows that for any $\langle m|$, the equation

$$i\hbar\frac{d|n\rangle}{dt}=\widehat{H}|n\rangle \tag{8.13}$$

must hold. This is precisely the time-dependent Schrödinger equation for a state $|n\rangle$, written in Dirac notation.[1] It corresponds to the description of the dynamics studied in Chapter 7, in which the time evolution of the system is expressed in the state vectors, the operators associated to the dynamical variables remaining fixed. For obvious reasons, this form of the theory is called the *Schrödinger representation* or *Schrödinger description*.

The above results confirm that Eq. (8.2), which implicitly contains any description, can be taken as the general evolution equation, abstracting from any reference to one or the other representation. In practice, however, a specific description is chosen as convenient, which may even be different from the two previous ones. An important example is the so-called *interaction description* studied in Section 8.6.6, which is a hybridization of the previous two, very useful for the study of complicated problems of systems in interaction.

8.3 The Dynamics of Expectation Values. Ehrenfest's Theorem

The evolution of the expectation value of a time-independent dynamical variable is described by (8.3) with $m=n$,

$$i\hbar\frac{d\langle\widehat{F}\rangle}{dt}=\langle[\widehat{F},\widehat{H}]\rangle, \tag{8.14}$$

with independence of the description used. In particular, for any $\widehat{F}$ commuting with the Hamiltonian, $d\langle\widehat{F}\rangle/dt=0$ and the quantity $\langle\widehat{F}\rangle$ is conserved. This is of course the case for the Hamiltonian itself, so if the Hamiltonian does not explicitly depend on time, the energy $E=\langle\widehat{H}\rangle$ is an integral of motion of the system. This is the quantum version of the classical law of conservation of energy.

Equation (8.14) applied to different dynamical (time-independent) variables F can be used to obtain a series of particular results, each of which appears in the literature under the name of Ehrenfest's equation; for this reason it is appropriate to call Eq. (8.14) itself *Ehrenfest's theorem*. Applying it to the position operator (in 1D, for simplicity) $\frac{d\langle\widehat{x}\rangle}{dt}=-\frac{i}{\hbar}\langle[\widehat{x},\widehat{H}]\rangle$, with $H=(p^2/2m)+V$, we get

$$\langle\widehat{p}\rangle=m\frac{d\langle\widehat{x}\rangle}{dt}. \tag{8.15}$$

If we *define* $\langle\widehat{p}\rangle\equiv m\langle\widehat{v}\rangle=m\langle\widehat{\dot{x}}\rangle$, it follows that

$$\frac{d\langle\widehat{x}\rangle}{dt}=\left\langle\frac{d\widehat{x}}{dt}\right\rangle=\langle\widehat{\dot{x}}\rangle, \tag{8.16}$$

[1] When going from symbolic states $|n\rangle$ to functions $\langle x|n\rangle=\varphi_n(x)$, it is necessary to make the substitution $d/dt\to\partial/\partial t$.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

and the operations of differentiating with respect to time and taking the expectation value are interchangeable. This is general, as can be seen by combining the expectation value of (8.1) (for time-independent F) with (8.14),

$$\left\langle \frac{d\widehat{F}}{dt} \right\rangle = \frac{1}{i\hbar} \langle [\widehat{F}, \widehat{H}] \rangle = \frac{d\langle \widehat{F} \rangle}{dt}. \tag{8.17}$$

We now take $\widehat{F} = \widehat{p}$ in (8.14) to obtain $\frac{d\langle \widehat{p} \rangle}{dt} = -\frac{i}{\hbar} \langle [\widehat{p}, \widehat{H}] \rangle$, whence

$$\frac{d\langle \widehat{p} \rangle}{dt} = \langle -\left(\frac{\partial \hat{V}}{\partial x} \right) \rangle = \langle f(\widehat{x}) \rangle. \tag{8.18}$$

Combining Eqs. (8.15) and (8.18), we get

$$m \frac{d^2 \langle \widehat{x} \rangle}{dt^2} = \langle f(\widehat{x}) \rangle. \tag{8.19}$$

The preceding results show that $\langle \widehat{x} \rangle$ and $\langle \widehat{p} \rangle$ satisfy *classical-like* relations in accordance with Ehrenfest's theorem. However, Eq. (8.19), which can be seen as the quantum version of Newton's second law, differs from it in an important way. Indeed, for the coordinate $\langle \widehat{x} \rangle$ of a classical particle we must write

$$m \frac{d^2 \langle x \rangle}{dt^2} = f(\langle x \rangle) \tag{8.20}$$

instead of (8.19). The force $f(\langle x \rangle)$ and the *mean* force $\langle f(x) \rangle$ are different quantities, since the former is a local function at $\langle x \rangle$, whereas $\langle f(x) \rangle$ depends on the value of f in the whole accessible space. The difference can be made explicit by writing x in terms of its mean value and its deviation Δx,

$$x = \bar{x} + \Delta x, \quad \bar{x} \equiv \langle x \rangle, \tag{8.21}$$

and expanding $f(x)$ around $\bar{x}$,

$$f(x) = f(\bar{x} + \Delta x) = f(\bar{x}) + \Delta x f'(\bar{x}) + \tfrac{1}{2} (\Delta x)^2 f''(\bar{x}) + \ldots \tag{8.22}$$

Taking the mean value of this expression gives, with $\langle \Delta x \rangle = 0$,

$$\langle f(x) \rangle = f(\bar{x}) + \tfrac{1}{2} \langle (\Delta x)^2 \rangle f''(\bar{x}) + \ldots \tag{8.23}$$

and substituting in (8.19) we get

$$m \frac{d^2 \bar{x}}{dt^2} = f(\bar{x}) + \tfrac{1}{2} \langle (\Delta x)^2 \rangle f''(\bar{x}) + \ldots, \tag{8.24}$$

which differs from Eq. (8.20) by the presence of terms that depend on higher-order moments $\langle (\Delta x)^n \rangle$. In other words, stochasticity makes the average quantum trajectory of the particles differ in general from the corresponding classical one. For the case of *linear* forces $f = a + bx$ (free particle, uniform electric field, harmonic oscillator and their linear combinations) the second and higher derivatives of the external force are all zero and the quantum expression (8.24) reduces to the classical one (8.20); however, the analogy is only formal, since in the latter case the absence of fluctuations is central.

The quantum Eq. (8.19) describes the acceleration of the average value $\langle x \rangle$ as determined by the value of the force $f(x)$ averaged over the entire accessible space. When referred to a single particle (located in the mean at $\langle x \rangle$), Eq. (8.20) introduces a nonlocal

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

element in the description. In Chapter 5 we found examples of this kind of nonlocalities when studying the dispersion of particles by a potential barrier. Such (apparent) nonlocalities are the result of reading (interpreting) the statistical description given by Eq. (8.19) in nonstatistical terms, as if it referred to a single particle, as is suggested by the Copenhagen point of view. Their appearance in the quantum description is one of the several arguments in favor of the ensemble interpretation of QM, as discussed in Section 10.1.2 in connection with the (nonlocal) quantum potential.

Exercise E8.2. Quantum virial theorem
Derive the quantum version of the virial theorem of classical mechanics for a particle subject to a potential V.

Solution. The virial theorem of classical mechanics is usually derived by analyzing the behavior of the time average of the quantity $\sum_i \boldsymbol{r}_i \cdot \boldsymbol{p}_i$, where the sum extends over all particles in the system.[2] For the derivation of a quantum version of this theorem, the same idea can be used, but applied to the average over the ensemble in a stationary state.

For a system in a stationary state, whose motion is restricted to a finite region of space, it must be true that

$$\frac{d}{dt}\langle \boldsymbol{r} \cdot \hat{\boldsymbol{p}} \rangle = 0. \tag{8.25}$$

On the other hand, from Eq. (8.14) it follows that

$$i\hbar \frac{d}{dt}\langle \boldsymbol{r} \cdot \hat{\boldsymbol{p}} \rangle = \langle [\boldsymbol{r} \cdot \hat{\boldsymbol{p}}, \widehat{H}] \rangle. \tag{8.26}$$

From

$$[x\widehat{p}_x, \widehat{H}] = [x\widehat{p}_x, \frac{\widehat{p}_x^2}{2m}] + [x\widehat{p}_x, V] = [x, \widehat{p}_x^2]\frac{\widehat{p}_x}{2m} + x[\widehat{p}_x, V] = i\hbar\frac{\widehat{p}_x^2}{m} - i\hbar x\frac{\partial V}{\partial x}, \tag{8.27}$$

we get

$$[\boldsymbol{r} \cdot \hat{\boldsymbol{p}}, \widehat{H}] = i\hbar\left(\frac{\widehat{\boldsymbol{p}}^2}{m} - \boldsymbol{r} \cdot \nabla V\right), \tag{8.28}$$

which when substituted in the preceding equation of motion gives

$$\frac{d}{dt}\langle \boldsymbol{r} \cdot \hat{\boldsymbol{p}} \rangle = 2\langle \widehat{T} \rangle - \langle \mathbf{r} \cdot \nabla V \rangle. \tag{8.29}$$

For the bounded stationary case, condition (8.25) gives the virial theorem[3]

$$2\langle \widehat{T} \rangle = \langle \boldsymbol{r} \cdot \nabla V \rangle. \tag{8.30}$$

Several particular cases are of interest. For example, for a central potential

$$2\langle \widehat{T} \rangle = \langle r\frac{\partial V}{\partial r} \rangle, \tag{8.31}$$

[2] See, e.g., Goldstein et al. (2011).
[3] The name reflects the fact that the quantity $\boldsymbol{r} \cdot \nabla V$ is called virial (from Latin *vis*, force).

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

and if in addition the potential is of the form $V = ar^n$, then

$$\langle \widehat{T} \rangle = \frac{n}{2} \langle V \rangle = \frac{n}{n+2} E. \tag{8.32}$$

For a harmonic oscillator ($n = 2$) we have $\langle \widehat{T} \rangle = \langle V \rangle = \frac{1}{2}E$, while for a Coulomb potential ($n = -1$), we have $\langle T \rangle = -\frac{1}{2}\langle V \rangle = -E$. If the quantum average is interpreted as a time average – which is equivalent to assuming that each member of the ensemble reproduces the ensemble over time, that is, that the system has ergodic properties – all the above results are in agreement with the corresponding classical ones.

8.4 Elements for a Statistical Description

In the following, we will discuss the most important statistical properties of a quantum system.

8.4.1 The meaning of eigenvalues

We have seen in a number of examples throughout the book that when a physical system is in an eigenstate of an operator, the expectation value of that operator coincides with its eigenvalue, that is,

$$\widehat{F}|n\rangle = F_n|n\rangle \;\Rightarrow\; F_{nn} = \langle n|\widehat{F}|n\rangle = F_n. \tag{8.33}$$

Expressed in the Schrödinger representation, if

$$\widehat{F}\psi_n = F_n\psi_n, \tag{8.34}$$

the expectation value of $\widehat{F}$ in the state ψ_n is

$$\langle \widehat{F} \rangle_n = \int \psi_n^* \widehat{F} \psi_n dx = F_n. \tag{8.35}$$

The statistical explanation for this is that the ensemble described by ψ_n has been constructed in such a way that each and every one of its members has exactly the value F_n of the variable F, so that by taking the average we get F_n as a result. For example, the solution of the stationary Schrödinger equation $\widehat{H}\psi_n = E\psi_n$ (which is an eigenvalue equation), is a state function ψ_n corresponding to particles that all have the same energy E_n, as we saw in Chapter 4. A second example is given by the momentum equation $\hat{p}\psi = -i\hbar(\partial\psi/\partial x) = p\psi$; the solution of this differential equation, $Ae^{ipx/\hbar}$, describes a stationary plane wave with well-defined momentum p.

It is only possible to assign a single, well-defined value to a dynamical variable F if the system is in an eigenstate of the corresponding operator $\hat{F}$. In the general case where ψ is not an eigenstate of $\hat{F}$, the value of the corresponding variable is distributed among the elements of the ensemble.

The preparation process to obtain a desired eigenstate is, of course, a matter of specific manipulation (preparation) of the ensemble, a very important subject but beyond our present scope; see, however, the comment in Section 8.4.4.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

8.4.2 Basic statistical elements

In Section 3.2.3 we introduced the variance or mean-square dispersion of $\widehat{F}$, defined as

$$\langle(\Delta\widehat{F})^2\rangle = \langle\widehat{F}^2\rangle - \langle\widehat{F}\rangle^2. \tag{8.36}$$

It is usual to also define the *standard deviation* (root mean square or *rms*), which is the square root of the variance and is sometimes written as ΔF or $\Delta_\psi F$ to make the dependence on the state explicit,

$$\Delta F \equiv (\Delta\widehat{F})_{\text{rms}} \equiv \sqrt{\langle(\widehat{F} - \langle\widehat{F}\rangle)^2\rangle} = \sqrt{\langle(\Delta\widehat{F})^2\rangle}. \tag{8.37}$$

When there is no risk of confusion, it is usual to write the average value of $\widehat{F}$ as $\langle\widehat{F}\rangle = \bar{F}$. Since, when applied to functions, the variance of F ($= \int (F - \bar{F})^2\rho(x)dx$) is a sum of squares of deviations, any deviation (positive or negative) of the variable F from its mean value $\bar{F}$ adds to the result; this means that the variance of a variable is zero if and only if the variable has *exactly* the same value for each member of the ensemble. Even though in the quantum case we are dealing with operators (and $(\Delta\widehat{F})^2$ is not necessarily a positive quantity), it is common to consider (8.36) as the definition of variance. Note, however, that the definition of the powers of an operator in the form

$$\widehat{F^2} = \hat{F}^2, \tag{8.38}$$

which is an integral part of the quantum formalism, is not the only one possible in principle, and the following conclusions depend crucially on it.[4]

8.4.3 Simultaneous well-defined variables

Suppose we set up a system in an eigenstate of $\hat{H}$, so that the energy has a well-defined value. Under these conditions, what other variables could be well defined? A well-known example of a wave function that is a simultaneous eigenfunction of two operators ($\hat{H}$ and $\hat{p}$ in this case) is the free particle described by a plane wave. We then have $(\hat{p}^2/2m)\varphi_p(x) = E\varphi_p(x)$, and $\hat{p}\varphi_p(x) = p\varphi_p(x)$. These eigenvalue equations have the common solution $\varphi_p(x) = Ae^{ipx/\hbar}$; the particles described by this solution have well-defined energy E and momentum p.

The general answer is that it is possible to set up the system so that two (or more) of its dynamical variables F, G have well-defined values *if and only if their respective operators commute*.

[4] Note that (8.38) expresses a relation between operators, not between the values assigned to them. Indeed, if one wanted to apply a similar relation between the values V that a dynamical variable $\hat{A}$ can take, it should be possible to write

$$V_\psi(F(\hat{A})) = F(V_\psi(\hat{A})),$$

which (hypothetically) states that in the given state ψ, the value of a function of A is equal to the function evaluated at the value of the variable over that state. However, the *Kocher and Specker theorem* (1967) states that such a function V_ψ *does not exist* if the corresponding Hilbert space has more than two dimensions. An immediate implication of this result is that in a Hilbert space with more than two dimensions (which means that there can be more than four linearly independent dynamical variables) there is no state for which it is possible to simultaneously assign definite values to each of the dynamical variables of the system.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

Here we show that the condition is necessary. By hypothesis, both $\widehat{F}$ and $\widehat{G}$ have well-defined values,

$$\widehat{F}\psi_n = F_n\psi_n, \quad \widehat{G}\psi_n = G_n\psi_n, \tag{8.39}$$

so that by applying $\widehat{G}$ from the left to the first equation

$$\widehat{G}\widehat{F}\psi_n = \widehat{G}F_n\psi_n = F_n\widehat{G}\psi_n = F_nG_n\psi_n, \tag{8.40}$$

and applying $\widehat{F}$ to the second equation

$$\widehat{F}\widehat{G}\psi_n = G_n\widehat{F}\psi_n = G_nF_n\psi_n, \tag{8.41}$$

we get $\widehat{F}\widehat{G}\psi_n = \widehat{G}\widehat{F}\psi_n$. Since this must hold for every ψ_n, we conclude that $\widehat{F}\widehat{G} = \widehat{G}\widehat{F}$. It is left to the student to prove that the condition is sufficient.

8.4.4 Well-defined and distributed variables

The preceding results suggest that once a starting operator has been selected, the remaining operators can be divided into two groups: those that commute with the selected operator and among themselves, and the rest of the operators. The first group is the *maximal set of commuting operators* (MSCO). Each operator can belong to one or the other group, this strongly depends on which was the initial selection; however, we know from the quantum canonical commutator $[x, p] = ih$ that not all operators can belong to the MSCO, that is, the noncommuting group is never empty. In fact, the number of variables in an MSCO is generally very small: 3, 4…, not much more.

The classification is not unambiguous, since it is based on an initial arbitrary choice of the reference operator. However, in each particular case we can add appropriate criteria to define the two groups uniquely; we will assume that this has been done. Under these conditions, it is possible to prepare the system – at least in principle; the "preparation" of the state is usually a practical task – in a common eigenstate of all the MSCO operators, with the result that all these variables are dispersion-free. This means that the remaining dynamical variables (the non-MSCO variables) will be distributed without exception. In other words, *every quantum state is necessarily dispersive.*

Each dynamical variable belonging to the MSCO group gives rise to a *quantum number*; the corresponding operator satisfies an eigenvalue equation and the corresponding eigenvalue (or a number derived from it) becomes a quantum number of the state. Therefore, we can expect a physical system to have a small amount of quantum numbers in general.

As an example, suppose that the chosen initial variable is the Hamiltonian for a central-force problem, with eigenvalue n; the angular momentum L is then added, with eigenvalue l, and the projection l_z with eigenvalue m completes the MSCO: the system has been prepared in state $|nlm\rangle$, which precises the basis for the description. If, given such a common eigenstate, we were to make a series of measurements to determine the numerical value of any variable of the MSCO group, we would obtain the same value each time (apart from the inevitable experimental errors).

On the other hand, a series of measurements on a given variable of the non-MSCO group, would give different results each time, unpredictable from case to case. If the

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

series of measurements is large enough, a law of distribution for that variable will eventually emerge. We see here one of the inevitable effects of quantum randomness: it is impossible to prepare a quantum system so that each of its dynamical variables has a well-defined value. This is a key feature that distinguishes quantum systems from classical ones and confirms the inevitability of the statistical approach.

8.4.4.1 Examples of well-defined and distributed variables

a) Consider first the case of particles moving in a potential $V(x)$. Then the momentum and the Hamiltonian operators do not commute, $[\widehat{p}, \widehat{H}] \neq 0$. So if we give all the particles the same energy, their momentum will be distributed; they will form a wave packet in momentum space.

b) A second example of great interest is that of an arbitrary pair of canonical variables. The fact that, for example, $\left[x, p\right] = ih$ means that a quantum system cannot be prepared so that all the members of the ensemble have exactly the same momentum and are simultaneously at the same point, that is, the product of the dispersions of x and p_x cannot vanish. In our idealization of the description of the free particle with a plane wave of well-defined momentum, the particles were uniformly distributed in space; only by distributing the momentum within a packet of plane waves can the system acquire finite dimensions in x-space.

c) It could be argued that even if we accept that most of the variables are distributed (those that do not belong to the MSCO), this may not be important in practice if the system is prepared so that the dispersions are made small enough as to be considered negligible. In the next section we will show that this is not possible, since the dispersions are usually significant when compared to the characteristic values of the corresponding variables.

8.5 The Heisenberg Inequalities and Their Meaning

To give quantitative form to the preceding discussion, we begin with two simple auxiliary results of general use. First, we show that $\langle \widehat{A}^\dagger \widehat{A} \rangle_\psi$ is nonnegative for any operator (not necessarily Hermitian) and any state $|\psi\rangle$. We use the representation $\widehat{A} = \sum_k a_k |k\rangle \langle k|$ (the coefficients a_k can be complex for $\hat{A}$ not Hermitian) and by inserting a pair of unit expansions we get

$$\begin{aligned}\langle \widehat{A}^\dagger \widehat{A} \rangle_\psi &= \langle \psi | \widehat{A}^\dagger \widehat{A} | \psi \rangle = \sum_{k,l} \langle \psi | a_k^* | k \rangle \langle k | a_l | l \rangle \langle l | \psi \rangle = \sum_{k,l} \langle \psi | a_k^* a_l | k \rangle \delta_{kl} \langle l | \psi \rangle \\ &= \sum_k |a_k|^2 \langle \psi | k \rangle \langle k | \psi \rangle = \sum_k |a_k|^2 |\langle k | \psi \rangle|^2 \geq 0, \end{aligned} \tag{8.42}$$

hence (recall that $\widehat{A}^\dagger$ contains the operation $\widehat{A}^*$)

$$\langle \widehat{A}^\dagger \widehat{A} \rangle \geq 0. \tag{8.43}$$

Now let $\widehat{A}$ and $\widehat{B}$ be two operators with commutator $i\widehat{C}$,

$$[\widehat{A}, \widehat{B}] = i\widehat{C}. \tag{8.44}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

The commutator of the deviations $\Delta\widehat{A}$ and $\Delta\widehat{B}$ is $[\Delta\widehat{A}, \Delta\widehat{B}] = [\widehat{A}-\overline{A}, \widehat{B}-\overline{B}] = [\widehat{A}, \widehat{B}]$; therefore,

$$[\Delta\widehat{A}, \Delta\widehat{B}] = i\widehat{C}. \tag{8.45}$$

This is our second observation; we now turn to the proof of Heisenberg's inequality, by considering the function $J(\alpha)$,

$$J(\alpha) = \langle(\alpha\widehat{A} + i\widehat{B})^{\dagger}(\alpha\widehat{A} + i\widehat{B})\rangle. \tag{8.46}$$

where α is a real parameter. From (8.43) applied to $\alpha\widehat{A} + i\widehat{B}$ it follows that

$$J(\alpha) \geq 0. \tag{8.47}$$

We will take $\widehat{A}$ and $\widehat{B}$ to be Hermitian, so $(\alpha\widehat{A} + i\widehat{B})^{\dagger} = \alpha\widehat{A} - i\widehat{B}$; substituting and expanding, we get

$$J(\alpha) = \alpha^2\langle\widehat{A}^2\rangle + \langle\widehat{B}^2\rangle + i\alpha\langle\widehat{A}\widehat{B} - \widehat{B}\widehat{A}\rangle \geq 0. \tag{8.48}$$

As a function of α, J describes a parabola in the upper half-plane, which takes its minimum value for $\alpha = \alpha_m$ and $J'(\alpha_m) = 0$ with

$$\alpha_m = -\frac{i\langle\widehat{A}\widehat{B} - \widehat{B}\widehat{A}\rangle}{2\langle\widehat{A}^2\rangle} = \frac{\langle\widehat{C}\rangle}{2\langle\widehat{A}^2\rangle}. \tag{8.49}$$

This minimum is

$$J_{\min} = J(\alpha_m) = \frac{\langle\widehat{C}\rangle^2}{4\langle\widehat{A}^2\rangle} + \langle\widehat{B}^2\rangle - \frac{\langle\widehat{C}\rangle^2}{2\langle\widehat{A}^2\rangle} = \langle\widehat{B}^2\rangle - \frac{\langle\widehat{C}\rangle^2}{4\langle\widehat{A}^2\rangle} \geq 0. \tag{8.50}$$

Multiplying the result by $\langle\widehat{A}^2\rangle$ and reorganizing gives

$$\langle\widehat{A}^2\rangle\langle\widehat{B}^2\rangle \geq \tfrac{1}{4}\langle\widehat{C}\rangle^2, \tag{8.51}$$

or using (8.45),

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle \geq \tfrac{1}{4}\langle\widehat{C}\rangle^2. \tag{8.52}$$

This is a general version of the Heisenberg inequality, a particular version of which was derived in Section 3.6 for the variances of $\hat{x}$ and $\hat{p}$,

$$\langle(\Delta\widehat{x})^2\rangle\langle(\Delta\widehat{p})^2\rangle \geq \tfrac{1}{4}\hbar^2. \tag{8.53}$$

In the general case of conjugate canonical variables A, B we have $\left|\langle\widehat{C}\rangle\right| = \hbar$ and the Heisenberg inequalities take the form

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle \geq \tfrac{1}{4}\hbar^2. \tag{8.54}$$

Equation (8.52) makes clear the meaning and content of Heisenberg's inequality: the product of the dispersions is bounded from below by the mean value of the commutator. This is an inviolable theorem of QM, relating to objective statistical properties of the system.

Exercise E8.3. A stronger Heisenberg inequality

Derive an inequality that is stronger than (8.52) by expressing the product $\hat{A}\hat{B}$ in terms of their commutator and anticommutator. *Hint*: use the Schwarz inequality.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

Solution. Proceeding as before, we write for $\overline{A} = \overline{B} = 0$, which is always possible; then

$$\begin{aligned}\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle &= \left[\int \left(\psi^*\hat{A}\right)\left(\hat{A}\psi\right)dx\right]\left[\int \left(\psi^*\hat{B}\right)\left(\hat{B}\psi\right)dx\right] \\ &= \left[\int \left(\hat{A}\psi\right)^\dagger\left(\hat{A}\psi\right)dx\right]\left[\int \left(\hat{B}\psi\right)^\dagger\left(\hat{B}\psi\right)dx\right] \\ &= \left[\int \left|\hat{A}\psi\right|^2 dx\right]\left[\int \left|\hat{B}\psi\right|^2 dx\right] \\ &\geq \left|\int \left(\hat{A}\psi\right)^\dagger\left(\hat{B}\psi\right)dx\right|^2 = \left|\int \psi^*\hat{A}\hat{B}\psi dx\right|^2, \end{aligned} \tag{8.55}$$

where we have used the Schwarz inequality. Introducing now the identity

$$\hat{A}\hat{B} = \tfrac{1}{2}\left[\hat{A},\hat{B}\right] + \tfrac{1}{2}\left\{\hat{A},\hat{B}\right\}, \tag{8.56}$$

where $\left\{\hat{A},\hat{B}\right\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ is the anticommutator, we get

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle \geq \left|\int \psi^*\hat{A}\hat{B}\psi dx\right|^2 = \left|\left\langle\hat{A}\hat{B}\right\rangle\right|^2 = \tfrac{1}{4}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle + \left\langle\left\{\hat{A},\hat{B}\right\}\right\rangle\right|^2. \tag{8.57}$$

For Hermitian operators $\left\langle\left[\hat{A},\hat{B}\right]\right\rangle^\dagger = -\left\langle\left[\hat{A},\hat{B}\right]\right\rangle$; this gives, after some simplification, the stronger relation

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle \geq \tfrac{1}{4}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|^2 + \tfrac{1}{4}\left|\left\{\left\langle\hat{A},\hat{B}\right\rangle\right\}\right|^2. \tag{8.58}$$

It is easy to show that the equal sign holds only if $\hat{A}$ and $\hat{B}$ are related by a constant of proportionality, that is, if they refer to the same state. The preceding result can also be obtained using the previous derivation, taking α as a complex parameter.

8.5.1 What do the Heisenberg inequalities tell us?

As already mentioned, the Heisenberg inequalities are commonly referred to in the literature as *uncertainty* or *indeterminacy relations*. To avoid unnecessary and misleading allusions, we prefer not to add such qualifiers, which imply specific (and different) interpretations, the former often subjective and the latter indeterministic.

Sometimes we read in texts on QM that Eq. (8.53) tells us that particle trajectories do not exist – as Heisenberg himself concluded. It is true that the quantum description does not contain the notion of trajectories and does not describe them; but it does allow us to determine some of their properties, such as the variances and other statistical moments of the position and momentum variables. According to Heisenberg's inequality, paths of equally prepared electrons differ from electron to electron in such a way that the product of the dispersions of x and p always satisfies (8.53), and similarly for any conjugate pair $\widehat{A}, \widehat{B}$; since (8.52) has a statistical meaning, it does not apply to a single case, but to an ensemble of realizations. This is true whether we observe them or not, it is a corollary of the formalism which does not include the act of observation.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

Note that the Heisenberg inequality does not imply that as the standard deviation of a variable decreases, the standard deviation of the corresponding conjugate canonical variable necessarily increases; in fact, the opposite may be true. To see this, consider the case of conjugate canonical variables,

$$\Delta_\psi q \Delta_\psi p \geq \tfrac{1}{2}\hbar, \tag{8.59}$$

for a particle subject to a binding potential. The more excited the bound state ψ is, the higher are the values of $\Delta_\psi q$ and $\Delta_\psi p$. When the excitation is reduced, it usually happens that both standard deviations decrease simultaneously, but their product still satisfies Heisenberg's inequality. For example, for the 1D harmonic oscillator studied in Chapter 9,

$$\langle(\Delta\widehat{x})^2\rangle = (n+\tfrac{1}{2})\frac{\hbar}{m\omega}; \quad \langle(\Delta\widehat{p})^2\rangle = (n+\tfrac{1}{2})\hbar m\omega, \tag{8.60}$$

where $n = 0, 1, 2, \ldots$ is the level of the excitation; thus,

$$\langle(\Delta\widehat{x})^2\rangle\langle(\Delta\widehat{p})^2\rangle = \tfrac{1}{4}\hbar^2(1+2n)^2 \geq \tfrac{1}{4}\hbar^2, \tag{8.61}$$

so that both dispersions can decrease simultaneously.

Heisenberg's inequalities are sometimes used to obtain semi-quantitative information about the dynamical behavior of a physical system. For example, consider the case of a particle in a stationary state, subject to a binding potential that depends only on x; (8.52) gives

$$\langle(\Delta\widehat{x})^2\rangle\langle(\Delta\widehat{H})^2\rangle \geq \frac{\hbar^2}{4m^2}\langle\widehat{p}\rangle^2. \tag{8.62}$$

Since $\langle(\Delta H)^2\rangle = 0$ and $\langle(\Delta x)^2\rangle < \infty$, we conclude that the mean value of p is zero (as shown with the examples of Chapter 5). Taking now the commutator

$$[\widehat{p}, \widehat{H}] = i\hbar\hat{f}, \tag{8.63}$$

where $\hat{f}(x)$ represents the external force, and using again Eq. (8.52), we obtain

$$\langle(\Delta\widehat{p})^2\rangle\langle(\Delta\widehat{H})^2\rangle \geq \tfrac{1}{4}\hbar^2\langle\hat{f}\rangle^2. \tag{8.64}$$

Therefore, for any real (i.e., with $\langle(\Delta\widehat{p})^2\rangle$ finite) bound eigenstate of the Hamiltonian, the mean value of the force is zero. This result is to be expected for any stationary state, classical or quantum.

Exercise E8.4. A minimum-dispersion packet

A state for which $\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle = \frac{1}{4}\langle\widehat{C}\rangle^2$ is called a minimum-dispersion packet with respect to the variables A and B. Construct a state in x-space, $\psi_{\min}(x)$, for which the Heisenberg inequality becomes an equality (remember that the substitution $\hat{A} \to \Delta\hat{A}$ can be made).

Solution. The definition of minimum dispersion requires the function $J(\alpha)$ in Eq. (8.47) to be zero, which only happens if

$$(\alpha\Delta\widehat{A} + i\Delta\widehat{B})\psi_{\min} = 0, \tag{8.65}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

as follows from Eq. (8.46). In this expression, α must have the value α_m that minimizes J, which is given by Eq. (8.49), $\alpha_m = \langle\widehat{C}\rangle/2\langle\widehat{A}^2\rangle$. The minimum-dispersion packet is therefore a solution of the differential equation

$$\left(\frac{\langle\widehat{C}\rangle}{2\langle(\Delta\widehat{A})^2\rangle}\Delta\widehat{A} + i\,\Delta\widehat{B}\right)\psi_{\min} = 0. \tag{8.66}$$

Taking $\widehat{A} = \widehat{x}$, $\widehat{B} = \widehat{p}$ and moving to the coordinate system with $\langle\widehat{x}\rangle = \langle\widehat{p}\rangle = 0$, $\langle\widehat{C}\rangle = \hbar$, we get

$$\left(\frac{x}{2\sigma^2} + \frac{\partial}{\partial x}\right)\psi_{\min} = 0, \quad \sigma^2 = \langle(\Delta x)^2\rangle, \tag{8.67}$$

whose solution,

$$\psi_{\text{mín}} = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{\frac{1}{2}} \exp\left[-\frac{(x-\langle x\rangle)^2}{4\sigma^2}\right], \tag{8.68}$$

is a Gaussian (normal) distribution with variance $\langle(\Delta\widehat{x})^2\rangle = \sigma^2$ and centered at $\langle\widehat{x}\rangle$.

For a harmonic oscillator, $m\omega\Delta x = \Delta p = \hbar/2$, which means that both quadratures have the same dispersion. As will be shown in Chapter 9, this solution is the coherent, minimal-dispersion packet.[5]

8.5.2 Combining equations of motion and the Heisenberg inequalities

To conclude this section, we will combine Ehrenfest's equation (8.14) with Heisenberg's inequality (8.52). If we set $\widehat{B} = \widehat{H}$ in the latter, we get

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{H})^2\rangle \geq \tfrac{1}{4}\langle\widehat{C}\rangle^2, \tag{8.69}$$

where

$$\left\langle\widehat{C}\right\rangle = -i\left\langle[\widehat{A},\widehat{H}]\right\rangle = \hbar\frac{d\langle\widehat{A}\rangle}{dt}, \tag{8.70}$$

as follows from Eq. (8.14). Therefore,

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{H})^2\rangle \geq \tfrac{1}{4}\hbar^2\left(\frac{d\langle\widehat{A}\rangle}{dt}\right)^2. \tag{8.71}$$

From this it follows, in particular, that when the system is in an eigenstate of either the Hamiltonian or the operator $\widehat{A}$, the average value $\langle\widehat{A}\rangle$ is constant. Equation (8.71) can be written in a slightly different form, which is obtained by dividing it by $(d\langle\widehat{A}\rangle/dt)^2$,

$$\langle(\Delta\widehat{H})^2\rangle\left\langle\left(\frac{\Delta\widehat{A}}{d\langle\widehat{A}\rangle/dt}\right)^2\right\rangle \geq \tfrac{1}{4}\hbar^2. \tag{8.72}$$

[5] For an oscillator in a *squeezed* state such that $\lambda^{-1}m\omega\Delta x = \lambda\Delta p = \hbar/2$ with $\lambda \neq 1$, the dispersion in one of the variables has increased at the expense of the other; their product remains minimal, but the energy increases. Squeezed states of light are an interesting topic in quantum optics and have been studied extensively experimentally since the 1980s.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

This result is known as the *Mandelstam–Tamm*[6,7] *inequality* or *relation* (1945) and can be interpreted as follows. We introduce a time τ_A defined as

$$\tau_A = \sqrt{\langle(\Delta\widehat{A})^2\rangle} \Big/ \left|\frac{d\langle\widehat{A}\rangle}{dt}\right|, \tag{8.73}$$

representing the mean time required by $\langle\widehat{A}\rangle$ to change by an amount of the order of its standard deviation, which we may call the *evolution time* of $\widehat{A}$. Equation (8.72) can then be written

$$\langle(\Delta\widehat{H})^2\rangle\tau_A^2 \geq \tfrac{1}{4}\hbar^2, \tag{8.74}$$

which shows that the evolution time is not arbitrarily short, but is bounded from below by the standard deviation of the energy,

$$\tau_A(\Delta H) \geq \frac{\hbar}{2}. \tag{8.75}$$

For an eigenstate of $\widehat{H}$, τ_A becomes infinite, which means that the dynamical variables then take an infinitely long time to change, or, in other words, that they do not change. From this point of view, τ_A is a specific measure of the "degree of stationarity" of the system.

8.6 Quantum Canonical Transformations

We are now equipped with the necessary elements to study the evolution of the quantum states using the propagator method introduced in Chapter 7. We then turn to an introduction to more powerful operator procedures that allow us to switch between different representations.

8.6.1 The evolution operator and the propagator

We will study the time evolution of a state $|\psi\rangle$ using Schrödinger's description. For a Hamiltonian $\widehat{H}$ that does not depend on time, the formal solution of the evolution equation (7.140), $i\hbar\frac{d|\psi\rangle}{dt} = \widehat{H}|\psi\rangle$, is

$$|\psi\rangle = e^{-\frac{i}{\hbar}\widehat{H}t}|\psi_0\rangle; \quad |\psi_0\rangle \equiv |\psi(t=0)\rangle. \tag{8.76}$$

This allows us to introduce the *evolution operator*

$$\widehat{S}(t) = e^{-\frac{i}{\hbar}\widehat{H}t}, \tag{8.77}$$

[6] Leonid Isaakovich Mandelstam (1879–1944) was a Russian-Soviet physicist co-discoverer of the Raman scattering; he founded one of the two major schools of theoretical physics in the Soviet Union, the other being due to L. Landau.

[7] Igor Yevgenyevich Tamm (1895–1971) was a Russian-Soviet theoretical physicist who received the 1958 Nobel Prize for his co-discovery of the Cherenkov radiation. He also predicted the phonon and together with A. Sakharov proposed the Tokamak system for the (successful) construction of the toroidal magnetic thermonuclear reactor.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

so that

$$|\psi(t)\rangle = \widehat{S}(t)|\psi_0\rangle. \tag{8.78}$$

Substituting this in (7.140) and simplifying gives the equation for the evolution operator itself,

$$i\hbar\frac{d\widehat{S}(t)}{dt} = \widehat{H}\widehat{S}(t). \tag{8.79}$$

Equation (8.78) is a formal way of writing an integral expression. To obtain the latter explicitly we multiply it from the left by $\langle x|$ and introduce on the right-hand side an expansion of the unit in terms of the basis; we thus obtain

$$\psi(x,t) = \int K(x,t|x't')|\psi(x',t')dx', \tag{8.80}$$

which is the same as Eq. (7.144), namely $\langle x|\psi(t)\rangle = \int K(x,t|x't'|\psi(x',t')dx'$, with $\psi(x,t) = \langle x|\psi\rangle$ and $t' = 0$. From this comparison it follows that the propagator from t' to $t \geq t'$ is given by

$$K(x,t|x',t') = \langle x|\widehat{S}(t-t')|x'\rangle = \langle x|e^{-\frac{i}{\hbar}\widehat{H}(t-t')}|x'\rangle, \tag{8.81}$$

which shows how the Hamiltonian takes (propagates) the state in x', t' to the state in x at a later time t.

An alternative convenient way to write the propagator in the general form discussed in Chapter 7 is to insert a pair of expansions of the unit and write

$$\begin{aligned} K(x,t|x',t') &= \sum_n \sum_{n'} \langle x|\ n\rangle\ \langle n|e^{-\frac{i}{\hbar}\widehat{H}(t-t')}\ |n'\rangle\langle n'\ |x'\rangle \\ &= \sum_n \sum_{n'} e^{-\frac{i}{\hbar}E_{n'}(t-t')}\delta_{nn'}\varphi_n(x)\varphi^*_{n'}(x'), \end{aligned} \tag{8.82}$$

which reduces to Eq. (7.145),

$$K(x,t|x',t') = \sum_n \psi_n(x,t)\psi^*_n(x',t'). \tag{8.83}$$

Similarly, by expanding $|\psi_0\rangle$ in terms of the eigenstates $|n\rangle$ of the Hamiltonian

$$|\psi_0\rangle = \sum_n c_n|n\rangle, \tag{8.84}$$

with $\widehat{H}|n\rangle = E_n|n\rangle$, we get

$$|\psi\rangle = e^{-\frac{i}{\hbar}\widehat{H}t}\sum_n c_n|n\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}|n\rangle, \tag{8.85}$$

where $\widehat{S}(t)$ has been interpreted in terms of its power series,

$$e^{-\frac{i}{\hbar}\widehat{H}t}|n\rangle = \sum_{k=0}^{\infty}\frac{1}{k!}\left(-\frac{i}{\hbar}t\right)^k\widehat{H}^k|n\rangle = \sum_{k=0}^{\infty}\frac{1}{k!}\left(-\frac{i}{\hbar}t\right)^k E_n^k|n\rangle = e^{-\frac{i}{\hbar}E_n t}|n\rangle. \tag{8.86}$$

Rewriting (8.85) in the coordinate representation, we obtain Eq. (7.141). It is common to interpret expressions like $\exp(-i\widehat{H}t/\hbar)$ in terms of their power series expansion.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

It may happen that the expansion is not convergent, in which case expressing the initial wave function in terms of the eigenfunctions of $\widehat{H}$ (as was done here) solves the problem.

From (8.77) we note that

$$\widehat{S}^{-1} = e^{\frac{i}{\hbar}\widehat{H}t} = \widehat{S}^{\dagger} \tag{8.87}$$

because $\widehat{H}$ is Hermitian. Therefore, $\widehat{S}^{\dagger} = \widehat{S}^{-1}$, which is the defining property of a unitary operator (see next section). This means that *the time evolution of the system is given by the action of a unitary operator acting on the initial state*. In classical mechanics, the time evolution of a dynamical system is a canonical transformation (i.e., if $f(0)$, $g(0)$ are canonically conjugate, $f(t)$, $g(t)$ are canonically conjugate at any time, see[4]). This general relationship points to the importance of the study of unitary transformations in QM, which will play the role of canonical transformations.

8.6.2 Properties of unitary operators

Let $\widehat{U}$ be a unitary operator,

$$\widehat{U}^{\dagger} = \widehat{U}^{-1}, \tag{8.88}$$

which we use to transform the state vector $|i\rangle$ into $|i'\rangle$ according to the rule

$$|i'\rangle = \widehat{U}|i\rangle, \quad \langle i'| = \langle i|\widehat{U}^{\dagger}. \tag{8.89}$$

The transformation preserves orthonormality because $\langle i'|j'\rangle = \langle i|\widehat{U}^{\dagger}\widehat{U}|j\rangle = \langle i|j\rangle$. This is a first reason for choosing unitary operators to transform state vectors into state vectors. The modified basis is still complete because the closure property is retained,

$$\sum_{i'} |i'\rangle\langle i'| = \sum_{i} \widehat{U}|i\rangle\langle i|\widehat{U}^{\dagger} = \widehat{U}\widehat{U}^{\dagger} = \widehat{\mathbb{I}}. \tag{8.90}$$

In other words, a unitary transformation does not modify the space, it only modifies the basis (like a rotation of the Cartesian coordinate axes in 3D space). The transformation can also be applied to operators, by writing

$$\widehat{F}' = \widehat{U}\widehat{F}U^{\dagger}. \tag{8.91}$$

Note that the matrix elements are invariant under the transformation,

$$F'_{ij} = \langle i'|\widehat{F}'|j'\rangle = \langle i|\widehat{U}^{\dagger}\widehat{F}'\widehat{U}|j\rangle = \langle i|\widehat{U}^{\dagger}\widehat{U}\widehat{F}\widehat{U}^{\dagger}\widehat{U}|j\rangle = \langle i|\widehat{F}|j\rangle = F_{ij}. \tag{8.92}$$

From the unitarity property $\widehat{U}^{\dagger}\widehat{U} = \widehat{U}\widehat{U}^{\dagger} = \mathbb{I}$ it follows that the inverse of the transformation (8.89)–(8.91) is

$$|i\rangle = \widehat{U}^{\dagger}|i'\rangle, \quad \widehat{F} = \widehat{U}^{\dagger}\widehat{F}'\widehat{U}. \tag{8.93}$$

Also the trace of the operator is invariant to a change in representation, because

$$\operatorname{tr}\widehat{F}' = \operatorname{tr}\widehat{U}\widehat{F}\widehat{U}^{-1} = \operatorname{tr}\widehat{F}\widehat{U}^{-1}\widehat{U} = \operatorname{tr}\widehat{F}. \tag{8.94}$$

Throughout the text we have already encountered several quantum unitary operators. Operations that preserve the norm or more generally, the scalar product of real vectors, as well as those that generate rotations, reflections and similar transformations, are

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

performed with orthogonal operators, which satisfy the condition $\hat{O}^{-1} = \hat{O}^T$, so that $\hat{O}\hat{O}^T = \hat{\mathbb{I}}$. The unitary operators are the generalization of the orthogonal operators to complex spaces (of any number of dimensions) $\hat{O} \to \hat{U}$, $\hat{O}^T \to \hat{U}^{T*} \equiv \hat{U}^\dagger$, and thus they satisfy the condition $\hat{U}^{-1} = \hat{U}^\dagger$.

It is clear that the product of two unitary operators is unitary, since each transformation separately preserves the scalar product. From this property it follows that the set of unitary operators (of a given dimension) contains the product of any pair of them; since it also contains the unit $\widehat{U} = \widehat{\mathbb{I}}$ and the inverse of each operator $\widehat{U}^{-1} = \widehat{U}^\dagger$, this set forms a continuous group of transformations, called *unitary transformations*, a generalization to the complex case of orthogonal transformations.

8.6.3 Eigenvectors of unitary operators

The eigenvalues of a unitary operator are complex numbers modulo 1, since

$$\langle u_n|\widehat{U}^\dagger\widehat{U}|u_n\rangle = \langle u_n|u_n\rangle = 1 = u_n^* u_n, \tag{8.95}$$

and we can therefore write

$$u_n = e^{ig_n},\ g_n \text{ real}. \tag{8.96}$$

We also have that

$$\langle u_n|u_m\rangle = \langle u_n|\widehat{U}^\dagger\widehat{U}|u_m\rangle = u_n^* u_m \langle u_n|u_m\rangle = e^{i(g_m - g_n)}\langle u_n|u_m\rangle, \tag{8.97}$$

with solution

$$\langle u_n|u_m\rangle = \delta_{nm}. \tag{8.98}$$

We conclude that the eigenvectors of a unitary operator belonging to different (complex) eigenvalues are orthogonal. Equation (8.96) suggests writing a unitary operator in the form (reminiscent of the time-evolution operator (8.77))

$$\widehat{U} = e^{i\widehat{G}}. \tag{8.99}$$

From $\widehat{U}^{-1} = \widehat{U}^\dagger$ we get $e^{-i\widehat{G}} = e^{-i\widehat{G}^\dagger}$, which shows that $\widehat{G}$ must be Hermitian. If $|g_n\rangle$ is an eigenvector of $\widehat{G}$ with real eigenvalue g_n, we have

$$\widehat{U}|g_n\rangle = e^{i\widehat{G}}|g_n\rangle = \sum_k \frac{1}{k!}(i\widehat{G})^k|g_n\rangle = \sum_k \frac{1}{k!}(ig_n)^k|g_n\rangle = e^{ig_n}|g_n\rangle = u_n|g_n\rangle, \tag{8.100}$$

which shows that the eigenvectors of $\widehat{G}$ are eigenvectors of the unitary operator $e^{i\widehat{G}}$.

Exercise E8.5. Invariance of the physical laws under a unitary transformation
Show that the prescribed transformation rules (8.89) and (8.91) keep the form of the physical laws invariant.

Solution. Consider the expression $|\psi\rangle = \widehat{F}|\varphi\rangle$; its transform is

$$|\psi'\rangle = \widehat{U}|\psi\rangle = \widehat{U}\widehat{F}|\varphi\rangle = \widehat{U}\widehat{U}^\dagger\widehat{F}'\widehat{U}\widehat{U}^\dagger|\varphi'\rangle = \widehat{F}'|\varphi'\rangle, \tag{8.101}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

which has exactly the form of the original relation $|\psi\rangle = \widehat{F}|\varphi\rangle$. To show the invariance of the equations of motion against the transformation (8.91), we multiply the equation of motion

$$i\hbar\dot{\widehat{A}} = [\widehat{A}, \widehat{H}] \tag{8.102}$$

by $\widehat{U}$ from the left and by $\widehat{U}^\dagger$ from the right, to obtain

$$i\hbar\widehat{U}\dot{\widehat{A}}\widehat{U}^\dagger = \widehat{U}[\widehat{A}, \widehat{H}]\widehat{U}^\dagger = \widehat{U}\widehat{A}\widehat{U}^\dagger\widehat{U}\widehat{H}\widehat{U}^\dagger - \widehat{U}\widehat{H}\widehat{U}^\dagger\widehat{U}\widehat{A}\widehat{U}^\dagger = \widehat{A}'\widehat{H}' - \widehat{H}'\widehat{A}', \tag{8.103}$$

that is,

$$i\hbar\dot{\widehat{A}}' = [\widehat{A}', \widehat{H}'], \tag{8.104}$$

which shows that the form of the equation of motion has not changed. From the same proof it follows that the canonical commutation relations also retain their form and, therefore, the quantization rules are invariant under the transformation. In this way it is shown that the unitary transformations performed with the rules (8.89) for the state vectors and (8.91) for the operators, leave the canonical equations of quantum mechanics invariant.

We thus confirm that unitary transformations are in general the quantum equivalent of canonical transformations; in particular, the time evolution of the state vectors, described by Eq. (8.78), is a canonical transformation (in evolution).

8.6.4 Projection operators

In Section 4.6 we saw that an operator of the form

$$\widehat{P}_a = |a\rangle\langle a| \tag{8.105}$$

is a projection operator. We will now briefly analyze such operators. Applying the operator $\widehat{P}_a$ to an arbitrary state $|Q\rangle$ we get

$$\widehat{P}_a|Q\rangle = |a\rangle\langle a|Q\rangle = c_Q(a)|a\rangle, \tag{8.106}$$

which is a vector in the $|a\rangle$ direction, with magnitude equal to the component $c_Q(a) = \langle a|Q\rangle$ of $|Q\rangle$ in the $|a\rangle$ direction. The operator $\widehat{P}_a$ thus projects any vector from the Hilbert space $\mathcal{H}$ into the direction (or the subspace) $|a\rangle$. The projection operators are Hermitian and idempotent, as follows from their definition,

$$\widehat{P}_a^\dagger = (|a\rangle\langle a|)^\dagger = |a\rangle\langle a| = \widehat{P}_a, \tag{8.107}$$

$$\widehat{P}_a^2 = |a\rangle\langle a|a\rangle\langle a| = |a\rangle\langle a| = \widehat{P}_a. \tag{8.108}$$

This last equation implies that the eigenvalues of a projector are 0 or 1. Conversely, any Hermitian operator $\widehat{P}$ that satisfies the equation $\widehat{P}^2 = \widehat{P}$ is a projector; it projects into the subspace of $\mathcal{H}$ that corresponds to its eigenvalue one. From $\widehat{P} = \widehat{P}^2 = \widehat{P}^n, n$ any positive integer, it follows that the most general function $f(\widehat{P}_a)$ of a projector has the form $f(\widehat{P}_a) = A + B\widehat{P}_a$, with A and B independent of $\widehat{P}_a$. Furthermore, since a projector has only one nonzero eigenvalue equal to 1, its trace is 1; note that according to (8.94) this property is independent of the representation.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

From the property of completeness it follows that the operator $1 - \widehat{P}$ is orthogonal to $\widehat{P}$; in fact, since $\widehat{P}$ is idempotent, we have that

$$\widehat{P}(1 - \widehat{P}) = \widehat{P} - \widehat{P}^2 = 0. \tag{8.109}$$

This means that the vectors $\widehat{P}|u\rangle$ and $(1 - \widehat{P})|u\rangle$ are orthogonal components for any state $|u\rangle$, and thus it is always possible to decompose a state into two orthogonal states,

$$|u\rangle = \widehat{P}|u\rangle + (1 - \widehat{P})|u\rangle. \tag{8.110}$$

The vector $\widehat{P}|u\rangle$ is an eigenvector of $\widehat{P}$ with eigenvalue 1, since

$$\widehat{P}\left(\widehat{P}|u\rangle\right) = \widehat{P}^2|u\rangle = \widehat{P}|u\rangle. \tag{8.111}$$

In turn, $(1 - \widehat{P})|u\rangle$ is an eigenvector of $\widehat{P}$ with eigenvalue 0,

$$\widehat{P}[(1 - \widehat{P})|u\rangle] = (\widehat{P} - \widehat{P}^2)|u\rangle = 0. \tag{8.112}$$

Note that when an expansion is made using the closure relation, projections are being made. For example,

$$|\psi\rangle = \sum_i |a_i\rangle\langle a_i|\psi\rangle = \sum_i \widehat{P}_i|\psi\rangle = \sum_i |\psi_i\rangle = \sum_i \langle a_i|\psi\rangle\,|a_i\rangle, \tag{8.113}$$

where $|\psi_i\rangle = \widehat{P}_i|\psi\rangle$ is the projection of $|\psi\rangle$ in the $|a_i\rangle$ direction.

8.6.5 Moving between descriptions

We have seen that unitary transformations in QM keep the normalization of the state functions and the fundamental laws of the theory invariant. Given two orthonormal bases in the same Hilbert space $\mathcal{H}$ we will now find the unitary operator that takes us from one basis to the other. Consider, for example, an operator $\widehat{Q}$ whose eigenfunctions $\{u_\mu\}$ we use to write the generic operator $\hat{A}$,

$$A_{\mu\nu} = \int u_\mu^* \hat{A} u_\nu dx. \tag{8.114}$$

Similarly, consider another operator $\hat{R}$, with eigenfunctions $\{\varphi_m\}$ and write now

$$A_{mn} = \int \varphi_m^* \hat{A} \varphi_n dx. \tag{8.115}$$

Let $\hat{U}$ be the operator that takes us from the Q-representation to the R-representation, that is,

$$\varphi = \hat{U}u, \quad \text{or} \quad \varphi_m = \sum_\lambda U_{\lambda m} u_\lambda. \tag{8.116}$$

From this expression it follows that

$$U_{\mu m=} \int u_\mu^* \varphi_m dx. \tag{8.117}$$

Now we can write by direct substitution

$$\begin{aligned} A_{mn} &= \int \varphi_m^* \hat{A} \varphi_n dx = \sum_{\lambda\sigma} U_{\lambda m}^* U_{\sigma n} \int dx u_\lambda^* \hat{A} u_\sigma \\ &= \sum_{\lambda\sigma} U_{\lambda m}^* U_{\sigma n} A_{\lambda\sigma} = \sum_{\lambda\sigma} \left(\hat{U}^\dagger\right)_{m\lambda} A_{\lambda\sigma} U_{\sigma n} = \left(\hat{U}^\dagger \hat{A} \hat{U}\right)_{mn}, \end{aligned} \tag{8.118}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

or adding the indexes R and Q as reminders,

$$\hat{A}_R = \hat{U}^\dagger \hat{A}_Q \hat{U}. \tag{8.119}$$

The transition from the Schrödinger description to the Heisenberg description, or vice versa, is also done by a unitary transformation, since it is obtained by the inverse application of the evolution operator (8.77), which "devolves" the state vector. To see this, we apply $\widehat{S}^\dagger = \widehat{S}^{-1}$ from the left to (8.78), $|\psi(t)\rangle = \widehat{S}(t)|\psi_0\rangle$, to get

$$|\psi_H\rangle \equiv \widehat{S}^\dagger |\psi_S\rangle = \widehat{S}^\dagger |\psi(t)\rangle = S^\dagger S|\psi_0\rangle = |\psi_0\rangle. \tag{8.120}$$

$|\psi_S\rangle \equiv |\psi\rangle = |\psi(t)\rangle$ is the state vector in the Schrödinger description, while $|\psi_H\rangle$ represents the state vector in the Heisenberg description. According to (8.91) and (8.120), if $\widehat{F}_S$ represents an operator in the Schrödinger description, its expression in the Heisenberg description is

$$\widehat{F}_H(t) = \widehat{S}^\dagger \widehat{F}_S \widehat{S} = e^{\frac{i}{\hbar}\widehat{H}t} \widehat{F}_S e^{-\frac{i}{\hbar}\widehat{H}t}, \tag{8.121}$$

from which it follows that, in general, $\widehat{F}_H$ depends on time and evolves (as we have already seen) according to the equation of motion

$$i\hbar \frac{d\widehat{F}_H}{dt} = [\widehat{F}_H, \widehat{H}_H], \tag{8.122}$$

obtained by differentiating (8.121) with respect to time. Note that for the Hamiltonian, $\widehat{H}_H = \widehat{H}_S$ because $\hat{H}$ commutes with itself in any representation.

Exercise E8.6. A detour: "quantum" description of a classical problem
In the context of classical physics, describe the evolution of a system in a Schrödinger version (functions, such as the probability density, evolve as in classical statistical mechanics), or in a Heisenberg version (dynamical variables evolve).

Solution. Consider the generic variable A of a 1D one-particle problem, with $A = A(q, p)$ at $t = 0$; we limit ourselves to the case of analytic functions that can be expressed in the form

$$A(q, p) = \sum_{n,m} \alpha_{nm} q^n p^m. \tag{8.123}$$

At time t we can do the expansion

$$A(q(t), p(t)) = \sum_{n,m} \alpha_{nm} q^n(t) p^m(t), \tag{8.124}$$

or alternatively write it in terms of q and p,

$$A_t(q, p) = \sum_{n,m} \alpha_{nm}(t) q^n p^m. \tag{8.125}$$

In the first case (Heisenberg description) A is expressed as the original function of the new (evolving) variables, while in the second case (Schrödinger description) it involves a new (evolving) function ($\alpha(t) \neq \alpha$ in general) and the original variables. From the

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

equations of motion it follows (now for an arbitrary number of dimensions), with $\hat{L}$ the Liouville operator, that

$$\frac{\partial A_t}{\partial t} = \sum_i \left(\frac{p_i}{m} \frac{\partial}{\partial q_i} + F_i \frac{\partial}{\partial p_i} \right) A_t(q, p) \equiv \hat{L} A_t(q, p). \tag{8.126}$$

Assuming that this equation is integrable, it can be written formally for time-independent forces in the form

$$A_t(q, p) = \left[e^{(t-t_0)\hat{L}} A \right] (q, p) = A(q(t), p(t)), \tag{8.127}$$

a result that establishes the connection between the two descriptions.

8.6.6 The interaction description

To deal with physical problems of two interacting subsystems, it is common to decompose the Hamiltonian into a sum of two contributions, one containing the Hamiltonians of the independent parts and the other describing their interaction. We will show that in these cases it is possible to construct an intermediate description between Schrödinger's and Heisenberg's, in which the state vector evolves only due to the action of the interaction Hamiltonian. This is the so-called *interaction description* (or *representation*) introduced in 1934 by Stückelberg,[8] and used successfully for the study of complex problems; in particular it played a fundamental role for the development of quantum electrodynamics.

We start by writing the Hamiltonian of the system in the form

$$\widehat{H} = \widehat{H}_0 + \widehat{V}, \tag{8.128}$$

where $\widehat{H}_0$ is the Hamiltonian of free – that is, noninteracting – fields (or particles), and $\widehat{V}$ represents the Hamiltonian of the interaction between them. We introduce a unitary transformation $\widehat{S}(t)$ defined in terms of the free Hamiltonian $\widehat{H}_0$ only, and with it we move from the original Schrödinger description to the interaction description; that is, we write

$$|\psi_I\rangle = \widehat{S}(t)|\psi_S\rangle, \tag{8.129}$$

where $|\psi_S\rangle$ corresponds to the Schrödinger description for the free Hamiltonian,

$$\widehat{S}(t) = e^{i\widehat{H}_0 t/\hbar}. \tag{8.130}$$

Substituting in the Schrödinger equation

$$i\hbar \frac{\partial |\psi_S\rangle}{\partial t} = (\widehat{H}_0 + \widehat{V})|\psi_S\rangle \tag{8.131}$$

and simplifying, we get (as the student can verify)

$$i\hbar \frac{\partial |\psi_I\rangle}{\partial t} = \widehat{V}_I |\psi_I\rangle, \tag{8.132}$$

[8] Ernst Carl Gerlach Stückelberg (1905–1984) was a renowned Swiss mathematician and physicist.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

where $\widehat{V}_I$ is the interaction Hamiltonian in the interaction description, that is,

$$\widehat{V}_I = \widehat{S}(t)\widehat{V}\,\widehat{S}^{-1}(t). \tag{8.133}$$

We see that in this description the state vector $|\psi_I\rangle$ evolves only due to the interaction between the subsystems; if it were zero, we would be making a usual Heisenberg description. On the other hand, if $\widehat{F}_S$ represents a generic operator in the Schrödinger description, then in the interaction description it is written as

$$\widehat{F}_I = \widehat{S}(t)\widehat{F}_S\widehat{S}^{\dagger}(t). \tag{8.134}$$

From here it follows that the evolution equation for $\widehat{F}_I$ is

$$i\hbar\frac{d\widehat{F}_I}{dt} = [\widehat{F}_I, \widehat{H}_0]. \tag{8.135}$$

This is a really important result; it shows that the time evolution of the operators in the interaction description is generated exclusively by the Hamiltonian of the free subsystems, even when they are in interaction. In other words, in the interaction description, the form of the fundamental dynamical equations is the *same* in the presence or absence of interaction. This, together with Eq. (8.132), makes this description extremely practical for the study of complicated systems, since an essential part of free systems theory, in particular, the set of evolution equations for *free fields,* remains applicable in the presence of interaction. Thus, having solved the problem for $\widehat{H}_0$, it remains only to solve Eq. (8.132) to determine $|\psi_I\rangle$.

8.6.6.1 *Perturbative method based on the interaction description

The perturbative method discussed here is used extensively in QED, including its relativistic version, and in many other problems. The task is to find the solution of the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(\hat{H}_0 + V\right)\Psi, \tag{8.136}$$

where the interaction Hamiltonian V may depend on time. In the interaction description, the wave function satisfies Eq. (8.132), with

$$V_I(t) = e^{i\hat{H}_0 t/\hbar}Ve^{-i\hat{H}_0 t/\hbar}, \tag{8.137}$$

and all other operators (except, of course, $\hat{H}_0$) evolve according to the same rule determined by $\hat{H}_0$. Indeed, Eq. (8.132) can be formally integrated to give

$$\Psi_I(t) = \hat{U}(t, t_0)\Psi_I(t_0), \tag{8.138}$$

where the new evolution operator $\hat{U}(t, t_0)$ evolves due to the perturbation (the old one evolved due to $\hat{H}_0$),

$$i\hbar\frac{d\hat{U}(t, t_0)}{dt} = V_I(t)\hat{U}(t, t_0), \quad \hat{U}(t_0, t_0) = \mathbb{I}, \tag{8.139}$$

so that

$$\hat{U}(t, t_0) = \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_I'(t')\hat{U}(t', t_0)dt'. \tag{8.140}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

This expression is well suited for a perturbative analysis, if the perturbation is sufficiently "small" so that $\hat{U}(t,t_0)$ remains close enough to the initial value $\mathbb{I}$. In such a case we can expand by successive iterations,

$$\begin{aligned}\hat{U}(t,t_0) &= \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\hat{U}(t',t_0)dt' \\ &= \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\hat{V}_I(t')\left[\mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t'} dt''\hat{V}_I(t'')\hat{U}(t'',t_0)\right] \\ &= \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\hat{V}_I(t')\left\{\mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t'} dt''\hat{V}_I(t'')\left[\mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t''} dt'''\hat{V}_I(t''')\hat{U}(t''',t_0)\right]\right\}\end{aligned} \tag{8.141}$$

and so on, so that

$$\hat{U}(t,t_0) = \mathbb{I} + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\hat{V}_I(t') + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt'\hat{V}_I(t')\int_{t_0}^{t'} dt''\hat{V}_I(t'') + \cdots \tag{8.142}$$

The term of order n contains n integrals, n factors V and n integration times, so that it is possible to write

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty}\hat{U}^{(n)}(t,t_0), \quad \hat{U}^{(0)}(t,t_0) = \mathbb{I}, \tag{8.143}$$

$$\hat{U}^{(1)}(t,t_0) = \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t')dt', \tag{8.144}$$

$$\hat{U}^{(2)}(t,t_0) = \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t}\hat{V}_I(t')dt'\int_{t_0}^{t'}\hat{V}_I(t'')dt'', \tag{8.145}$$

and so on. The last expression can be conveniently rewritten by changing the order of integration with the help of the Heaviside $\Theta(t)$ function,

$$\begin{aligned}\int_{t_0}^{t}\hat{V}_I(t')dt'\int_{t_0}^{t'}\hat{V}_I(t'')dt'' &= \int_{t_0}^{t}dt'\int_{t_0}^{t}dt''\Theta(t'-t'')\hat{V}_I(t')\hat{V}_I(t'') \\ &= \int_{t_0}^{t}dt''\int_{t_0}^{t}dt'\Theta(t'-t'')\hat{V}_I(t')\hat{V}_I(t'') \\ &= \int_{t_0}^{t}dt''\int_{t''}^{t}dt'\hat{V}_I(t')\hat{V}_I(t'') \\ &= \tfrac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{V}_I(t')\hat{V}_I(t'') \\ &\quad + \tfrac{1}{2}\int_{t_0}^{t}dt'\int_{t'}^{t}dt''\hat{V}_I(t'')\hat{V}_I(t') \\ &= \hat{\mathsf{T}}\tfrac{1}{2}\int_{t_0}^{t}dt'\int_{t_0}^{t}dt''\hat{V}_I(t')\hat{V}_I(t'').\end{aligned} \tag{8.146}$$

The last but one equality was obtained by exchanging t' and t''. To write the final result, we introduced the *chronological operator* $\hat{\mathsf{T}}$, which orders the factors to the right in descending order of time; for example,

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

$$\hat{\mathsf{T}}\hat{V}_I(t')\hat{V}_I(t'') = \begin{cases} \hat{V}_I(t')\hat{V}_I(t'') & \text{if } t' \geq t'', \\ \hat{V}_I(t'')\hat{V}_I(t') & \text{if } t'' \geq t'. \end{cases} \tag{8.147}$$

When reordering the factors chronologically they should be taken as commutative. The multiple integral of order n contains n terms, but using $\hat{\mathsf{T}}$ reduces them to a single one extending from t_0 to t, preceded by a factor $1/n!$, just as in the case of $n = 2$ above. So we get

$$\hat{U}^{(n)}(t, t_0) = \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \hat{\mathsf{T}} \int_{t_0}^{t} \hat{V}_I(t_1)dt_1 \cdots \int_{t_0}^{t} \hat{V}_I(t_n)dt_n. \tag{8.148}$$

Summing up these terms gives the final result from (8.142), expressed in synthetic form,

$$\hat{U}(t, t_0) = \hat{\mathsf{T}} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')dt'\right). \tag{8.149}$$

An analysis of this result helps to understand the origin of the chronological operator. Deriving with respect to time gives

$$\begin{aligned} i\hbar\frac{d}{dt}\hat{U}(t, t_0) &= i\hbar\frac{d}{dt}\hat{\mathsf{T}} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')dt'\right) \\ &= \hat{\mathsf{T}}\hat{V}_I(t) \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')dt'\right) \\ &= \hat{V}_I(t)\hat{\mathsf{T}} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')dt'\right) = \hat{V}_I(t)\hat{U}(t, t_0), \end{aligned} \tag{8.150}$$

which coincides with Eq. (8.139). Without the chronological operator, the order of the factor $\hat{V}_I(t)$ that comes from the derivative of the exponent would remain imprecise. The $\hat{\mathsf{T}}$ sends this factor to the extreme left because its argument has the maximum value t, forcing the correct expression. Taking this into account, the series of equalities in (8.150) is equivalent to a derivation of (8.149).

Exercise E8.7. First-order transition amplitude

Use the preceding method to obtain a formula for the transition amplitude between energy eigenstates, up to first order.

Solution. Consider the eigenstate ψ_n of $\hat{H}_0$; the transition amplitude to another eigenstate ψ_k is

$$\begin{aligned} A_{nk}(t) &\equiv \langle\psi_k|\, \Psi_{In}(t)\rangle = \langle\psi_k|\, U(t, t_0)\, |\psi_n\rangle \\ &= \langle\psi_k|\, I - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')dt' + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} \hat{V}_I(t')dt' \int_{t_0}^{t'} \hat{V}_I(t'')dt'' + \cdots |\psi_n\rangle \\ &\quad + \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \hat{\mathsf{T}} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, \langle\psi_k|\, \hat{V}_I(t')\hat{V}_I(t'')\, |\psi_n\rangle + \ldots \end{aligned} \tag{8.151}$$

From (8.137) we can write for the first-order transition amplitude

$$A_{nk}^{(1)}(t) = \langle\psi_k|\, U^{(1)}(t, t_0)\, |\psi_n\rangle = -\frac{i}{\hbar}\int_{t_0}^{t} \langle\psi_k|\, \hat{V}_I\, |\psi_n\rangle\, e^{i\omega_{kn}t'}dt'. \tag{8.152}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

Thus, at $t \to \infty$ the transition probability is to first order in perturbation theory given by

$$w_{nk}^{(1)} = \left|A_{nk}^{(1)}\right|^2 = \left|\langle\psi_k|\, U^{(1)}(t,t_0)\,|\psi_n\rangle\right|^2 = \frac{1}{\hbar^2}\left|\int_{t_0}^{\infty}\langle\psi_k|\,\hat{V}_I\,|\psi_n\rangle\, e^{i\omega_{kn}t}dt\right|^2. \quad (8.153)$$

This result coincides with the formula obtained in Section 17.1 using time-dependent perturbation theory.

8.7 *Integrals of Motion and Symmetries: Noether's Theorem

We have learned from classical mechanics that it is possible to establish a relation between the integrals of motion of a dynamical system and the symmetries of its Hamiltonian (or equivalently, of its Lagrangian or its action function). Successfully developed by Emmy Noether in 1915[9] as a theorem of classical dynamics, this result was subsequently extended to QM. Noether's theorem has become one of the most powerful tools for the study of dynamical systems, both classical and quantum, as will become clear from the brief introduction to the subject in the following sections, or by exploring any advanced text on classical or quantum field theory.

There is a simple connection between the constants of motion and the infinitesimal transformations of the coordinate system that leave the Hamiltonian invariant. For example, the infinitesimal transformation of the generalized coordinate q_i into $q_i + \delta q_i$ transforms H into $H + \delta H$, where $\delta H = (\partial H/\partial q_i)\delta q_i$ (to first order in δq_i); if H is invariant under this infinitesimal transformation, then $\partial H/\partial q_i = 0$ and it follows from $\dot{p}_i = -\partial H/\partial q_i$ that p_i is a constant of the motion. This particular symmetry occurs when H does not depend on q_i (which is then called an ignorable or cyclic coordinate); it then turns out that *the momentum associated with an ignorable coordinate is conserved*. For example, the spatial homogeneity of the free-particle Hamiltonian $H = p_x^2/2m$ leads to the conservation of the linear momentum p_x.

8.7.1 Quantum Noether's theorem

Let $\widehat{G}$ be a Hermitian operator used as the generator to construct the unitary operator $\widehat{U}$

$$\widehat{U} = e^{i\alpha\widehat{G}}, \quad (8.154)$$

where α is a real parameter; taking $\alpha \to \delta\alpha$ infinitesimal for the moment, we can write to first order

$$\widehat{U} = 1 + i\delta\alpha\widehat{G}. \quad (8.155)$$

[9] Amalie Emmy Noether (1882–1935) was an outstanding German mathematician and logician who was denied an official position at any university because of her gender. Several scientists, including Albert Einstein, Norbert Wiener, David Hilbert, Pavel Alexandrov, Jean Dieudonné, and Hermann Weyl, consider her as the most important woman in the history of mathematics. In 1915 Hilbert invited her out of step to work in a corner at the University in Göttingen.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

$\widehat{G}$ is the *generator of the infinitesimal transformation* $\widehat{U}$ and $\delta\alpha$ is the *parameter* of the transformation. If $\widehat{H}$ is the initial Hamiltonian, the transformed Hamiltonian $\widehat{H}_U$ is given by Eq. (8.91); expanding to first order gives

$$\widehat{H}_U = \widehat{U}\widehat{H}\widehat{U}^{-1} = (1 + i\delta\alpha\widehat{G})\widehat{H}(1 - i\delta\alpha\widehat{G}) = \widehat{H} + i\delta\alpha(\widehat{G}\widehat{H} - \widehat{H}\widehat{G}), \tag{8.156}$$

namely

$$\widehat{H}_U = \widehat{H} + \delta\widehat{H} = \widehat{H} + i\delta\alpha[\widehat{G}, \widehat{H}]. \tag{8.157}$$

For this transformation to leave the Hamiltonian invariant $\widehat{H}_U = \widehat{H}$, it is required that $\delta H = i\delta\alpha[\widehat{G}, \widehat{H}] = 0$ and since $\delta\alpha \neq 0$, it follows that

$$[\widehat{G}, \widehat{H}] = 0. \tag{8.158}$$

This means that $\widehat{G}$ is conserved. Therefore, *the operators representing constants of motion of the system generate unitary infinitesimal transformations that leave the Hamiltonian unchanged*. Or alternatively, if $\widehat{H}$ is invariant under a unitary infinitesimal transformation, then the generator of the transformation is an integral of motion. For example, if $\widehat{H}$ is homogeneous with respect to spatial coordinates, it will be invariant under an infinitesimal translation and momentum will be conserved; in this case, the generator of the transformation is the momentum operator. Similarly, the spatial isotropy of $\widehat{H}$ will guarantee its invariance against infinitesimal rotations generated by the angular momentum operator, which will be conserved, and so on.

The set of operators that commute with the Hamiltonian forms a group, which is called the *group of the Schrödinger equation*. A set of operators forms a group if it contains: (i) the identity operator; (ii) the product operators $\widehat{A}\widehat{B}$ and $\widehat{B}\widehat{A}$ for each pair of operators $\widehat{A}$ and $\widehat{B}$ of the set; (iii) the inverse operator $\widehat{A}^{-1}$ for each operator $\widehat{A}$ of the set, such that $\widehat{A}^{-1}\widehat{A} = \widehat{A}\widehat{A}^{-1} = \hat{1}$. We can see that if $\widehat{A}$ and $\widehat{B}$ commute with $\widehat{H}$, then the operators $\widehat{A}\widehat{B}$, $\widehat{B}\widehat{A}$, $\widehat{A}^{-1}$, $\widehat{B}^{-1}$ also commute with $\widehat{H}$; furthermore, it is obvious that $\widehat{H}$ commutes with $\widehat{1}$. So the set of operators that commute with the Hamiltonian forms a group.

8.7.2 Finite unitary transformations

It is possible to apply the previous arguments to the case of finite unitary transformations. To see this, let us consider a Hermitian operator $\widehat{G}$ that commutes with the Hamiltonian, so that $\widehat{G}$ corresponds to a conserved quantity. The operator $\widehat{G}$ generates a continuous symmetry transformation $\widehat{U}_\alpha = e^{i\alpha\widehat{G}}$, that leaves $\widehat{H}$ invariant, since from (8.158) it follows that

$$\widehat{H}_\alpha = \widehat{U}_\alpha\widehat{H}\widehat{U^\dagger}_\alpha = \widehat{H}\widehat{U}_\alpha\widehat{U}_\alpha^\dagger = \widehat{H}. \tag{8.159}$$

With this we verify that every operator that commutes with the Hamiltonian – and therefore corresponds to a conserved quantity – generates a continuous symmetry transformation of the Hamiltonian. Alternatively, we can say that unitary operators whose generators are conserved generate symmetry transformations of the Hamiltonian. Note that the reverse is not necessarily true: the generator of a finite symmetry transformation of the Hamiltonian does not necessarily commute with it.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

So far we have only dealt with the changes that are induced in the Hamiltonian, but it is possible to study the general case. Let $\widehat{F}$ be a generic dynamical variable; a unitary infinitesimal transformation changes it to $\widehat{F}' = \widehat{F} + \delta\widehat{F}$ with $\widehat{F}'$ given by (8.91) and $\widehat{U}$ by (8.155), so we get

$$\begin{aligned}\widehat{F}' &= \widehat{F} + \delta\widehat{F} = \widehat{U}\widehat{F}\widehat{U}^\dagger = (1 + i\delta\alpha\widehat{G})\widehat{F}(1 - i\delta\alpha\widehat{G}) \\ &= \widehat{F} + i\delta\alpha(\widehat{G}\widehat{F} - \widehat{F}\widehat{G}),\end{aligned} \tag{8.160}$$

and thus

$$\delta\widehat{F} = i\delta\alpha[\widehat{G}, \widehat{F}], \tag{8.161}$$

where $\widehat{G}$ is the generator of the infinitesimal transformation and $\delta\alpha$ its parameter,

$$\widehat{U} = 1 + i\delta\alpha\widehat{G}. \tag{8.162}$$

Equation (8.161) – often written in the form of a functional derivative $\delta\widehat{F}/\delta\alpha = i[\widehat{G}, \widehat{F}]$ – is important, since it establishes the general relationship between the variation $\delta\widehat{F}$ of the dynamical variable $\widehat{F}$ and the generator $\widehat{G}$ of the applied infinitesimal transformation. In particular, if we take $\widehat{G} = \hat{H}$ and $\delta\alpha = \delta t/\hbar$ (as required by a dimensional analysis), we get the evolution equation

$$i\hbar\delta\widehat{F}/\delta t = i\hbar\dot{\widehat{F}} = [\widehat{F}, \widehat{H}], \tag{8.163}$$

which again shows the Hamiltonian as the generator of time translations – and thus of the evolution of the system.

8.7.2.1 The rotation operator

We will now use these ideas applied in reverse, to construct the generator of infinitesimal rotations. The Hamiltonian of an isotropic system with central interactions is invariant under infinitesimal rotations $\widehat{T}_{\delta\varphi}$ about an axis in any direction $\widehat{\mathbf{n}}$ passing through the origin. If $\delta\varphi$ is the infinitesimal angle of the rotation, we write

$$\delta\boldsymbol{\varphi} = \widehat{\mathbf{n}}\delta\varphi. \tag{8.164}$$

Applying this operator to $\psi(\boldsymbol{r})$ and using the formula $\boldsymbol{a}\cdot\boldsymbol{b}\times\boldsymbol{c} = \boldsymbol{a}\times\boldsymbol{b}\cdot\boldsymbol{c}$ we get

$$\widehat{T}_{\delta\varphi}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} - \delta\boldsymbol{\varphi}\times\boldsymbol{r}) = \psi(\boldsymbol{r}) - \delta\boldsymbol{\varphi}\times\boldsymbol{r}\cdot\nabla\psi = (1 - \delta\boldsymbol{\varphi}\cdot\boldsymbol{r}\times\nabla)\psi(\boldsymbol{r}). \tag{8.165}$$

With $\widehat{\boldsymbol{L}} = \boldsymbol{r}\times\widehat{\boldsymbol{p}}$, $\widehat{T}_{\delta\varphi}$ takes the form

$$\widehat{T}_{\delta\varphi} = 1 - \frac{i}{\hbar}\boldsymbol{\delta\varphi}\cdot\widehat{\boldsymbol{L}}. \tag{8.166}$$

Therefore, the *rotation operator* that performs a finite rotation of the coordinate system around the axis $\widehat{\mathbf{n}}$ by the angle φ is

$$\widehat{T}_{\widehat{\mathbf{n}}}(\varphi) = e^{-\frac{i}{\hbar}\varphi\widehat{\mathbf{n}}\cdot\widehat{\boldsymbol{L}}}. \tag{8.167}$$

To complete the example, let us apply Eq. (8.161) (noting the change in the sign of $\delta\alpha$) to the operator $\widehat{G} = x\widehat{p}_y - y\widehat{p}_x = \widehat{L}_z$. We have

$$\begin{aligned}x' &= x + i\delta\alpha[\widehat{x}, \widehat{L}_z] = x + i\delta\alpha\left[x(x\widehat{p}_y - y\widehat{p}_x) - (x\widehat{p}_y - y\widehat{p}_x)x\right] \\ &= x + i\delta\alpha y[-x\widehat{p}_x + \widehat{p}_x x] = x + \hbar\delta\alpha y = x - \epsilon y,\end{aligned} \tag{8.168}$$

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

where we have put $\epsilon = -\hbar\delta\alpha$. Analogously we get

$$y' = y + \epsilon x, \quad z' = z. \tag{8.169}$$

Similarly,

$$\begin{aligned} p'_x &= \widehat{p}_x + i\delta\alpha[\widehat{p}_x, \widehat{L}_z] = \widehat{p}_x + i\delta\alpha[\widehat{p}_x x - x\widehat{p}_x]p_y \\ &= \widehat{p}_x + \hbar\delta\alpha\,\widehat{p}_y = \widehat{p}_x - \epsilon\widehat{p}_y, \end{aligned} \tag{8.170}$$

$$p'_y = \widehat{p}_y + \epsilon\widehat{p}_x, \quad p'_z = \widehat{p}_z. \tag{8.171}$$

These results show, as expected, that $\widehat{L}_z$ is the generator of rotations about the z-axis.

We take the opportunity to observe that the application of Eq. (8.167) to a spin $\hbar\boldsymbol{\sigma}/2$, with $\boldsymbol{\sigma}$ the vector constructed with Pauli matrices, leads to

$$\widehat{T}_{\widehat{\mathbf{n}}}(\varphi) = e^{-\frac{i}{2}\varphi\widehat{\mathbf{n}}\cdot\widehat{\boldsymbol{\sigma}}}. \tag{8.172}$$

This result has two properties, both peculiar and important. One of them is related to the properties of the Pauli 2×2 matrices, the other to the half rotation angle $\varphi/2$. Together they explain the strange rotation properties of spinors, in particular the fact that they are not invariant with respect to a full rotation by the angle 2π, which leads to a change of sign of the spinor, thus essentially distinguishing spinors from tensors, the latter being, by definition, insensitive to a 2π rotation.

Other important conclusions can be drawn from the preceding results. On the one hand, it is clear that the transformation law $x \to x' = x + (\hbar\delta\alpha)\,y$ due to an infinitesimal rotation around the z-axis, applies to *any* vector operator, which leads us to write more generally that

$$\hat{A}_x \to \hat{A}'_x = \hat{A}_x + (\hbar\delta\alpha)\,\hat{A}_y = \hat{A}_x + i\delta\alpha\left[\hat{A}_x, \hat{L}_z\right], \tag{8.173}$$

whence

$$\left[\hat{L}_z, \hat{A}_x\right] = i\hbar\hat{A}_y. \tag{8.174}$$

Noting that in this expression the indices are in cyclic order, we can write more generally

$$\left[\hat{L}_i, \hat{A}_j\right] = i\hbar\varepsilon_{ijk}\hat{A}_k, \tag{8.175}$$

where ε_{ijk} is the Levi–Civita totally antisymmetric 3D tensor. This law expresses the commutators of *any* vector $\hat{A}$ and the angular momentum operator. In fact, it is often used as the *definition* of a vector operator, namely as the three-component operator that satisfies these commutation rules. In particular, angular momentum is a vector operator, so applying this rule to it with $\hat{A}_i = \hat{L}_i$ gives the commutation rules of the components of the angular momentum operator, namely

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\varepsilon_{ijk}\hat{L}_k. \tag{8.176}$$

In Chapter 11 we will have the opportunity to review and make use of these results.

Note that in the cases analyzed the generator of the transformation is the conjugate canonical variable of the transformed variable. In fact, this relation can be used in general to define the pairs of conjugate canonical variables. It is not difficult to relate this result to the structure of the commutators of these variables, but the development of this observation is left to the student.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

8.7.3 Discrete symmetries: Parity

Discrete symmetries are symmetries that describe noncontinuous changes in a system. In geometry, for example, a square has discrete rotational symmetry, since only rotations by multiples of $\pi/2$ preserve the original shape of the square. Here we will discuss one of the most important symmetries in physics, the parity symmetry.

For this purpose we introduce the parity operator $\widehat{P}$ in coordinate space,[10] which produces a mirror reflection of the coordinates x_i or, equivalently, a reflection of the *polar vectors* (such as $\boldsymbol{r}$ and $\boldsymbol{p}$; see what follows) about the origin, leaving the *axial vectors* (such as $\boldsymbol{L}$) unchanged. By definition, $\hat{P}$ satisfies the following relations

$$\boldsymbol{r}_P \equiv \widehat{P}\boldsymbol{r}\widehat{P} = -\boldsymbol{r}, \tag{8.177}$$

$$\boldsymbol{p}_P \equiv \widehat{P}\boldsymbol{p}\widehat{P} = -\boldsymbol{p}. \tag{8.178}$$

When $\widehat{P}$ acts on a function of the coordinates, one gets

$$\widehat{P}\psi(\boldsymbol{r}) = a\psi(-\boldsymbol{r}), \tag{8.179}$$

or $\widehat{P}\psi(\boldsymbol{r}) = \langle \boldsymbol{r}|\ \widehat{P}\ |\psi\rangle = \langle -\boldsymbol{r}|\ \psi\rangle$. Applying the operator $\widehat{P}$ to (8.179) we get

$$\widehat{P}^2\psi(\boldsymbol{r}) = \widehat{P}a\psi(-\boldsymbol{r}) = a^2\psi(\boldsymbol{r}) = \psi(\boldsymbol{r}), \tag{8.180}$$

thus $\widehat{P}^2 = 1$; eigenfunctions of $\widehat{P}$ with eigenvalue +1, i.e., $\psi(-\boldsymbol{r}) = \psi(\boldsymbol{r})$, have even parity, and those with eigenvalue -1, that is, $\psi(-\boldsymbol{r}) = -\psi(\boldsymbol{r})$, have odd parity. Note that $\widehat{P}$ is a unitary operator, since it is Hermitian with square equal to 1.

When $\widehat{H}(-\boldsymbol{r}) = \widehat{H}(\boldsymbol{r})$, that is, when the system is invariant with respect to a reflection about the origin, the operator $\widehat{P}$ commutes with the Hamiltonian. This happens in many important cases, including the free particle, 1D square potentials, central potentials, and so on. In these cases, the parity is an integral of motion, so the eigenvalue of $\widehat{P}$ is preserved during the evolution of the system.

Vectors that transform like $\boldsymbol{r}$ or $\boldsymbol{p}$ (i.e., that change the sign of their components against mirror reflection) are called *polar vectors*. Note that since the angular-momentum operator is the product of two (polar) vectors, $\hat{\boldsymbol{L}} = \boldsymbol{r} \times \boldsymbol{p}$, it is invariant under a mirror reflection of the coordinates. Vectors such as angular momentum, spin, and the magnetic field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$, are examples of *axial vectors* or *pseudo-vectors*; their components do not change sign with the specular reflection generated by $\widehat{P}$.

Just as there are two types of vectors with respect to the parity operator, there are the corresponding *scalars* and *pseudo scalars*. A product $\boldsymbol{A} \cdot \boldsymbol{B}$ with both factors $\boldsymbol{A}$ and $\boldsymbol{B}$ polar or axial vectors is a scalar; when one factor is a polar vector and the other an axial vector, the result is a pseudo-scalar; for example, $\boldsymbol{r} \cdot \boldsymbol{L}$ is pseudo scalar.

Particles may also possess an *intrinsic* parity, expressed in the form of a phase factor that arises as an eigenvalue of the parity operation. In this case too, the operator P is unitary, since $PP^* = P^*P = 1$. Thus

$$\widehat{P}\psi = e^{i\phi}\psi, \tag{8.181}$$

where the phase factor must be determined experimentally (or, where appropriate, by the corresponding theory). For example, the pions $(\pi^0, \pi^{\pm})$ have zero spin and

[10] Not to be confused with the projection operators $\hat{P}$ introduced previously.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

parity -1, which indicates that they are *pseudo-scalar* particles. As will be seen in Chapter 15, a rotation of 2π does not change the wave function of bosons (integer-spin particles), so it is appropriate to set $a^2 = 1$ for them, giving $a = \pm 1$. In contrast, the wave function of fermions (half-integer-spin particles) is only invariant against rotations of 4π, so $a^4 = 1$ and $\pm 1, \pm i$.

8.7.3.1 Time inversion

The operation usually called *time inversion* – which should more properly be called motion inversion – is defined by the relations ($\hat{\boldsymbol{J}}$ stands for the total angular-momentum operator)

$$\hat{T}\hat{\boldsymbol{r}}\hat{T}^{-1} = \hat{\boldsymbol{r}}, \quad \hat{T}\hat{\boldsymbol{p}}\hat{T}^{-1} = -\hat{\boldsymbol{p}}, \quad \hat{T}\hat{\boldsymbol{J}}\hat{T}^{-1} = -\hat{\boldsymbol{J}}. \tag{8.182}$$

In order for the fundamental commutation rules not to change with time inversion, it is required that $\hat{T}$ be an *antilinear* and *antiunitary* operator.

An operator $\hat{F}$ is antilinear if

$$\hat{F}\left(a\left|\varphi\right\rangle + b\left|\psi\right\rangle\right) = a^*\hat{F}\left|\varphi\right\rangle + b^*\hat{F}\left|\psi\right\rangle. \tag{8.183}$$

The conjugation operator $\widehat{K}$ is such that $\widehat{K}\varphi = \varphi^*$ for any φ, so it is easy to conclude that $\widehat{K}$ is an antilinear operator. The product of $\widehat{K}$ with a unitary operator is antiunitary; hence, in particular, $\widehat{K}$ is antiunitary. These properties make it difficult to define the action of this operator on the bras and kets and complicate the theory; for that reason we do not insist on this topic here. The point is discussed in more advanced textbooks on QM.

Problems

P8.1 Show that the commutator of two variables that are conserved is also a conserved quantity.

P8.2 Prove the validity of the following expression of the virial theorem for a system of several particles, where α denotes the particles and i, j are their Cartesian coordinates,

$$\sum_{\alpha}\left\langle -\frac{1}{m^{\alpha}}\hat{p}_i^{\alpha}\hat{p}_j^{\alpha} + x_i^{\alpha}\frac{\partial V}{\partial x_j^{\alpha}}\right\rangle = 0. \tag{8.184}$$

P8.3 Show that an attractive potential of the type $V \sim r^n$ only produces stable orbits if $n > -2$.

P8.4 Show that for an electron subject to the one-dimensional potential $V = -Cx$ with $C > 0$, the momentum dispersion Δp is constant.

P8.5 Show that

$$\frac{d\langle(\Delta x)^2\rangle}{dt} = \frac{1}{m}\langle\hat{x}\hat{p} + \hat{p}\hat{x}\rangle - \frac{2}{m}\bar{x}\bar{p}. \tag{8.185}$$

P8.6 In Section 8.4 we proved that if two dynamical variables F, G have simultaneous well-defined values, their respective operators must commute.

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press

Show that this condition is also sufficient, that is, if $\widehat{F}$ and $\widehat{G}$ commute, they have simultaneous well-defined values.

P8.7 Study the motion of a packet of free particles in the Heisenberg description. *Hint:* calculate the dispersions of x and p as functions of time.

P8.8 Show that the transformation $\hat{U}$ given by Eqs. (8.114)–(8.119) is unitary.

P8.9 Use the projection operators to construct an expression for the function $f(\hat{A})$, where $\hat{A}$ is an operator with eigenvectors $|n\rangle$ and eigenvalues a_n.

P8.10 Consider the two-dimensional problem of a particle of mass m moving on the xy-plane under the action of a radial force $f(r)$. Analyze the symmetries of the Hamiltonian and find the associated constants of motion.

Bibliographical Notes

Three highly recommended, very different textbooks are Feynman, Leighton, and Sands (1971), Bohm (1989), and Cohen-Tannoudji et al. (1977).

https://doi.org/10.1017/9781009679633.009 Published online by Cambridge University Press