Chapter 3

Postulates of Quantum Mechanics

3.1 Introduction

The formalism of quantum mechanics is based on a number of postulates. These postulates are in turn based on a wide range of experimental observations; the underlying physical ideas of these experimental observations have been briefly mentioned in Chapter 1. In this chapter we present a formal discussion of these postulates, and how they can be used to extract quantitative information about microphysical systems.

These postulates cannot be derived; they result from experiment. They represent the minimal set of assumptions needed to develop the theory of quantum mechanics. But how does one find out about the validity of these postulates? Their validity cannot be determined directly; only an indirect inferential statement is possible. For this, one has to turn to the theory built upon these postulates: if the theory works, the postulates will be valid; otherwise they will make no sense. Quantum theory not only works, but works extremely well, and this represents its experimental justification. It has a very penetrating qualitative as well as quantitative prediction power; this prediction power has been verified by a rich collection of experiments. So the accurate prediction power of quantum theory gives irrefutable evidence to the validity of the postulates upon which the theory is built.

3.2 The Basic Postulates of Quantum Mechanics

According to classical mechanics, the state of a particle is specified, at any time t, by two fundamental dynamical variables: the position $\vec{r}(t)$ and the momentum $\vec{p}(t)$. Any other physical quantity, relevant to the system, can be calculated in terms of these two dynamical variables. In addition, knowing these variables at a time t, we can predict, using for instance Hamilton's equations $dx/dt = \partial H/\partial p$ and $dp/dt = -\partial H/\partial x$, the values of these variables at any later time t'.

The quantum mechanical counterparts to these ideas are specified by postulates, which enable us to understand:

- how a quantum state is described mathematically at a given time t,
- how to calculate the various physical quantities from this quantum state, and

- knowing the system's state at a time t, how to find the state at any later time t'; that is, how to describe the time evolution of a system.

The answers to these questions are provided by the following set of five postulates.

Postulate 1: State of a system
The state of any physical system is specified, at each time t, by a state vector $|\psi(t)\rangle$ in a Hilbert space $\mathcal{H}$; $|\psi(t)\rangle$ contains (and serves as the basis to extract) all the needed information about the system. Any superposition of state vectors is also a state vector.

Postulate 2: Observables and operators
To every physically measurable quantity A, called an observable or dynamical variable, there corresponds a linear Hermitian operator $\hat{A}$ whose eigenvectors form a complete basis.

Postulate 3: Measurements and eigenvalues of operators
The measurement of an observable A may be represented formally by the action of $\hat{A}$ on a state vector $|\psi(t)\rangle$. The only possible result of such a measurement is one of the eigenvalues a_n (which are real) of the operator $\hat{A}$. If the result of a measurement of A on a state $|\psi(t)\rangle$ is a_n, the state of the system *immediately after* the measurement changes to $|\psi_n\rangle$:

$$\hat{A}|\psi(t)\rangle = a_n|\psi_n\rangle, \tag{3.1}$$

where $a_n = \langle\psi_n|\psi(t)\rangle$. **Note:** a_n is the component of $|\psi(t)\rangle$ when projected[1] onto the eigenvector $|\psi_n\rangle$.

Postulate 4: Probabilistic outcome of measurements

- **Discrete spectra**: When measuring an observable A of a system in a state $|\psi\rangle$, the probability of obtaining one of the nondegenerate eigenvalues a_n of the corresponding operator $\hat{A}$ is given by

$$P_n(a_n) = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|a_n|^2}{\langle\psi|\psi\rangle}, \tag{3.2}$$

  where $|\psi_n\rangle$ is the eigenstate of $\hat{A}$ with eigenvalue a_n. If the eigenvalue a_n is m-degenerate, P_n becomes

$$P_n(a_n) = \frac{\sum_{j=1}^{m}|\langle\psi_n^j|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{\sum_{j=1}^{m}|a_n^{(j)}|^2}{\langle\psi|\psi\rangle}. \tag{3.3}$$

  The act of measurement changes the state of the system from $|\psi\rangle$ to $|\psi_n\rangle$. If the system is already in an eigenstate $|\psi_n\rangle$ of $\hat{A}$, a measurement of A yields with certainty the corresponding eigenvalue a_n: $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$.

- **Continuous spectra:** The relation (3.2), which is valid for discrete spectra, can be extended to determine the probability density that a measurement of $\hat{A}$ yields a value between a and $a + da$ on a system which is initially in a state $|\psi\rangle$:

$$\frac{dP(a)}{da} = \frac{|\psi(a)|^2}{\langle\psi|\psi\rangle} = \frac{|\psi(a)|^2}{\int_{-\infty}^{+\infty}|\psi(a')|^2 da'}; \tag{3.4}$$

  for instance, the probability density for finding a particle between x and $x + dx$ is given by $dP(x)/dx = |\psi(x)|^2/\langle\psi|\psi\rangle$.

[1] To see this, we need only to expand $|\psi(t)\rangle$ in terms of the eigenvectors of $\hat{A}$ which form a complete basis: $|\psi(t)\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\psi(t)\rangle = \sum_n a_n|\psi_n\rangle$.

Postulate 5: Time evolution of a system
The time evolution of the state vector $|\psi(t)\rangle$ of a system is governed by the time-dependent *Schrödinger equation*

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle, \tag{3.5}$$

where $\hat{H}$ is the Hamiltonian operator corresponding to the total energy of the system.

Remark
These postulates fall into two categories:

- The first four describe the system at a given time.

- The fifth shows how this description evolves in time.

In the rest of this chapter we are going to consider the physical implications of each one of the four postulates. Namely, we shall look at the state of a quantum system and its interpretation, the physical observables, measurements in quantum mechanics, and finally the time evolution of quantum systems.

3.3 The State of a System

To describe a system in quantum mechanics, we use a mathematical entity (a complex function) belonging to a Hilbert space, the state vector $|\psi(t)\rangle$, which contains all the information we need to know about the system and from which all needed physical quantities can be computed. As discussed in Chapter 2, the state vector $|\psi(t)\rangle$ may be represented in two ways:

- A wave function $\psi(\vec{r}, t)$ in the position space: $\quad \psi(\vec{r}, t) = \langle \vec{r}|\psi(t)\rangle$.

- A momentum wave function $\Psi(\vec{p}, t)$ in the momentum space: $\quad \Psi(\vec{p}, t) = \langle \vec{p}|\psi(t)\rangle$.

So, for instance, to describe the state of a one-dimensional particle in quantum mechanics we use a complex function $\psi(x, t)$ instead of two real real numbers (x, p) in classical physics.

The wave functions to be used are only those that correspond to physical systems. What are the mathematical requirements that a wave function must satisfy to represent a physical system? Wave functions $\psi(x)$ that are physically acceptable must, along with their first derivatives $d\psi(x)/dx$, be *finite*, *continuous*, and *single-valued everywhere*. As will be discussed in Chapter 4, we will examine the underlying physics behind the continuity conditions of $\psi(x)$ and $d\psi(x)/dx$ (we will see that $\psi(x)$ and $d\psi(x)/dx$ must be be continuous because the probability density and the linear momentum are continuous functions of x).

3.3.1 Probability Density

What about the physical meaning of a wave function? Only the square of its norm, $|\psi(\vec{r}, t)|^2$, has meaning. According to Born's probabilistic interpretation, the square of the norm of $\psi(\vec{r}, t)$,

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2, \tag{3.6}$$

represents a position probability density; that is, the quantity $|\psi(\vec{r},t)|^2 d^3r$ represents the probability of finding the particle at time t in a volume element d^3r located between $\vec{r}$ and $\vec{r}+d\vec{r}$. Therefore, the total probability of finding the system somewhere in space is equal to 1:

$$\int |\psi(\vec{r},t)|^2 d^3r = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} |\psi(\vec{r},t)|^2 dz = 1. \tag{3.7}$$

A wave function $\psi(\vec{r},t)$ satisfying this relation is said to be *normalized*. We may mention that $\psi(\vec{r})$ has the physical dimensions of $1/\sqrt{L^3}$, where L is a length. Hence, the physical dimensions of $|\psi(\vec{r})|^2$ is $1/L^3$: $\left[|\psi(\vec{r})|^2\right] = 1/L^3$.

Note that the wave functions $\psi(\vec{r},t)$ and $e^{i\alpha}\psi(\vec{r},t)$, where α is a real number, represent the same state.

Example 3.1 (Physical and unphysical wave functions)
Which among the following functions represent physically acceptable wave functions: $f(x) = 3\sin \pi x$, $g(x) = 4 - |x|$, $h^2(x) = 5x$, and $e(x) = x^2$.

Solution
Among these functions only $f(x) = 3\sin \pi x$ represents a physically acceptable wave function, since $f(x)$ and its derivative are finite, continuous, single-valued everywhere, and integrable.

The other functions cannot be wave functions, since $g(x) = 4 - |x|$ is not continuous, not finite, and not square integrable; $h^2(x) = 5x$ is neither finite nor square integrable; and $e(x) = x^2$ is neither finite nor square integrable.

3.3.2 The Superposition Principle

The state of a system does not have to be represented by a *single* wave function; it can be represented by a *superposition* of two or more wave functions. An example from the macroscopic world is a vibrating string; its state can be represented by a single wave or by the superposition (linear combination) of many waves.

If $\psi_1(\vec{r},t)$ and $\psi_2(\vec{r},t)$ separately satisfy the Schrödinger equation, then the wave function $\psi(\vec{r},t) = \alpha_1\psi_1(\vec{r},t) + \alpha_2\psi_2(\vec{r},t)$ also satisfies the Schrödinger equation, where α_1 and α_2 are complex numbers. The Schrödinger equation is a linear equation. So in general, according to the superposition principle, the linear superposition of many wave functions (which describe the various permissible physical states of a system) gives a new wave function which represents a possible physical state of the system:

$$|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle, \tag{3.8}$$

where the α_i are complex numbers. The quantity

$$P = \left|\sum_i \alpha_i |\psi_i\rangle\right|^2, \tag{3.9}$$

represents the probability for this superposition. If the states $|\psi_i\rangle$ are mutually *orthonormal*, the probability will be equal to the sum of the individual probabilities:

$$P = \left|\sum_i \alpha_i |\psi_i\rangle\right|^2 = \sum_i |\alpha_i|^2 = P_1 + P_2 + P_3 + \cdots, \tag{3.10}$$

where $P_i = |\alpha_i|^2$; P_i is the probability of finding the system in the state $|\psi_i\rangle$.

Example 3.2

Consider a system whose state is given in terms of an orthonormal set of three vectors: $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ as

$$|\psi\rangle = \frac{\sqrt{3}}{3}|\phi_1\rangle + \frac{2}{3}|\phi_2\rangle + \frac{\sqrt{2}}{3}|\phi_3\rangle.$$

(a) Verify that $|\psi\rangle$ is normalized. Then, calculate the probability of finding the system in any one of the states $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$. Verify that the total probability is equal to one.

(b) Consider now an ensemble of 810 identical systems, each one of them in the state $|\psi\rangle$. If measurements are done on all of them, how many systems will be found in each of the states $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$?

Solution

(a) Using the orthonormality condition $\langle\phi_j|\phi_k\rangle = \delta_{jk}$ where $j, k = 1, 2, 3$, we can verify that $|\psi\rangle$ is normalized:

$$\langle\psi|\psi\rangle = \frac{1}{3}\langle\phi_1|\phi_1\rangle + \frac{4}{9}\langle\phi_2|\phi_2\rangle + \frac{2}{9}\langle\phi_3|\phi_3\rangle = \frac{1}{3} + \frac{4}{9} + \frac{2}{9} = 1. \tag{3.11}$$

Since $|\psi\rangle$ is normalized, the probability of finding the system in $|\phi_1\rangle$ is given by

$$P_1 = |\langle\phi_1|\psi\rangle|^2 = \left|\frac{\sqrt{3}}{3}\langle\phi_1|\phi_1\rangle + \frac{2}{3}\langle\phi_1|\phi_2\rangle + \frac{\sqrt{2}}{3}\langle\phi_1|\phi_3\rangle\right|^2 = \frac{1}{3}, \tag{3.12}$$

since $\langle\phi_1|\phi_1\rangle = 1$ and $\langle\phi_1|\phi_2\rangle = \langle\phi_1|\phi_3\rangle = 0$.

Similarly, from the relations $\langle\phi_2|\phi_2\rangle = 1$ and $\langle\phi_2|\phi_1\rangle = \langle\phi_2|\phi_3\rangle = 0$, we obtain the probability of finding the system in $|\phi_2\rangle$:

$$P_2 = |\langle\phi_2|\psi\rangle|^2 = \left|\frac{2}{3}\langle\phi_2|\phi_2\rangle\right|^2 = \frac{4}{9}. \tag{3.13}$$

As for $\langle\phi_3|\phi_3\rangle = 1$ and $\langle\phi_3|\phi_1\rangle = \langle\phi_3|\phi_2\rangle = 0$, they lead to the probability of finding the system in $|\phi_3\rangle$:

$$P_3 = |\langle\phi_3|\psi\rangle|^2 = \left|\frac{\sqrt{2}}{3}\langle\phi_3|\phi_3\rangle\right|^2 = \frac{2}{9}. \tag{3.14}$$

As expected, the total probability is equal to one:

$$P = P_1 + P_2 + P_3 = \frac{1}{3} + \frac{4}{9} + \frac{2}{9} = 1. \tag{3.15}$$

(b) The number of systems that will be found in the state $|\phi_1\rangle$ is

$$N_1 = 810 \times P_1 = \frac{810}{3} = 270. \tag{3.16}$$

Likewise, the number of systems that will be found in states $|\phi_2\rangle$ and $|\phi_3\rangle$ are given, respectively, by

$$N_2 = 810 \times P_2 = \frac{810 \times 4}{9} = 360, \qquad N_3 = 810 \times P_3 = \frac{810 \times 2}{9} = 180. \tag{3.17}$$

3.4 Observables and Operators

An observable is a dynamical variable that can be measured; the dynamical variables encountered most in classical mechanics are the position, linear momentum, angular momentum, and energy. How do we mathematically represent these and other variables in quantum mechanics?

According to the second postulate, a *Hermitian operator* is associated with every *physical observable*. In the preceding chapter, we have seen that the position representation of the linear momentum operator is given in one-dimensional space by $\hat{P} = -i\hbar\partial/\partial x$ and in three-dimensional space by $\hat{\vec{P}} = -i\hbar\vec{\nabla}$.

In general, any function, $f(\vec{r}, \vec{p})$, which depends on the position and momentum variables, $\vec{r}$ and $\vec{p}$, can be "*quantized*" or made into a function of operators by replacing $\vec{r}$ and $\vec{p}$ with their corresponding operators:

$$f(\vec{r}, \vec{p}) \quad \longrightarrow \quad F(\hat{\vec{R}}, \hat{\vec{P}}) = f(\hat{\vec{R}}, -i\hbar\vec{\nabla}), \tag{3.18}$$

or $f(x, p) \to F(\hat{X},\ -i\hbar\partial/\partial x)$. For instance, the operator corresponding to the Hamiltonian

$$H = \frac{1}{2m}\vec{p}^{\,2} + V(\vec{r}, t) \tag{3.19}$$

is given in the position representation by

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\hat{\vec{R}}, t), \tag{3.20}$$

where ∇^2 is the Laplacian operator; it is given in Cartesian coordinates by: $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$.

Since the momentum operator $\hat{\vec{P}}$ is Hermitian, and if the potential $V(\hat{\vec{R}}, t)$ is a real function, the Hamiltonian (3.19) is Hermitian. We saw in Chapter 2 that the eigenvalues of Hermitian operators are real. Hence, the spectrum of the Hamiltonian, which consists of the entire set of its eigenvalues, is real. This spectrum can be discrete, continuous, or a mixture of both. In the case of *bound* states, the Hamiltonian has a *discrete* spectrum of values and a *continuous* spectrum for *unbound* states. In general, an operator will have bound or unbound spectra in the same manner that the corresponding classical variable has bound or unbound orbits. As for $\hat{\vec{R}}$ and $\hat{\vec{P}}$, they have continuous spectra, since r and p may take a continuum of values.

Table 3.1 Some observables and their corresponding operators.

Observable	Corresponding operator
$\vec{r}$	$\hat{\vec{R}}$
$\vec{p}$	$\hat{\vec{P}} = -i\hbar\vec{\nabla}$
$T = \frac{p^2}{2m}$	$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$
$E = \frac{p^2}{2m} + V(\vec{r}, t)$	$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\hat{\vec{R}}, t)$
$\vec{L} = \vec{r} \times \vec{p}$	$\hat{\vec{L}} = -i\hbar\hat{\vec{R}} \times \vec{\nabla}$

According to Postulate 5, the total energy E for time-dependent systems is associated to the operator

$$\hat{H} = i\hbar\frac{\partial}{\partial t}. \tag{3.21}$$

This can be seen as follows. The wave function of a free particle of momentum $\vec{p}$ and total energy E is given by $\psi(\vec{r}, t) = Ae^{i(\vec{p}\cdot\vec{r}-Et)/\hbar}$, where A is a constant. The time derivative of $\psi(\vec{r}, t)$ yields

$$i\hbar\frac{\partial\psi(\vec{r}, t)}{\partial t} = E\psi(\vec{r}, t). \tag{3.22}$$

Let us look at the eigenfunctions and eigenvalues of the momentum operator $\hat{\vec{P}}$. The eigenvalue equation

$$-i\hbar\vec{\nabla}\psi(\vec{r}) = \vec{p}\psi(\vec{r}) \tag{3.23}$$

yields the eigenfunction $\psi(\vec{r})$ corresponding to the eigenvalue $\vec{p}$ such that $|\psi(\vec{r})|^2 d^3r$ is the probability of finding the particle with a momentum $\vec{p}$ in the volume element d^3r centered about $\vec{r}$. The solution to the eigenvalue equation (3.23) is

$$\psi(\vec{r}) = Ae^{i\vec{p}\cdot\vec{r}/\hbar}, \tag{3.24}$$

where A is a normalization constant. Since $\vec{p} = \hbar\vec{k}$ is the eigenvalue of the operator $\hat{\vec{P}}$, the eigenfunction (3.24) reduces to $\psi(\vec{r}) = Ae^{i\vec{k}\cdot\vec{r}}$; hence the eigenvalue equation (3.23) becomes

$$\hat{\vec{P}}\psi(\vec{r}) = \hbar\vec{k}\psi(\vec{r}). \tag{3.25}$$

To summarize, there is a one-to-one correspondence between observables and operators (Table 3.1).

Example 3.3 (Orbital angular momentum)
Find the operator representing the classical orbital angular momentum.

Solution
The classical expression for the orbital angular momentum of a particle whose position and linear momentum are $\vec{r}$ and $\vec{p}$ is given by $\vec{L} = \vec{r} \times \vec{p} = l_x\vec{i} + l_y\vec{j} + l_z\vec{k}$, where $l_x = yp_z - zp_y$, $l_y = zp_x - xp_z$, $l_z = xp_y - yp_x$.

To find the operator representing the classical angular momentum, we need simply to replace $\vec{r}$ and $\vec{p}$ with their corresponding operators $\hat{\vec{R}}$ and $\hat{\vec{P}} = -i\hbar\vec{\nabla}$: $\hat{\vec{L}} = -i\hbar\hat{\vec{R}} \times \vec{\nabla}$. This leads to

$$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y = -i\hbar\left(\hat{Y}\frac{\partial}{\partial z} - \hat{Z}\frac{\partial}{\partial y}\right), \tag{3.26}$$

$$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z = -i\hbar\left(\hat{Z}\frac{\partial}{\partial x} - \hat{X}\frac{\partial}{\partial Z}\right), \tag{3.27}$$

$$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x = -i\hbar\left(\hat{X}\frac{\partial}{\partial y} - \hat{Y}\frac{\partial}{\partial x}\right). \tag{3.28}$$

Recall that in classical mechanics the position and momentum components commute, $xp_x = p_x x$, and so do the components of the angular momentum, $l_x l_y = l_y l_x$. In quantum mechanics, however, this is not the case, since $\hat{X}\hat{P}_x = \hat{P}_x\hat{X} + i\hbar$ and, as will be shown in Chapter 5, $\hat{L}_x\hat{L}_y = \hat{L}_y\hat{L}_x + i\hbar\hat{L}_z$, and so on.

3.5 Measurement in Quantum Mechanics

Quantum theory is about the results of measurement; it says nothing about what might happen in the physical world outside the context of measurement. So the emphasis is on measurement.

3.5.1 How Measurements Disturb Systems

In classical physics it is possible to perform measurements on a system without disturbing it significantly. In quantum mechanics, however, the measurement process perturbs the system significantly. While carrying out measurements on classical systems, this perturbation does exist, but it is small enough that it can be neglected. In atomic and subatomic systems, however, the act of measurement induces nonnegligible or significant disturbances.

As an illustration, consider an experiment that measures the position of a hydrogenic electron. For this, we need to bombard the electron with electromagnetic radiation (photons). If we want to determine the position accurately, the wavelength of the radiation must be sufficiently short. Since the electronic orbit is of the order of 10^{-10} m, we must use a radiation whose wavelength is smaller than 10^{-10} m. That is, we need to bombard the electron with photons of energies higher than

$$h\nu = h\frac{c}{\lambda} = h\frac{3 \times 10^8}{10^{-10}} \sim 10^4 \text{ eV}. \tag{3.29}$$

When such photons strike the electron, not only will they perturb it, they will knock it completely off its orbit; recall that the ionization energy of the hydrogen atom is about 13.5 eV. Thus, the mere act of measuring the position of the electron disturbs it appreciably.

Let us now discuss the general concept of measurement in quantum mechanics. *The act of measurement generally changes the state of the system.* In theory we can represent the measuring device by an operator so that, after carrying out the measurement, the system will be in one of the eigenstates of the operator. Consider a system which is in a state $|\psi\rangle$. Before measuring an observable A, the state $|\psi\rangle$ can be represented by a linear superposition of eigenstates $|\psi_n\rangle$

of the corresponding operator $\hat{A}$:

$$|\psi\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n a_n|\psi_n\rangle. \tag{3.30}$$

According to Postulate 4, the act of measuring A changes the state of the system from $|\psi\rangle$ to one of the eigenstates $|\psi_n\rangle$ of the operator $\hat{A}$, and the result obtained is the eigenvalue a_n. The only *exception* to this rule is when the *system is already in one of the eigenstates of the observable being measured.* For instance, if the system is in the eigenstate $|\psi_n\rangle$, a measurement of the observable A yields with certainty (i.e., with probability = 1) the value a_n without changing the state $|\psi_n\rangle$.

Before a measurement, we do not know in advance with certainty in which eigenstate, among the various states $|\psi_n\rangle$, a system will be after the measurement; only a probabilistic outcome is possible. Postulate 4 states that the probability of finding the system in one particular nondegenerate eigenstate $|\psi_n\rangle$ is given by

$$P_n = \frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle}. \tag{3.31}$$

Note that the wave function does not predict the results of individual measurements; it instead determines the probability distribution, $P = |\psi|^2$, over measurements on many identical systems in the same state.

Finally, we may state that quantum mechanics is the mechanics applicable to objects for which measurements necessarily interfere with the state of the system. Quantum mechanically, we cannot ignore the effects of the measuring equipment on the system, for they are important. In general, certain measurements cannot be performed without major disturbances to other properties of the quantum system. In conclusion, *it is the effects of the interference by the equipment on the system which is the essence of quantum mechanics*.

3.5.2 Expectation Values

The expectation value $\langle\hat{A}\rangle$ of $\hat{A}$ with respect to a state $|\psi\rangle$ is defined by

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{3.32}$$

For instance, the energy of a system is given by the expectation value of the Hamiltonian: $E = \langle\hat{H}\rangle = \langle\psi|\hat{H}|\psi\rangle/\langle\psi|\psi\rangle$.

In essence, the expectation value $\langle\hat{A}\rangle$ represents the average result of measuring $\hat{A}$ on the state $|\ \psi\rangle$. To see this, using the complete set of eigenvectors $|\psi_n\rangle$ of $\hat{A}$ as a basis (i.e., $\hat{A}$ is diagonal in ψ_n), we can rewrite $\langle\hat{A}\rangle$ as follows:

$$\langle\hat{A}\rangle = \frac{1}{\langle\psi|\psi\rangle}\sum_{nm}\langle\psi|\psi_m\rangle\langle\psi_m|\hat{A}|\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n a_n\frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle}, \tag{3.33}$$

where we have used $\langle\psi_m|\hat{A}|\psi_n\rangle = a_n\delta_{nm}$. Since the quantity $|\langle\psi_n|\psi\rangle|^2/\langle\psi|\psi\rangle$ gives the probability P_n of finding the value a_n after measuring the observable A, we can indeed interpret $\langle\hat{A}\rangle$ as an *average* of a series of measurements of A:

$$\boxed{\langle\hat{A}\rangle = \sum_n a_n\frac{|\langle\psi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \sum_n a_n P_n.} \tag{3.34}$$

That is, the expectation value of an observable is obtained by adding all permissible eigenvalues a_n, with each a_n multiplied by the corresponding probability P_n.

The relation (3.34), which is valid for *discrete* spectra, can be extended to a *continuous* distribution of probabilities $P(a)$ as follows:

$$\langle \hat{A} \rangle = \frac{\int_{-\infty}^{+\infty} a\, |\psi(a)|^2 da}{\int_{-\infty}^{+\infty} |\psi(a)|^2 da} = \int_{-\infty}^{+\infty} a\, dP(a). \tag{3.35}$$

The expectation value of an observable can be obtained physically as follows: prepare a very large number of *identical* systems each in the *same* state $|\psi\rangle$. The observable A is then measured on all these identical systems; the results of these measurements are a_1, a_2, ..., a_n, ...; the corresponding probabilities of occurrence are P_1, P_2, ..., P_n, ... The average value of all these repeated measurements is called the expectation value of $\hat{A}$ with respect to the state $|\psi\rangle$.

Note that the process of obtaining different results when measuring the same observable on many identically prepared systems is contrary to classical physics, where these measurements must give the same outcome. In quantum mechanics, however, we can predict only the probability of obtaining a certain value for an observable.

Example 3.4

Consider a system whose state is given in terms of a complete and orthonormal set of five vectors $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, $|\phi_4\rangle$, $|\phi_5\rangle$ as follows:

$$|\psi\rangle = \frac{1}{\sqrt{19}}|\phi_1\rangle + \frac{2}{\sqrt{19}}|\phi_2\rangle + \sqrt{\frac{2}{19}}|\phi_3\rangle + \sqrt{\frac{3}{19}}|\phi_4\rangle + \sqrt{\frac{5}{19}}|\phi_5\rangle,$$

where $|\phi_n\rangle$ are eigenstates to the system's Hamiltonian, $\hat{H}|\phi_n\rangle = n\varepsilon_0|\phi_n\rangle$ with $n = 1, 2, 3, 4, 5$, and where ε_0 has the dimensions of energy.

(a) If the energy is measured on a large number of identical systems that are all initially in the same state $|\psi\rangle$, what values would one obtain and with what probabilities?

(b) Find the average energy of one such system.

Solution

First, note that $|\psi\rangle$ is not normalized:

$$\langle\psi|\psi\rangle = \sum_{n=1}^{5} a_n^2 \langle\phi_n|\phi_n\rangle = \sum_{n=1}^{5} a_n^2 = \frac{1}{19} + \frac{4}{19} + \frac{2}{19} + \frac{3}{19} + \frac{5}{19} = \frac{15}{19}, \tag{3.36}$$

since $\langle\phi_j|\phi_k\rangle = \delta_{jk}$ with $j, k = 1, 2, 3, 4, 5$.

(a) Since $E_n = \langle\phi_n|\hat{H}|\phi_n\rangle = n\varepsilon_0$ $(n = 1, 2, 3, 4, 5)$, the various measurements of the energy of the system yield the values $E_1 = \varepsilon_0$, $E_2 = 2\varepsilon_0$, $E_3 = 3\varepsilon_0$, $E_4 = 4\varepsilon_0$, $E_5 = 5\varepsilon_0$ with the following probabilities:

$$P_1(E_1) = \frac{|\langle\phi_1|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\frac{1}{\sqrt{19}}\langle\phi_1|\phi_1\rangle\right|^2 \times \frac{19}{15} = \frac{1}{15}, \tag{3.37}$$

$$P_2(E_2) = \frac{|\langle\phi_2|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\frac{2}{\sqrt{19}}\langle\phi_2|\phi_2\rangle\right|^2 \times \frac{19}{15} = \frac{4}{15}, \tag{3.38}$$

$$P_3(E_3) = \frac{|\langle\phi_3|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\sqrt{\frac{2}{19}}\langle\phi_3|\phi_3\rangle\right|^2 \times \frac{19}{15} = \frac{2}{15}, \tag{3.39}$$

$$P_4(E_4) = \frac{|\langle\phi_4|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\sqrt{\frac{3}{19}}\langle\phi_4|\phi_4\rangle\right|^2 \times \frac{19}{15} = \frac{3}{15}, \tag{3.40}$$

and

$$P_5(E_5) = \frac{|\langle\phi_5|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \left|\sqrt{\frac{5}{19}}\langle\phi_5|\phi_5\rangle\right|^2 \times \frac{19}{15} = \frac{5}{15}, \tag{3.41}$$

(b) The average energy of a system is given by

$$E = \sum_{j=1}^{5} P_j E_j = \frac{1}{15}\varepsilon_0 + \frac{8}{15}\varepsilon_0 + \frac{6}{15}\varepsilon_0 + \frac{12}{15}\varepsilon_0 + \frac{25}{15}\varepsilon_0 = \frac{52}{15}\varepsilon_0. \tag{3.42}$$

This energy can also be obtained from the expectation value of the Hamiltonian:

$$\begin{aligned} E &= \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{19}{15}\sum_{n=1}^{5} a_n^2\langle\phi_n|\hat{H}|\phi_n\rangle = \frac{19}{15}\left(\frac{1}{19} + \frac{8}{19} + \frac{6}{19} + \frac{12}{19} + \frac{25}{19}\right)\varepsilon_0 \\ &= \frac{52}{15}\varepsilon_0, \end{aligned} \tag{3.43}$$

where the values of the coefficients a_n^2 are listed in (3.36).

3.5.3 Complete Sets of Commuting Operators (CSCO)

Two observables A and B are said to be *compatible* when their corresponding operators commute, $[\hat{A}, \hat{B}] = 0$; observables corresponding to noncommuting operators are said to be *non-compatible*.

In what follows we are going to consider the task of measuring two observables A and B on a given system. Since the act of measurement generally *perturbs* the system, the result of measuring A and B therefore depends on the *order* in which they are carried out. Measuring A first and then B leads[2] in general to results that are different from those obtained by measuring B first and then A. How does this take place?

If $\hat{A}$ and $\hat{B}$ do not commute and if the system is in an eigenstate $|\psi_n^{(a)}\rangle$ of $\hat{A}$, a measurement of A yields with certainty a value a_n, since $\hat{A}|\psi_n^{(a)}\rangle = a_n|\psi_n^{(a)}\rangle$. Then, when we measure B, the state of the system will be left in one of the eigenstates of B. If we measure A again, we will find a value which will be different from a_n. What is this new value? We cannot answer this question with certainty: only a probabilistic outcome is possible. For this, we need to expand the eigenstates of B in terms of those of A, and thus provide a probabilistic answer as to the value of measuring A. *So if $\hat{A}$ and $\hat{B}$ do not commute, they cannot be measured simultaneously; the order in which they are measured matters.*

[2]The act of measuring A first and then B is represented by the action of product $\hat{B}\hat{A}$ of their corresponding operators on the state vector.

What happens when A and B commute? We can show that the results of their measurements will not depend on the order in which they are carried out. Before showing this, let us mention a useful theorem.

Theorem 3.1 *If two observables are compatible, their corresponding operators possess a set of common (or simultaneous) eigenstates (this theorem holds for both degenerate and nondegenerate eigenstates).*

Proof
We provide here a proof for the nondegenerate case only. If $|\psi_n\rangle$ is a nondegenerate eigenstate of $\hat{A}$, $\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle$, we have

$$\langle\psi_m|[\hat{A}, \hat{B}]|\psi_n\rangle = (a_m - a_n)\langle\psi_m|\hat{B}|\psi_n\rangle = 0, \tag{3.44}$$

since $\hat{A}$ and $\hat{B}$ commute. So $\langle\psi_m|\hat{B}|\psi_n\rangle$ must vanish unless $a_n = a_m$. That is,

$$\langle\psi_m|\hat{B}|\psi_n\rangle = \langle\psi_n|\hat{B}|\psi_n\rangle \propto \delta_{nm}. \tag{3.45}$$

Hence the $|\psi_n\rangle$ are *joint* or *simultaneous* eigenstates of $\hat{A}$ and $\hat{B}$ (this completes the proof).

Denoting the simultaneous eigenstate of $\hat{A}$ and $\hat{B}$ by $|\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}\rangle$, we have

$$\hat{A}|\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}\rangle = a_{n_1}|\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}\rangle, \tag{3.46}$$
$$\hat{B}|\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}\rangle = b_{n_2}|\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}\rangle. \tag{3.47}$$

Theorem 3.1 can be generalized to the case of many mutually compatible observables A, B, C, ... These compatible observables possess a *complete* set of *joint eigenstates*

$$|\psi_n\rangle = |\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}, \psi_{n_3}^{(c)}, \ldots\rangle. \tag{3.48}$$

The completeness and orthonormality conditions of this set are

$$\sum_{n_1}\sum_{n_2}\sum_{n_3}\cdots|\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}, \psi_{n_3}^{(c)}, \ldots\rangle\langle\psi_{n_1}^{(a)}, \psi_{n_2}^{(b)}, \psi_{n_3}^{(c)}, \ldots| = 1; \tag{3.49}$$

$$\langle\psi_{n'}|\psi_n\rangle = \delta_{n'n} = \delta_{n_1'n_1}\delta_{n_2'n_2}\delta_{n_3'n_3}\cdots. \tag{3.50}$$

Let us now show why, when two observables A and B are compatible, the order in which we carry out their measurements is irrelevant. Measuring A first, we would find a value a_n and would leave the system in an eigenstate of A. According to Theorem 3.1, this eigenstate is also an eigenstate of B. Thus a measurement of B yields with certainty b_n without affecting the state of the system. In this way, if we measure A again, we obtain with certainty the same initial value a_n. Similarly, another measurement of B will yield b_n and will leave the system in the same joint eigenstate of A and B. Thus, if two observables A and B are compatible, and if the system is initially in an eigenstate of one of their operators, their measurements not only yield precise values (eigenvalues) but they will not depend on the order in which the measurements were performed. In this case, A and B are said to be *simultaneously measurable. So compatible observables can be measured simultaneously with arbitrary accuracy; noncompatible observables cannot*.

What happens if an operator, say $\hat{A}$, has *degenerate* eigenvalues? The specification of one eigenvalue does not uniquely determine the state of the system. Among the degenerate eigenstates of $\hat{A}$, only a subset of them are also eigenstates of $\hat{B}$. Thus, the set of states that are joint eigenstates of both $\hat{A}$ and $\hat{B}$ is not complete. To resolve the degeneracy, we can introduce a third operator $\hat{C}$ which commutes with both $\hat{A}$ and $\hat{B}$; then we can construct a set of joint eigenstates of $\hat{A}$, $\hat{B}$, and $\hat{C}$ that is complete. If the degeneracy persists, we may introduce a fourth operator $\hat{D}$ that commutes with the previous three and then look for their joint eigenstates which form a complete set. Continuing in this way, we will ultimately exhaust all the operators (that is, there are no more independent operators) which commute with each other. When that happens, we have then obtained a *complete set of commuting operators* (CSCO). Only then will the state of the system be specified unambiguously, for the joint eigenstates of the CSCO are determined uniquely and will form a complete set (recall that a complete set of eigenvectors of an operator is called a basis). We should, at this level, state the following definition.

Definition: A set of Hermitian operators, $\hat{A}$, $\hat{B}$, $\hat{C}$, ..., is called a CSCO if the operators mutually commute and if the set of their common eigenstates is complete and not degenerate (i.e., unique).

The complete commuting set may sometimes consist of only one operator. *Any operator with nondegenerate eigenvalues constitutes, all by itself, a CSCO.* For instance, the position operator $\hat{X}$ of a one-dimensional, spinless particle provides a complete set. Its momentum operator $\hat{P}$ is also a complete set; together, however, $\hat{X}$ and $\hat{P}$ cannot form a CSCO, for they do not commute. In three-dimensional problems, the three-coordinate position operators $\hat{X}$, $\hat{Y}$, and $\hat{Z}$ form a CSCO; similarly, the components of the momentum operator $\hat{P}_x$, $\hat{P}_y$, and $\hat{P}_z$ also form a CSCO. In the case of spherically symmetric three-dimensional potentials, the set $\hat{H}$, $\hat{\vec{L}}^2$, $\hat{L}_z$ forms a CSCO. Note that in this case of spherical symmetry, we need three operators to form a CSCO because $\hat{H}$, $\hat{\vec{L}}^2$, and $\hat{L}_z$ are all degenerate; hence the complete and unique determination of the wave function cannot be achieved with one operator or with two.

In summary, when a given operator, say $\hat{A}$, is degenerate, the wave function cannot be determined uniquely unless we introduce one or more additional operators so as to form a complete commuting set.

3.5.4 Measurement and the Uncertainty Relations

We have seen in Chapter 2 that the uncertainty condition pertaining to the measurement of any two observables A and B is given by

$$\Delta A \Delta B \geq \frac{1}{2}|\langle[\hat{A},\ \hat{B}]\rangle|, \tag{3.51}$$

where $\Delta A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$.

Let us illustrate this on the joint measurement of the position and momentum observables. Since these observables are not compatible, their simultaneous measurement with infinite accuracy is not possible; that is, since $[\hat{X}, \hat{P}] = i\hbar$ there exists no state which is a simultaneous eigenstate of $\hat{X}$ and $\hat{P}$. For the case of the position and momentum operators, the relation (3.51) yields

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{3.52}$$

This condition shows that the position and momentum of a microscopic system cannot be measured with infinite accuracy both at once. If the position is measured with an uncertainty Δx, the uncertainty associated with its momentum measurement cannot be smaller than $\hbar/2\Delta x$. This is due to *the interference between the two measurements*. If we measure the position first, we perturb the system by changing its state to an eigenstate of the position operator; then the measurement of the momentum throws the system into an eigenstate of the momentum operator.

Another interesting application of the uncertainty relation (3.51) is to the orbital angular momentum of a particle. Since its components satisfy the commutator $[\hat{L}_x, \ \hat{L}_y] = i\hbar\hat{L}_z$, we obtain

$$\Delta L_x \Delta L_y \geq \frac{1}{2}\hbar|\langle\hat{L}_z\rangle|. \tag{3.53}$$

We can obtain the other two inequalities by means of a cyclic permutation of x, y, and z. If $\langle\hat{L}_z\rangle = 0$, $\hat{L}_x$ and $\hat{L}_y$ will have sharp values simultaneously. This occurs when the particle is in an s state. In fact, when a particle is in an s state, we have $\langle\hat{L}_x\rangle = \langle\hat{L}_y\rangle = \langle\hat{L}_z\rangle = 0$; hence all the components of orbital angular momentum will have sharp values simultaneously.

3.6 Time Evolution of the System's State

3.6.1 Time Evolution Operator

We want to examine here how quantum states evolve in time. That is, given the initial state $|\psi(t_0)\rangle$, how does one find the state $|\psi(t)\rangle$ at any later time t? The two states can be related by means of a linear operator $\hat{U}(t, t_0)$ such that

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle \qquad (t > t_0); \tag{3.54}$$

$\hat{U}(t, t_0)$ is known as the *time evolution operator* or *propagator*. From (3.54), we infer that

$$\hat{U}(t_0, t_0) = \hat{I}, \tag{3.55}$$

where $\hat{I}$ is the unit (identity) operator.

The issue now is to find $\hat{U}(t, t_0)$. For this, we need simply to substitute (3.54) into the time-dependent Schrödinger equation (3.5):

$$i\hbar\frac{\partial}{\partial t}\left(\hat{U}(t, t_0)|\psi(t_0)\rangle\right) = \hat{H}\left(\hat{U}(t, t_0)|\psi(t_0)\rangle\right) \tag{3.56}$$

or

$$\frac{\partial\hat{U}(t, t_0)}{\partial t} = -\frac{i}{\hbar}\hat{H}\hat{U}(t, t_0). \tag{3.57}$$

The integration of this differential equation depends on whether or not the Hamiltonian depends on time. If it does not depend on time, and taking into account the initial condition (3.55), we can easily ascertain that the integration of (3.57) leads to

$$\boxed{\hat{U}(t, t_0) = e^{-i(t-t_0)\hat{H}/\hbar} \qquad \text{and} \qquad |\psi(t)\rangle = e^{-i(t-t_0)\hat{H}/\hbar}|\psi(t_0)\rangle.} \tag{3.58}$$

We will show in Section 3.7 that the operator $\hat{U}(t, t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$ represents a finite time translation.

If, on the other hand, $\hat{H}$ depends on time the integration of (3.57) becomes less trivial. We will deal with this issue in Chapter 10 when we look at time-dependent potentials or at the time-dependent perturbation theory. In this chapter, and in all chapters up to Chapter 10, we will consider only Hamiltonians that do not depend on time.

Note that $\hat{U}(t, t_0)$ is a unitary operator, since

$$\hat{U}(t, t_0)\hat{U}^\dagger(t, t_0) = \hat{U}(t, t_0)\hat{U}^{-1}(t, t_0) = e^{-i(t-t_0)\hat{H}/\hbar}e^{i(t-t_0)\hat{H}/\hbar} = \hat{I} \tag{3.59}$$

or $\hat{U}^\dagger = \hat{U}^{-1}$.

3.6.2 Stationary States: Time-Independent Potentials

In the position representation, the time-dependent Schrödinger equation (3.5) for a particle of mass m moving in a time-dependent potential $\hat{V}(\vec{r}, t)$ can be written as follows:

$$\boxed{i\hbar\frac{\partial\Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}, t) + \hat{V}(\vec{r}, t)\Psi(\vec{r}, t).} \tag{3.60}$$

Now, let us consider the particular case of *time-independent* potentials: $\hat{V}(\vec{r}, t) = \hat{V}(\vec{r})$. In this case the Hamiltonian operator will also be time independent, and hence the Schrödinger equation will have solutions that are *separable*, i.e., solutions that consist of a product of two functions, one depending only on $\vec{r}$ and the other only on time:

$$\Psi(\vec{r}, t) = \psi(\vec{r})f(t). \tag{3.61}$$

Substituting (3.61) into (3.60) and dividing both sides by $\psi(\vec{r})f(t)$, we obtain

$$i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = \frac{1}{\psi(\vec{r})}\left[-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + \hat{V}(\vec{r})\psi(\vec{r})\right]. \tag{3.62}$$

Since the left-hand side depends only on time and the right-hand side depends only on $\vec{r}$, both sides must be equal to a constant; this constant, which we denote by E, has the dimensions of energy. We can therefore break (3.62) into two separate differential equations, one depending on time only,

$$i\hbar\frac{df(t)}{dt} = Ef(t), \tag{3.63}$$

and the other on the space variable $\vec{r}$,

$$\boxed{\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}).} \tag{3.64}$$

This equation is known as the *time-independent* Schrödinger equation for a particle of mass m moving in a time-independent potential $\hat{V}(\vec{r})$.

The solutions to (3.63) can be written as $f(t) = e^{-iEt/\hbar}$; hence the state (3.61) becomes

$$\Psi(\vec{r}, t) = \psi(\vec{r})e^{-iEt/\hbar}. \tag{3.65}$$

This particular solution of the Schrödinger equation (3.60) for a *time-independent potential* is called a *stationary state*. Why is this state called *stationary*? The reason is obvious: the probability density is stationary, i.e., it does not depend on time:

$$|\Psi(\vec{r}, t)|^2 = |\psi(\vec{r})e^{-iEt/\hbar}|^2 = |\psi(\vec{r})|^2. \tag{3.66}$$

Note that such a state has a precise value for the energy, $E = \hbar\omega$.

In summary, stationary states, which are given by the solutions of (3.64), exist only for time-independent potentials. The set of energy levels that are solutions to this equation are called the *energy spectrum* of the system. The states corresponding to discrete and continuous spectra are called *bound* and *unbound* states, respectively. We will consider these questions in detail in Chapter 4.

The most general solution to the time-dependent Schrödinger equation (3.60) can be written as an expansion in terms of the stationary states $\psi_n(\vec{r})\exp(-iE_nt/\hbar)$:

$$\Psi(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r}) \exp\left(-\frac{iE_n t}{\hbar}\right), \tag{3.67}$$

where $c_n = \langle \psi_n | \Psi(t=0)\rangle = \int \psi_n^*(\vec{r})\psi(\vec{r})\, d^3r$. The general solution (3.67) is not a stationary state, because a linear superposition of stationary states is not necessarily a stationary state.

Remark

The time-dependent and time-independent Schrödinger equations are given in one dimension by (see (3.60) and (3.64))

$$\boxed{i\hbar\frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + \hat{V}(x,t)\Psi(x,t),} \tag{3.68}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \hat{V}(x)\psi(x) = E\psi(x).} \tag{3.69}$$

3.6.3 Schrödinger Equation and Wave Packets

Can we derive the Schrödinger equation (3.5) formally from first principles? No, we cannot; we can only postulate it. What we can do, however, is to provide an educated guess on the formal steps leading to it. *Wave packets* offer the formal tool to achieve that. We are going to show how to start from a wave packet and end up with the Schrödinger equation.

As seen in Chapter 1, the wave packet representing a particle of energy E and momentum p moving in a potential V is given by

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\tilde{\phi}(p)\exp\left[\frac{i}{\hbar}(px - Et)\right]dp \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\tilde{\phi}(p)\exp\left[\frac{i}{\hbar}\left(px - \left(\frac{p^2}{2m} + V\right)t\right)\right]dp;\end{aligned} \tag{3.70}$$

recall that wave packets unify the corpuscular (E and p) and the wave (k and ω) features of particles: $k = p/\hbar$, $\hbar\omega = E = p^2/(2m) + V$. A partial time derivative of (3.70) yields

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\tilde{\phi}(p)\left(\frac{p^2}{2m} + V\right)\exp\left[\frac{i}{\hbar}\left(px - \left(\frac{p^2}{2m} + V\right)t\right)\right]dp. \tag{3.71}$$

Since $p^2/(2m) = -(\hbar^2/2m)\partial^2/\partial x^2$ and assuming that V is constant, we can take the term $-(\hbar^2/2m)\partial^2/\partial x^2 + V$ outside the integral sign, for it does not depend on p:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\tilde{\phi}(p)\exp\left[\frac{i}{\hbar}\left(px - \left(\frac{p^2}{2m} + V\right)t\right)\right]dp. \tag{3.72}$$

This can be written as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\Psi(x,t). \tag{3.73}$$

Now, since this equation is valid for spatially varying potentials $V = V(x)$, we see that we have ended up with the Schrödinger equation (3.68).

3.6.4 The Conservation of Probability

Since the Hamiltonian operator is Hermitian, we can show that the norm $\langle\Psi(t)|\Psi(t)\rangle$, which is given by

$$\langle\Psi(t)|\Psi(t)\rangle = \int |\Psi(\vec{r},t)|^2\, d^3r, \tag{3.74}$$

is time independent. This means, if $|\Psi(t)\rangle$ is normalized, it stays normalized for all subsequent times. This is a direct consequence of the hermiticity of $\hat{H}$.

To prove that $\langle\Psi(t)|\Psi(t)\rangle$ is constant, we need simply to show that its time derivative is zero. First, the time derivative of $\langle\Psi(t)|\Psi(t)\rangle$ is

$$\frac{d}{dt}\langle\Psi(t)|\Psi(t)\rangle = \left(\frac{d}{dt}\langle\Psi(t)|\right)|\Psi(t)\rangle + \langle\Psi(t)|\left(\frac{d|\Psi(t)\rangle}{dt}\right), \tag{3.75}$$

where $d|\Psi(t)\rangle/dt$ and $d\langle\Psi(t)|/dt$ can be obtained from (3.5):

$$\frac{d}{dt}|\Psi(t)\rangle = -\frac{i}{\hbar}\hat{H}|\Psi(t)\rangle, \tag{3.76}$$

$$\frac{d}{dt}\langle\Psi(t)| = \frac{i}{\hbar}\langle\Psi(t)|\hat{H}^\dagger = \frac{i}{\hbar}\langle\Psi(t)|\hat{H}. \tag{3.77}$$

Inserting these two equations into (3.75), we end up with

$$\frac{d}{dt}\langle\Psi(t)|\Psi(t)\rangle = \left(\frac{i}{\hbar} - \frac{i}{\hbar}\right)\langle\Psi(t)|\hat{H}|\Psi(t)\rangle = 0. \tag{3.78}$$

Thus, the probability density $\langle\Psi|\Psi\rangle$ does not evolve in time.

In what follows we are going to calculate the probability density in the position representation. For this, we need to invoke the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + \hat{V}(\vec{r},t)\Psi(\vec{r},t) \tag{3.79}$$

and its complex conjugate

$$-i\hbar\frac{\partial\Psi^*(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi^*(\vec{r},t) + \hat{V}(\vec{r},t)\Psi^*(\vec{r},t). \tag{3.80}$$

Multiplying both sides of (3.79) by $\Psi^*(\vec{r}, t)$ and both sides of (3.80) by $\Psi(\vec{r}, t)$, and subtracting the two resulting equations, we obtain

$$i\hbar \frac{\partial}{\partial t}\left[\Psi^*(\vec{r}, t)\Psi(\vec{r}, t)\right] = -\frac{\hbar^2}{2m}\left[\Psi^*(\vec{r}, t)\nabla^2\Psi(\vec{r}, t) - \Psi\nabla^2\Psi^*\right]. \tag{3.81}$$

We can rewrite this equation as

$$\boxed{\frac{\partial \rho(\vec{r}, t)}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0,} \tag{3.82}$$

where $\rho(\vec{r}, t)$ and $\vec{J}$ are given by

$$\boxed{\rho(\vec{r}, t) = \Psi^*(\vec{r}, t)\Psi(\vec{r}, t), \qquad \vec{J}(\vec{r}, t) = \frac{i\hbar}{2m}\left(\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi\right);} \tag{3.83}$$

$\rho(\vec{r}, t)$ is called the *probability density*, while $\vec{J}(\vec{r}, t)$ is the *probability current density*, or simply the *current density*, or even the particle density flux. By analogy with charge conservation in electrodynamics, equation (3.82) is interpreted as the *conservation of probability*.

Let us find the relationship between the density operators $\hat{\rho}(t)$ and $\hat{\rho}(t_0)$. Since $|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi(t_0)\rangle$ and $\langle\Psi(t)| = \langle\Psi(t_0)|\hat{U}^\dagger(t, t_0)$, we have

$$\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)| = \hat{U}(t, t_0)|\Psi(0)\rangle\langle\Psi(0)|\hat{U}^\dagger(t, t_0). \tag{3.84}$$

This is known as the *density operator* for the state $|\Psi(t)\rangle$. Hence knowing $\hat{\rho}(t_0)$ we can calculate $\hat{\rho}(t)$ as follows:

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t, t_0). \tag{3.85}$$

3.6.5 Time Evolution of Expectation Values

We want to look here at the time dependence of the expectation value of a linear operator; if the state $|\Psi(t)\rangle$ is normalized, the expectation value is given by

$$\langle\hat{A}\rangle = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle. \tag{3.86}$$

Using (3.76) and (3.77), we can write $d\langle\hat{A}\rangle/dt$ as follows:

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle\Psi(t)|\hat{A}\hat{H} - \hat{H}\hat{A}|\Psi(t)\rangle + \langle\Psi(t)|\frac{\partial A}{\partial t}|\Psi(t)\rangle \tag{3.87}$$

or

$$\boxed{\frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A}, \hat{H}]\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle.} \tag{3.88}$$

Two important results stem from this relation. First, if the observable A does not depend explicitly on time, the term $\partial\hat{A}/\partial t$ will vanish, so the rate of change of the expectation value of $\hat{A}$ is given by $\langle[\hat{A}, \hat{H}]\rangle/i\hbar$. Second, besides not depending explicitly on time, if the observable A commutes with the Hamiltonian, the quantity $d\langle\hat{A}\rangle/dt$ will then be zero; hence the expectation value $\langle \hat{A} \rangle$ will be constant in time. So if $\hat{A}$ commutes with the Hamiltonian and is not dependent on time, the observable A is said to be a *constant of the motion*; that is, *the expectation value of an operator that does not depend on time and that commutes with the Hamiltonian is constant in time*:

$$\boxed{\text{If} \quad [\hat{H}, \hat{A}] = 0 \quad \text{and} \quad \frac{\partial \hat{A}}{\partial t} = 0 \implies \frac{d\langle \hat{A} \rangle}{dt} = 0 \implies \langle \hat{A} \rangle = \text{constant.}} \tag{3.89}$$

For instance, we can verify that the energy, the linear momentum, and the angular momentum of an isolated system are conserved: $d\langle \hat{H} \rangle/dt = 0$, $d\langle \hat{\vec{P}} \rangle/dt = 0$, and $d\langle \hat{\vec{L}} \rangle/dt = 0$. This implies that the expectation values of $\hat{H}$, $\hat{\vec{P}}$, and $\hat{\vec{L}}$ are constant. Recall from classical physics that the conservation of energy, linear momentum, and angular momentum are consequences of the following symmetries, respectively: homogeneity of time, homogeneity of space, and isotropy of space. We will show in the following section that these symmetries are associated, respectively, with invariances in time translation, space translation, and space rotation.

As an example, let us consider the time evolution of the expectation value of the density operator $\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$; see (3.84). From (3.5), which leads to $\partial|\Psi(t)\rangle/\partial t = (1/i\hbar)\hat{H}|\Psi(t)\rangle$ and $\partial\langle\Psi(t)|/\partial t = -(1/i\hbar)\langle\Psi(t)|\hat{H}$, we have

$$\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{1}{i\hbar}\hat{H}|\Psi(t)\rangle\langle\Psi(t)| - \frac{1}{i\hbar}|\Psi(t)\rangle\langle\Psi(t)|\hat{H} = -\frac{1}{i\hbar}[\hat{\rho}(t), \hat{H}]. \tag{3.90}$$

A substitution of this relation into (3.88) leads to

$$\frac{d}{dt}\langle \hat{\rho}(t) \rangle = \frac{1}{i\hbar}\langle [\hat{\rho}(t), \hat{H}] \rangle + \langle \frac{\partial \hat{\rho}(t)}{\partial t} \rangle = \frac{1}{i\hbar}\langle [\hat{\rho}(t), \hat{H}] \rangle - \frac{1}{i\hbar}\langle [\hat{\rho}(t), \hat{H}] \rangle = 0. \tag{3.91}$$

So the density operator is a constant of the motion. In fact, we can easily show that

$$\begin{aligned} \langle [\hat{\rho}(t), \hat{H}] \rangle &= \langle \Psi(t)|[|\Psi(t)\rangle\langle\Psi(t)|, \hat{H}]|\Psi(t)\rangle \\ &= \langle \Psi(t)|\Psi(t)\rangle\langle\Psi(t)|\hat{H}|\Psi(t)\rangle - \langle\Psi(t)|\hat{H}|\Psi(t)\rangle\langle\Psi(t)|\Psi(t)\rangle \\ &= 0, \end{aligned} \tag{3.92}$$

which, when combined with (3.90), yields $\langle \partial\hat{\rho}(t)/\partial t \rangle = 0$.

Finally, we should note that the constants of motion are nothing but observables that can be measured simultaneously with the energy to arbitrary accuracy. If a system has a complete set of commuting operators (CSCO), the number of these operators is given by the total number of constants of the motion.

3.7 Symmetries and Conservation Laws

We are interested here in symmetries that leave the Hamiltonian of an *isolated* system invariant. We will show that for each such symmetry there corresponds an observable which is a constant of the motion. The invariance principles relevant to our study are the time translation invariance and the space translation invariance. We may recall from classical physics that whenever a system is invariant under space translations, its total momentum is conserved; and whenever it is invariant under rotations, its total angular momentum is also conserved.

To prepare the stage for symmetries and conservation laws in quantum mechanics, we are going to examine the properties of infinitesimal and finite unitary transformations that are most essential to these invariance principles.

3.7.1 Infinitesimal Unitary Transformations

In Chapter 2 we saw that the transformations of a state vector $|\psi\rangle$ and an operator $\hat{A}$ under an infinitesimal unitary transformation $U_\varepsilon(\hat{G}) = \hat{I} + i\varepsilon\hat{G}$ are given by

$$|\psi'\rangle = (\hat{I} + i\varepsilon\hat{G})|\psi\rangle = |\psi\rangle + \delta|\psi\rangle, \tag{3.93}$$
$$\hat{A}' = (\hat{I} + i\varepsilon\hat{G})\hat{A}(\hat{I} - i\varepsilon\hat{G}) \simeq \hat{A} + i\varepsilon[\hat{G}, \hat{A}], \tag{3.94}$$

where ε and $\hat{G}$ are called the parameter and the generator of the transformation, respectively.

Let us consider two important applications of infinitesimal unitary transformations: time and space translations.

3.7.1.1 Time Translations: $\hat{G} = \hat{H}/\hbar$

The application of $\hat{U}_{\delta t}(\hat{H}) = \hat{I} + (i/\hbar)\delta t\,\hat{H}$ on a state $|\psi(t)\rangle$ gives

$$\left(\hat{I} + \frac{i}{\hbar}\,\delta t\,\hat{H}\right)|\psi(t)\rangle = |\psi(t)\rangle + \left(\frac{i}{\hbar}\delta t\right)\hat{H}|\psi(t)\rangle. \tag{3.95}$$

Since $\hat{H}|\psi(t)\rangle = i\hbar\partial|\psi(t)\rangle/\partial t$ we have

$$\boxed{\left(\hat{I} + \frac{i}{\hbar}\,\delta t\,\hat{H}\right)|\psi(t)\rangle = |\psi(t)\rangle - \delta t\frac{\partial|\psi(t)\rangle}{\partial t} \simeq |\psi(t - \delta t)\rangle,} \tag{3.96}$$

because $|\psi(t)\rangle - \delta t\,\partial|\psi(t)\rangle/\partial t$ is nothing but the first-order Taylor expansion of $|\psi(t-\delta t)\rangle$. We conclude from (3.96) that the application of $\hat{U}_{\delta t}(\hat{H})$ to $|\psi(t)\rangle$ generates a state $|\psi(t-\delta t)\rangle$ which consists simply of a *time translation* of $|\psi(t)\rangle$ by an amount equal to δt. *The Hamiltonian in* $(\hat{I}+(i/\hbar)\delta t\,\hat{H})$ *is thus the generator of infinitesimal time translations*. Note that this translation preserves the shape of the state $|\psi(t)\rangle$, for its overall shape is merely translated in time by δt.

3.7.1.2 Spatial Translations: $\hat{G} = \hat{P}_x/\hbar$

The application of $\hat{U}_\varepsilon(\hat{P}_x) = \hat{I} + (i/\hbar)\varepsilon\hat{P}_x$ to $\psi(x)$ gives

$$\left(\hat{I} + \frac{i}{\hbar}\varepsilon\hat{P}_x\right)\psi(x) = \psi(x) + \left(\frac{i}{\hbar}\varepsilon\right)\hat{P}_x\psi(x). \tag{3.97}$$

Since $\hat{P}_x = -i\hbar\partial/\partial x$ and since the first-order Taylor expansion of $\psi(x+\varepsilon)$ is given by $\psi(x+\varepsilon) = \psi(x) + \varepsilon\partial\psi(x)/\partial x$, we have

$$\boxed{\left(\hat{I} + \frac{i}{\hbar}\varepsilon\hat{P}_x\right)\psi(x) = \psi(x) + \varepsilon\frac{\partial\psi(x)}{\partial x} \simeq \psi(x+\varepsilon).} \tag{3.98}$$

So, when $\hat{U}_\varepsilon(\hat{P}_x)$ acts on a wave function, it translates it spatially by an amount equal to ε.

Using $[\hat{X},\ \hat{P}_x] = i\hbar$ we infer from (3.94) that the position operator $\hat{X}$ transforms as follows:

$$\hat{X}' = \left(\hat{I} + \frac{i}{\hbar}\varepsilon\hat{P}_x\right)\hat{X}\left(\hat{I} - \frac{i}{\hbar}\varepsilon\hat{P}_x\right) \simeq \hat{X} + \frac{i}{\hbar}\varepsilon[\hat{P}_x, \hat{X}] = \hat{X} + \varepsilon. \tag{3.99}$$

The relations (3.98) and (3.99) show that the *linear momentum operator in* $(\hat{I} + (i/\hbar)\varepsilon\hat{P}_x)$ *is a generator of infinitesimal spatial translations*.

3.7.2 Finite Unitary Transformations

In Chapter 2 we saw that a *finite* unitary transformation can be constructed by performing a succession of infinitesimal transformations. For instance, by applying a single infinitesimal time translation N times in steps of τ/N, we can generate a finite time translation

$$\hat{U}_\tau(\hat{H}) = \lim_{N\to+\infty}\prod_{k=1}^{N}\left(\hat{I}+\frac{i}{\hbar}\frac{\tau}{N}\hat{H}\right) = \lim_{N\to+\infty}\left(\hat{I}+\frac{i}{\hbar}\tau\hat{H}\right)^N = \exp\left(\frac{i}{\hbar}\tau\hat{H}\right), \tag{3.100}$$

where the Hamiltonian is the generator of finite time translations. We should note that the time evolution operator $\hat{U}(t, t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$, displayed in (3.58), represents a finite unitary transformation where $\hat{H}$ is the generator of the time translation.

By analogy with (3.96) we can show that the application of $\hat{U}_\tau(\hat{H})$ to $|\psi(t)\rangle$ yields

$$\boxed{\hat{U}_\tau(\hat{H})|\psi(t)\rangle = \exp\left(\frac{i}{\hbar}\tau\hat{H}\right)|\psi(t)\rangle = |\psi(t-\tau)\rangle,} \tag{3.101}$$

where $|\psi(t-\tau)\rangle$ is merely a time translation of $|\psi(t)\rangle$.

Similarly, we can infer from (3.98) that the application of $\hat{U}_{\vec{a}}(\hat{\vec{P}}) = \exp(i\vec{a}\cdot\hat{\vec{P}}/\hbar)$ to a wave function causes it to be translated in space by a vector $\vec{a}$:

$$\boxed{\hat{U}_{\vec{a}}(\hat{\vec{P}})\psi(\vec{r}) = \exp\left(\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right)\psi(\vec{r}) = \psi(\vec{r}+\vec{a}).} \tag{3.102}$$

To calculate the transformed position vector operator $\hat{\vec{R}}\,'$, let us invoke a relation we derived in Chapter 2:

$$\hat{A}' = e^{i\alpha\hat{G}}\hat{A}e^{-i\alpha\hat{G}} = \hat{A} + i\alpha[\hat{G}, \hat{A}] + \frac{(i\alpha)^2}{2!}[\hat{G}, [\hat{G}, \hat{A}]] + \frac{(i\alpha)^3}{3!}[\hat{G}, [\hat{G}, [\hat{G}, \hat{A}]]] + \cdots. \tag{3.103}$$

An application of this relation to the spatial translation operator $\hat{U}_{\vec{a}}(\hat{\vec{P}})$ yields

$$\hat{\vec{R}}\,' = \exp\left(\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right)\hat{\vec{R}}\exp\left(-\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right) = \hat{\vec{R}} + \frac{i}{\hbar}[\vec{a}\cdot\hat{\vec{P}}, \hat{\vec{R}}] = \hat{\vec{R}} + \vec{a}. \tag{3.104}$$

In deriving this, we have used the fact that $[\vec{a}\cdot\hat{\vec{P}}, \hat{\vec{R}}] = -i\hbar\vec{a}$ and that the other commutators are zero, notably $[\vec{a}\cdot\hat{\vec{P}}, [\vec{a}\cdot\hat{\vec{P}}, \hat{\vec{R}}]] = 0$. From (3.102) and (3.104), we see that *the linear momentum in* $\exp(i\vec{a}\cdot\hat{\vec{P}}/\hbar)$ *is a generator of finite spatial translations*.

3.7.3 Symmetries and Conservation Laws

We want to show here that every invariance principle of $\hat{H}$ is connected with a conservation law.

The Hamiltonian of a system transforms under a unitary transformation $e^{i\alpha\hat{G}}$ as follows; see (3.103):

$$\hat{H}' = e^{i\alpha\hat{G}}\hat{H}e^{-i\alpha\hat{G}} = \hat{H} + i\alpha[\hat{G}, \hat{H}] + \frac{(i\alpha)^2}{2!}[\hat{G}, [\hat{G}, \hat{H}]] + \frac{(i\alpha)^3}{3!}[\hat{G}, [\hat{G}, [\hat{G}, \hat{H}]]] + \cdots. \tag{3.105}$$

If $\hat{H}$ commutes with $\hat{G}$, it also commutes with the unitary transformation $\hat{U}_\alpha(\hat{G}) = e^{i\alpha\hat{G}}$. In this case we may infer two important conclusions. On the one hand, there is an *invariance principle*: the Hamiltonian is invariant under the transformation $\hat{U}_\alpha(\hat{G})$, since

$$\hat{H}' = e^{i\alpha\hat{G}}\hat{H}e^{-i\alpha\hat{G}} = e^{i\alpha\hat{G}}e^{-i\alpha\hat{G}}\hat{H} = \hat{H}. \tag{3.106}$$

On the other hand, if in addition to $[\hat{G},\ \hat{H}] = 0$, the operator $\hat{G}$ does not depend on time explicitly, there is a *conservation law*: equation (3.88) shows that $\hat{G}$ is a *constant of the motion*, since

$$\frac{d}{dt}\langle\hat{G}\rangle = \frac{1}{i\hbar}\langle[\hat{G}, \hat{H}]\rangle + \langle\frac{\partial\hat{G}}{\partial t}\rangle = 0. \tag{3.107}$$

We say that $\hat{G}$ is conserved.

So whenever the Hamiltonian is invariant under a unitary transformation, the generator of the transformation is conserved. We may say, in general, that *for every invariance symmetry of the Hamiltonian, there corresponds a conservation law.*

3.7.3.1 Conservation of Energy and Linear Momentum

Let us consider two interesting applications pertaining to the invariance of the Hamiltonian of an *isolated* system with respect to time translations and to space translations. First, let us consider time translations. As shown in (3.58), time translations are generated in the case of time-independent Hamiltonians by the evolution operator $\hat{U}(t, t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$. Since $\hat{H}$ commutes with the generator of the time translation (which is given by $\hat{H}$ itself), it is invariant under time translations. *As $\hat{H}$ is invariant under time translations, the energy of an isolated system is conserved*. We should note that if the system is invariant under time translations, this means there is a symmetry of time homogeneity. Time homogeneity implies that the time-displaced state $\psi(t-\tau)$, like $\psi(t)$, satisfies the Schrödinger equation.

The second application pertains to the spatial translations, or to transformations under $\hat{U}_{\vec{a}}(\hat{\vec{P}}) = \exp(i\vec{a}\cdot\hat{\vec{P}}/\hbar)$, of an isolated system. The linear momentum is invariant under $\hat{U}_{\vec{a}}(\hat{\vec{P}})$ and the position operator transforms according to (3.104):

$$\hat{\vec{P}}' = \hat{\vec{P}}, \qquad \hat{\vec{R}}' = \hat{\vec{R}} + \vec{a}. \tag{3.108}$$

For instance, since the Hamiltonian of a free particle does not depend on the coordinates, it commutes with the linear momentum $[\hat{H}, \hat{\vec{P}}] = 0$. The Hamiltonian is then invariant under spatial translations, since

$$\hat{H}' = \exp\left(\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right)\hat{H}\exp\left(-\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right) = \exp\left(\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right)\exp\left(-\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{P}}\right)\hat{H} = \hat{H}. \tag{3.109}$$

Since $[\hat{H}, \hat{\vec{P}}] = 0$ and since the linear momentum operator does not depend explicitly on time, we infer from (3.88) that $\hat{\vec{P}}$ is a constant of the motion, since

$$\frac{d}{dt}\langle\hat{\vec{P}}\rangle = \frac{1}{i\hbar}\langle[\hat{\vec{P}}, \hat{H}]\rangle + \langle\frac{\partial\hat{\vec{P}}}{\partial t}\rangle = 0. \tag{3.110}$$

So if $[\hat{H},\ \hat{\vec{P}}] = 0$ the *Hamiltonian will be invariant under spatial translations and the linear momentum will be conserved*. A more general case where the linear momentum is a constant of the motion is provided by an isolated system, for its total linear momentum is conserved. Note that the invariance of the system under spatial translations means there is a symmetry of spatial homogeneity. The requirement for the homogeneity of space implies that the spatially displaced wave function $\psi(\vec{r}+\vec{a})$, much like $\psi(\vec{r})$, satisfies the Schrödinger equation.

In summary, the symmetry of time homogeneity gives rise to the conservation of energy, whereas the symmetry of space homogeneity gives rise to the conservation of linear momentum.

In Chapter 7 we will see that the symmetry of space isotropy, or the invariance of the Hamiltonian with respect to space rotations, leads to conservation of the angular momentum.

Parity operator

The unitary transformations we have considered so far, time translations and space translations, are *continuous*. We may consider now a *discrete* unitary transformation, the *parity*. As seen in Chapter 2, the parity transformation consists of an inversion or reflection through the origin of the coordinate system:

$$\hat{\mathcal{P}}\psi(\vec{r}) = \psi(-\vec{r}). \tag{3.111}$$

If the parity operator commutes with the system's Hamiltonian,

$$[\hat{H},\ \hat{\mathcal{P}}] = 0, \tag{3.112}$$

the *parity will be conserved*, and hence a constant of the motion. In this case the Hamiltonian and the parity operator have simultaneous eigenstates. For instance, we will see in Chapter 4 that the wave functions of a particle moving in a symmetric potential, $\hat{V}(\vec{r}) = \hat{V}(-\vec{r})$, have definite parities: they can be only even or odd. Similarly, we can ascertain that the parity of an isolated system is a constant of the motion.

3.8 Connecting Quantum to Classical Mechanics

3.8.1 Poisson Brackets and Commutators

To establish a connection between quantum mechanics and classical mechanics, we may look at the time evolution of observables.

Before describing the time evolution of a dynamical variable within the context of classical mechanics, let us review the main ideas of the mathematical tool relevant to this description, the *Poisson bracket*. The Poisson bracket between two dynamical variables A and B is defined in terms of the generalized coordinates q_i and the momenta p_i of the system:

$$\{A, B\} = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} \right). \tag{3.113}$$

Since the variables q_i are independent of p_i, we have $\partial q_j/\partial p_k = 0$, $\partial p_j/\partial q_k = 0$; thus we can show that

$$\{q_j, q_k\} = \{p_j, p_k\} = 0, \qquad \{q_j, p_k\} = \delta_{jk}. \tag{3.114}$$

Using (3.113) we can easily infer the following properties of the Poisson brackets:

- Antisymmetry

$$\{A,\ B\} = -\{B,\ A\} \tag{3.115}$$

- Linearity

$$\{A,\ \alpha B + \beta C + \gamma D + \cdots\} = \alpha\{A,\ B\} + \beta\{A,\ C\} + \gamma\{A,\ D\} + \cdots \tag{3.116}$$

- Complex conjugate

$$\{A,\ B\}^* = \{A^*,\ B^*\} \tag{3.117}$$

- Distributivity

$$\{A,\ BC\} = \{A,\ B\}C + B\{A,\ C\}, \qquad \{AB,\ C\} = A\{B,\ C\} + \{A,\ C\}B \tag{3.118}$$

- Jacobi identity

$$\{A, \{B,\ C\}\} + \{B,\ \{C,\ A\}\} + \{C,\ \{A,\ B\}\} = 0 \tag{3.119}$$

- Using $df^n(x)/dx = nf^{n-1}(x)df(x)/dx$, we can show that

$$\{A,\ B^n\} = nB^{n-1}\{A,\ B\}, \qquad \{A^n,\ B\} = nA^{n-1}\{A,\ B\} \tag{3.120}$$

These properties are similar to the properties of the quantum mechanical commutators seen in Chapter 2.

The total time derivative of a dynamical variable A is given by

$$\frac{dA}{dt} = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial q_j}{\partial t} + \frac{\partial A}{\partial p_j}\frac{\partial p_j}{\partial t}\right) + \frac{\partial A}{\partial t} = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial H}{\partial p_j}\right) + \frac{\partial A}{\partial t}; \tag{3.121}$$

in deriving this relation we have used the Hamilton equations of classical mechanics:

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j}, \qquad \frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j}, \tag{3.122}$$

where H is the Hamiltonian of the system. The total time evolution of a dynamical variable A is thus given by the following equation of motion:

$$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t}. \tag{3.123}$$

Note that if A does not depend explicitly on time, its time evolution is given simply by $dA/dt = \{A, H\}$. If $dA/dt = 0$ or $\{A, H\} = 0$, A is said to be a *constant of the motion*.

Comparing the classical relation (3.123) with its quantum mechanical counterpart (3.88),

$$\frac{d}{dt}\langle \hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A}, \hat{H}]\rangle + \langle\frac{\partial \hat{A}}{\partial t}\rangle, \tag{3.124}$$

we see that they are identical only if we identify the Poisson bracket $\{A, H\}$ with the commutator $[\hat{A}, \hat{H}]/(i\hbar)$. We may thus infer the following general rule. The Poisson bracket of any pair of classical variables can be obtained from the commutator between the corresponding pair of quantum operators by dividing it by $i\hbar$:

$$\boxed{\frac{1}{i\hbar}[\hat{A}, \hat{B}] \longrightarrow \{A, B\}_{classical}.} \tag{3.125}$$

Note that the expressions of classical mechanics can be derived from their quantum counterparts, but the opposite is not possible. That is, dividing quantum mechanical expressions by $i\hbar$ leads to their classical analog, but multiplying classical mechanical expressions by $i\hbar$ doesn't necessarily lead to their quantum counterparts.

Example 3.5

(a) Evaluate the Poisson bracket $\{x, p\}$ between the position, x, and momentum, p, variables.

(b) Compare the commutator $\left[\hat{X}, \hat{P}\right]$ with Poisson bracket $\{x, p\}$ calculated in Part (a).

Solution

(a) Applying the general relation

$$\{A, B\} = \sum_j \left(\frac{\partial A}{\partial x_j}\frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial x_j}\right) \tag{3.126}$$

to x and p, we can readily evaluate the given Poisson bracket:

$$\begin{aligned} \{x, p\} &= \frac{\partial(x)}{\partial x}\frac{\partial(p)}{\partial p} - \frac{\partial(x)}{\partial p}\frac{\partial(p)}{\partial x} \\ &= \frac{\partial(x)}{\partial x}\frac{\partial(p)}{\partial p} \\ &= 1. \end{aligned} \tag{3.127}$$

(b) Using the fact that $[\hat{X}, \hat{P}] = i\hbar$, we see that

$$\frac{1}{i\hbar}[\hat{X}, \hat{P}] = 1, \tag{3.128}$$

which is equal to the Poisson bracket (3.127); that is,

$$\frac{1}{i\hbar}[\hat{X}, \hat{P}] = \{x, p\}_{classical} = 1. \tag{3.129}$$

This result is in agreement with Eq. (3.125).

3.8.2 The Ehrenfest Theorem

If quantum mechanics is to be more general than classical mechanics, it must contain classical mechanics as a limiting case. To illustrate this idea, let us look at the time evolution of the expectation values of the position and momentum operators, $\hat{\vec{R}}$ and $\hat{\vec{P}}$, of a particle moving in a potential $\hat{V}(\vec{r})$, and then compare these relations with their classical counterparts.

Since the position and the momentum observables do not depend explicitly on time, within the context of wave mechanics, the terms $\langle \partial\hat{\vec{R}}/\partial t\rangle$ and $\langle \partial\hat{\vec{P}}/\partial t\rangle$ are zero. Hence, inserting

$\hat{H} = \hat{\vec{P}}^2/(2m) + \hat{V}(\hat{\vec{R}}, t)$ into (3.88) and using the fact that $\hat{\vec{R}}$ commutes with $\hat{V}(\hat{\vec{R}}, t)$, we can write

$$\frac{d}{dt}\langle\hat{\vec{R}}\rangle = \frac{1}{i\hbar}\langle[\hat{\vec{R}}, \hat{H}]\rangle = \frac{1}{i\hbar}\langle[\hat{\vec{R}}, \frac{\hat{\vec{P}}^2}{2m} + \hat{V}(\hat{\vec{R}}, t)]\rangle = \frac{1}{2im\hbar}\langle[\hat{\vec{R}}, \hat{\vec{P}}^2]\rangle. \tag{3.130}$$

Since

$$[\hat{\vec{R}}, \hat{\vec{P}}^2] = 2i\hbar\hat{\vec{P}}, \tag{3.131}$$

we have

$$\boxed{\frac{d}{dt}\langle\hat{\vec{R}}\rangle = \frac{1}{m}\langle\hat{\vec{P}}\rangle.} \tag{3.132}$$

As for $d\langle\hat{\vec{P}}\rangle/dt$, we can infer its expression from a treatment analogous to $d\langle\hat{\vec{R}}\rangle/dt$. Using

$$[\hat{\vec{P}}, \hat{V}(\hat{\vec{R}}, t)] = -i\hbar\vec{\nabla}\hat{V}(\vec{R}, t), \tag{3.133}$$

we can write

$$\boxed{\frac{d}{dt}\langle\hat{\vec{P}}\rangle = \frac{1}{i\hbar}\langle[\hat{\vec{P}}, \hat{V}(\hat{\vec{R}}, t)]\rangle = -\langle\vec{\nabla}\hat{V}(\hat{\vec{R}}, t)\rangle.} \tag{3.134}$$

The two relations (3.132) and (3.134), expressing the time evolution of the expectation values of the position and momentum operators, are known as the *Ehrenfest theorem*, or Ehrenfest equations. Their respective forms are reminiscent of the Hamilton–Jacobi equations of classical mechanics,

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m}, \qquad \frac{d\vec{p}}{dt} = -\vec{\nabla}V(\vec{r}), \tag{3.135}$$

which reduce to Newton's equation of motion for a *classical* particle of mass m, position $\vec{r}$, and momentum $\vec{p}$:

$$\frac{d\vec{p}}{dt} = m\frac{d^2\vec{r}}{dt^2} = -\vec{\nabla}V(\vec{r}). \tag{3.136}$$

Notice $\hbar$ has completely disappeared in the Ehrenfest equations (3.132) and (3.134). These two equations certainly establish a connection between quantum mechanics and classical mechanics. We can, within this context, view the center of the wave packet as moving like a classical particle when subject to a potential $V(\vec{r})$.

3.8.3 Quantum Mechanics and Classical Mechanics

In Chapter 1 we focused mainly on those experimental observations which confirm the failure of classical physics at the microscopic level. We should bear in mind, however, that classical physics works perfectly well within the realm of the macroscopic world. Thus, if the theory of quantum mechanics is to be considered more general than classical physics, it must yield accurate results not only on the microscopic scale but at the classical limit as well.

How does one decide on when to use classical or quantum mechanics to describe the motion of a given system? That is, how do we know when a classical description is good enough or when a quantum description becomes a must? The answer is provided by comparing the size of those quantities of the system that have the dimensions of an action with the Planck constant, h. Since, as shown in (3.125), the quantum relations are characterized by h, we can state that if the value of the action of a system is too large compared to h, this system can be accurately described by means of classical physics. Otherwise, the use of a quantal description becomes unavoidable. One should recall that, for microscopic systems, the size of action variables is of the order of h; for instance, the angular momentum of the hydrogen atom is $L = n\hbar$, where n is finite.

Another equivalent way of defining the classical limit is by means of "*length*." Since $\lambda = h/p$ the classical domain can be specified by the limit $\lambda \to 0$. This means that, when the de Broglie wavelength of a system is too small compared to its size, the system can be described accurately by means of classical physics.

In summary, the classical limit can be described as the limit $h \to 0$ or, equivalently, as the limit $\lambda \to 0$. In these limits the results of quantum mechanics should be similar to those of classical physics:

$$\lim_{h\to 0} \text{ Quantum Mechanics} \longrightarrow \text{Classical Mechanics}, \tag{3.137}$$

$$\lim_{\lambda\to 0} \text{ Quantum Mechanics} \longrightarrow \text{Classical Mechanics}. \tag{3.138}$$

Classical mechanics can thus be regarded as the short wavelength limit of quantum mechanics. In this way, quantum mechanics contains classical mechanics as a limiting case. So, in the limit of $h \to 0$ or $\lambda \to 0$, quantum dynamical quantities should have, as proposed by Bohr, a one-to-one correspondence with their classical counterparts. This is the essence of the *correspondence principle*.

But how does one reconcile, in the classical limit, the probabilistic nature of quantum mechanics with the determinism of classical physics? The answer is quite straightforward: quantum *fluctuations* must become negligible or even vanish when $h \to 0$, for Heisenberg's uncertainty principle would acquire the status of *certainty*; when $h \to 0$, the fluctuations in the position and momentum will vanish, $\Delta x \to 0$ and $\Delta p \to 0$. Thus, the position and momentum can be measured simultaneously with arbitrary accuracy. This implies that the probabilistic assessments of dynamical quantities by quantum mechanics must give way to exact calculations (these ideas will be discussed further when we study the WKB method in Chapter 9).

So, for those cases where the action variables of a system are too large compared to h (or, equivalently, when the lengths of this system are too large compared to its de Broglie wavelength), quantum mechanics gives the same results as classical mechanics.

In the rest of this text, we will deal with the various applications of the Schrödinger equation. We start, in Chapter 4, with the simple case of one-dimensional systems and later on consider more realistic systems.

3.9 Solved Problems

Problem 3.1

A particle of mass m, which moves freely inside an infinite potential well of length a, has the following initial wave function at $t = 0$:

$$\psi(x, 0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right),$$

where A is a real constant.

(a) Find A so that $\psi(x, 0)$ is normalized.

(b) If measurements of the energy are carried out, what are the values that will be found and what are the corresponding probabilities? Calculate the average energy.

(c) Find the wave function $\psi(x, t)$ at any later time t.

(d) Determine the probability of finding the system at a time t in the state $\varphi(x, t) = \sqrt{2/a}\sin(5\pi x/a)\exp(-iE_5 t/\hbar)$; then determine the probability of finding it in the state $\chi(x, t) = \sqrt{2/a}\sin(2\pi x/a)\exp(-iE_2 t/\hbar)$.

Solution

Since the functions

$$\phi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \tag{3.139}$$

are orthonormal,

$$\langle\phi_n|\phi_m\rangle = \int_0^a \phi_n^*(x)\phi_m(x)\,dx = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right)dx = \delta_{nm}, \tag{3.140}$$

it is more convenient to write $\psi(x, 0)$ in terms of $\phi_n(x)$:

$$\begin{aligned}\psi(x,0) &= \frac{A}{\sqrt{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)\\ &= \frac{A}{\sqrt{2}}\phi_1(x) + \sqrt{\frac{3}{10}}\phi_3(x) + \frac{1}{\sqrt{10}}\phi_5(x).\end{aligned} \tag{3.141}$$

(a) Since $\langle\phi_n|\phi_m\rangle = \delta_{nm}$ the normalization of $\psi(x, 0)$ yields

$$1 = \langle\psi|\psi\rangle = \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10}, \tag{3.142}$$

or $A = \sqrt{6/5}$; hence

$$\psi(x,0) = \sqrt{\frac{3}{5}}\phi_1(x) + \sqrt{\frac{3}{10}}\phi_3(x) + \frac{1}{\sqrt{10}}\phi_5(x). \tag{3.143}$$

(b) Since the second derivative of (3.139) is given by $d^2\phi_n(x)/dx^2 = -(n^2\pi^2/a^2)\phi_n(x)$, and since the Hamiltonian of a free particle is $\hat{H} = -(\hbar^2/2m)d^2/dx^2$, the expectation value of $\hat{H}$ with respect to $\phi_n(x)$ is

$$E_n = \langle\phi_n|\hat{H}|\phi_n\rangle = -\frac{\hbar^2}{2m}\int_0^a \phi_n^*(x)\frac{d^2\phi_n(x)}{dx^2}dx = \frac{n^2\pi^2\hbar^2}{2ma^2}. \tag{3.144}$$

If a measurement is carried out on the system, we would obtain $E_n = n^2\pi^2\hbar^2/(2ma^2)$ with a corresponding probability of $P_n(E_n) = |\langle\phi_n|\psi\rangle|^2$. Since the initial wave function (3.143) contains only three eigenstates of $\hat{H}$, $\phi_1(x)$, $\phi_3(x)$, and $\phi_5(x)$, the results of the energy measurements along with the corresponding probabilities are

$$E_1 = \langle\phi_1|\hat{H}|\phi_1\rangle = \frac{\pi^2\hbar^2}{2ma^2}, \qquad P_1(E_1) = |\langle\phi_1|\psi\rangle|^2 = \frac{3}{5}, \tag{3.145}$$

$$E_3 = \langle\phi_3|\hat{H}|\phi_3\rangle = \frac{9\pi^2\hbar^2}{2ma^2}, \qquad P_3(E_3) = |\langle\phi_3|\psi\rangle|^2 = \frac{3}{10}, \tag{3.146}$$

$$E_5 = \langle\phi_5|\hat{H}|\phi_5\rangle = \frac{25\pi^2\hbar^2}{2ma^2}, \qquad P_5(E_5) = |\langle\phi_5|\psi\rangle|^2 = \frac{1}{10}. \tag{3.147}$$

The average energy is

$$E = \sum_n P_n E_n = \frac{3}{5}E_1 + \frac{3}{10}E_3 + \frac{1}{10}E_5 = \frac{29\pi^2\hbar^2}{10ma^2}. \tag{3.148}$$

(c) As the initial state $\psi(x, 0)$ is given by (3.143), the wave function $\psi(x, t)$ at any later time t is

$$\psi(x, t) = \sqrt{\frac{3}{5}}\phi_1(x)e^{-iE_1t/\hbar} + \sqrt{\frac{3}{10}}\phi_3(x)e^{-iE_3t/\hbar} + \frac{1}{\sqrt{10}}\phi_5(x)e^{-iE_5t/\hbar}, \tag{3.149}$$

where the expressions of E_n are listed in (3.144) and $\phi_n(x)$ in (3.139).

(d) First, let us express $\varphi(x, t)$ in terms of $\phi_n(x)$:

$$\varphi(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{5\pi x}{a}\right) e^{-iE_5t/\hbar} = \phi_5(x)e^{-iE_5t/\hbar}. \tag{3.150}$$

The probability of finding the system at a time t in the state $\varphi(x, t)$ is

$$P = |\langle\varphi|\psi\rangle|^2 = \left|\int_0^a \varphi^*(x, t)\psi(x, t)\, dx\right|^2 = \frac{1}{10}\left|\int_0^a \phi_5^*(x)\phi_5(x)\, dx\right|^2 = \frac{1}{10}, \tag{3.151}$$

since $\langle\varphi|\phi_1\rangle = \langle\varphi|\phi_3\rangle = 0$ and $\langle\varphi|\phi_5\rangle = \exp(iE_5t/\hbar)$.

Similarly, since $\chi(x, t) = \sqrt{2/a}\sin(2\pi x/a)\exp(-iE_2t/\hbar) = \phi_2(x)\exp(-iE_2t/\hbar)$, we can easily show that the probability for finding the system in the state $\chi(x, t)$ is zero:

$$P = |\langle\chi|\psi\rangle|^2 = \left|\int_0^a \chi^*(x, t)\psi(x, t)\, dx\right|^2 = 0, \tag{3.152}$$

since $\langle\chi|\phi_1\rangle = \langle\chi|\phi_3\rangle = \langle\chi|\phi_5\rangle = 0$.

Problem 3.2

A particle of mass m, which moves freely inside an infinite potential well of length a, is initially in the state $\psi(x, 0) = \sqrt{3/5a}\sin(3\pi x/a) + (1/\sqrt{5a})\sin(5\pi x/a)$.

(a) Find $\psi(x, t)$ at any later time t.

(b) Calculate the probability density $\rho(x, t)$ and the current density, $\vec{J}(x, t)$.

(c) Verify that the probability is conserved, i.e., $\partial\rho/\partial t + \vec{\nabla}\cdot\vec{J}(x, t) = 0$.

Solution

(a) Since $\psi(x, 0)$ can be expressed in terms of $\phi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ as

$$\psi(x, 0) = \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right) = \sqrt{\frac{3}{10}}\phi_3(x) + \frac{1}{\sqrt{10}}\phi_5(x), \tag{3.153}$$

we can write

$$\begin{aligned}\psi(x, t) &= \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right)e^{-iE_3t/\hbar} + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)e^{-iE_5t/\hbar} \\ &= \sqrt{\frac{3}{10}}\phi_3(x)e^{-iE_3t/\hbar} + \frac{1}{\sqrt{10}}\phi_5(x)e^{-iE_5t/\hbar},\end{aligned} \tag{3.154}$$

where the expressions for E_n are listed in (3.144): $E_n = n^2\pi^2\hbar^2/(2ma^2)$.

(b) Since $\rho(x,t) = \psi^*(x,t)\psi(x,t)$, where $\psi(x,t)$ is given by (3.154), we can write

$$\rho(x,t) = \frac{3}{10}\phi_3^2(x) + \frac{\sqrt{3}}{10}\phi_3(x)\phi_5(x)\left[e^{i(E_3-E_5)t/\hbar} + e^{-i(E_3-E_5)t/\hbar}\right] + \frac{1}{10}\phi_5^2(x). \quad (3.155)$$

From (3.144) we have $E_3 - E_5 = 9E_1 - 25E_1 = -16E_1 = -8\pi^2\hbar^2/(ma^2)$. Thus, $\rho(x,t)$ becomes

$$\begin{aligned}\rho(x,t) &= \frac{3}{10}\phi_3^2(x) + \frac{\sqrt{3}}{5}\phi_3(x)\phi_5(x)\cos\left(\frac{16E_1t}{\hbar}\right) + \frac{1}{10}\phi_5^2(x)\\ &= \frac{3}{5a}\sin^2\left(\frac{3\pi x}{a}\right) + \frac{2\sqrt{3}}{5a}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{16E_1t}{\hbar}\right)\\ &\quad + \frac{1}{5a}\sin^2\left(\frac{5\pi x}{a}\right). \end{aligned} \quad (3.156)$$

Since the system is one-dimensional, the action of the gradient operator on $\psi(x,t)$ and $\psi^*(x,t)$ is given by $\vec{\nabla}\psi(x,t) = (d\psi(x,t)/dx)\vec{i}$ and $\vec{\nabla}\psi^*(x,t) = (d\psi^*(x,t)/dx)\vec{i}$. We can thus write the current density $\vec{J}(x,t) = (i\hbar/2m)\left(\psi(x,t)\vec{\nabla}\psi^*(x,t) - \psi^*(x,t)\vec{\nabla}\psi(x,t)\right)$ as

$$\vec{J}(x,t) = \frac{i\hbar}{2m}\left(\psi(x,t)\frac{d\psi^*(x,t)}{dx} - \psi^*(x,t)\frac{d\psi(x,t)}{dx}\right)\vec{i}. \quad (3.157)$$

Using (3.154) we have

$$\frac{d\psi(x,t)}{dx} = \frac{3\pi}{a}\sqrt{\frac{3}{5a}}\cos\left(\frac{3\pi x}{a}\right)e^{-iE_3t/\hbar} + \frac{5\pi}{a}\frac{1}{\sqrt{5a}}\cos\left(\frac{5\pi x}{a}\right)e^{-iE_5t/\hbar}, \quad (3.158)$$

$$\frac{d\psi^*(x,t)}{dx} = \frac{3\pi}{a}\sqrt{\frac{3}{5a}}\cos\left(\frac{3\pi x}{a}\right)e^{iE_3t/\hbar} + \frac{5\pi}{a}\frac{1}{\sqrt{5a}}\cos\left(\frac{5\pi x}{a}\right)e^{iE_5t/\hbar}. \quad (3.159)$$

A straightforward calculation yields

$$\begin{aligned}\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx} &= -2i\pi\frac{\sqrt{3}}{5a^2}\left[5\sin\left(\frac{3\pi x}{a}\right)\cos\left(\frac{5\pi x}{a}\right) - 3\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{3\pi x}{a}\right)\right]\\ &\quad\times\sin\left(\frac{E_3-E_5}{\hbar}t\right). \end{aligned} \quad (3.160)$$

Inserting this into (3.157) and using $E_3 - E_5 = -16E_1$, we have

$$\vec{J}(x,t) = -\frac{\pi\hbar}{m}\frac{\sqrt{3}}{5a^2}\left[5\sin\left(\frac{3\pi x}{a}\right)\cos\left(\frac{5\pi x}{a}\right) - 3\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{3\pi x}{a}\right)\right]\sin\left(\frac{16E_1t}{\hbar}\right)\vec{i}. \quad (3.161)$$

(c) Performing the time derivative of (3.156) and using the expression $32\sqrt{3}E_1/(5a\hbar) = 16\pi^2\hbar\sqrt{3}/(5ma^3)$, since $E_1 = \pi^2\hbar^2/(2ma^2)$, we obtain

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= -\frac{32\sqrt{3}E_1}{5a\hbar}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\sin\left(\frac{16E_1t}{\hbar}\right)\\ &= -\frac{16\pi^2\hbar\sqrt{3}}{5ma^3}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\sin\left(\frac{16E_1t}{\hbar}\right), \end{aligned} \quad (3.162)$$

Now, taking the divergence of (3.161), we end up with

$$\vec{\nabla}\cdot\vec{J}(x,t) = \frac{dJ(x,t)}{dx} = \frac{16\pi^2\hbar\sqrt{3}}{5ma^3}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\sin\left(\frac{16E_1 t}{\hbar}\right). \tag{3.163}$$

The addition of (3.162) and (3.163) confirms the conservation of probability:

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{J}(x,t) = 0. \tag{3.164}$$

Problem 3.3

Consider a one-dimensional particle which is confined within the region $0 \le x \le a$ and whose wave function is $\Psi(x,t) = \sin(\pi x/a)\exp(-i\omega t)$.

(a) Find the potential $V(x)$.

(b) Calculate the probability of finding the particle in the interval $a/4 \le x \le 3a/4$.

Solution

(a) Since the first time derivative and the second x derivative of $\Psi(x,t)$ are given by $\partial\Psi(x,t)/\partial t = -i\omega\Psi(x,t)$ and $\partial^2\Psi(x,t)/\partial x^2 = -(\pi^2/a^2)\Psi(x,t)$, the Schrödinger equation (3.68) yields

$$i\hbar(-i\omega)\Psi(x,t) = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\Psi(x,t) + \hat{V}(x,t)\Psi(x,t). \tag{3.165}$$

Hence $V(x,t)$ is time independent and given by $V(x) = \hbar\omega - \hbar^2\pi^2/(2ma^2)$.

(b) The probability of finding the particle in the interval $a/4 \le x \le 3a/4$ can be obtained from (3.4):

$$P = \frac{\int_{a/4}^{3a/4}|\psi(x)|^2 dx}{\int_0^a |\psi(x)|^2 dx} = \frac{\int_{a/4}^{3a/4}\sin^2(\pi x/a)\,dx}{\int_0^a \sin^2(\pi x/a)\,dx} = \frac{2+\pi}{2\pi} = 0.82 \tag{3.166}$$

Problem 3.4

A system is initially in the state $|\psi_0\rangle = [\sqrt{2}|\phi_1\rangle + \sqrt{3}|\phi_2\rangle + |\phi_3\rangle + |\phi_4\rangle]/\sqrt{7}$, where $|\phi_n\rangle$ are eigenstates of the system's Hamiltonian such that $\hat{H}|\phi_n\rangle = n^2\mathcal{E}_0|\phi_n\rangle$.

(a) If energy is measured, what values will be obtained and with what probabilities?

(b) Consider an operator $\hat{A}$ whose action on $|\phi_n\rangle$ is defined by $\hat{A}|\phi_n\rangle = (n+1)a_0|\phi_n\rangle$. If A is measured, what values will be obtained and with what probabilities?

(c) Suppose that a measurement of the energy yields $4\mathcal{E}_0$. If we measure A immediately afterwards, what value will be obtained?

Solution

(a) A measurement of the energy yields $E_n = \langle\phi_n|\hat{H}|\phi_n\rangle = n^2\mathcal{E}_0$, that is

$$E_1 = \mathcal{E}_0, \quad E_2 = 4\mathcal{E}_0, \quad E_3 = 9\mathcal{E}_0, \quad E_4 = 16\mathcal{E}_0. \tag{3.167}$$

Since $|\ \psi_0\rangle$ is normalized, $\langle\psi_0\ |\ \psi_0\rangle = (2+3+1+1)/7 = 1$, and using (3.2), we can write the probabilities corresponding to (3.167) as $P(E_n) = |\langle\phi_n|\psi_0\rangle|^2/\langle\psi_0\ |\ \psi_0\rangle = |\langle\phi_n|\psi_0\rangle|^2$; hence, using the fact that $\langle \phi_n | \phi_m \rangle = \delta_{nm}$, we have

$$P(E_1) = \left| \sqrt{\frac{2}{7}} \langle \phi_1 | \phi_1 \rangle \right|^2 = \frac{2}{7}, \qquad P(E_2) = \left| \sqrt{\frac{3}{7}} \langle \phi_2 | \phi_2 \rangle \right|^2 = \frac{3}{7}, \tag{3.168}$$

$$P(E_3) = \left| \frac{1}{\sqrt{7}} \langle \phi_3 | \phi_3 \rangle \right|^2 = \frac{1}{7}, \qquad P(E_4) = \left| \frac{1}{\sqrt{7}} \langle \phi_4 | \phi_4 \rangle \right|^2 = \frac{1}{7}. \tag{3.169}$$

(b) Similarly, a measurement of the observable $\hat{A}$ yields $a_n = \langle \phi_n | \hat{A} | \phi_n \rangle = (n+1)a_0$; that is,

$$a_1 = 2a_0, \quad a_2 = 3a_0, \quad a_3 = 4a_0, \quad a_4 = 5a_0. \tag{3.170}$$

Again, using (3.2) and since $| \psi_0 \rangle$ is normalized, we can ascertain that the probabilities corresponding to the values (3.170) are given by $P(a_n) = |\langle \phi_n | \psi_0 \rangle|^2 / \langle \psi_0 \mid \psi_0 \rangle = |\langle \phi_n | \psi_0 \rangle|^2$, or

$$P(a_1) = \left| \sqrt{\frac{2}{7}} \langle \phi_1 | \phi_1 \rangle \right|^2 = \frac{2}{7}, \qquad P(a_2) = \left| \sqrt{\frac{3}{7}} \langle \phi_2 | \phi_2 \rangle \right|^2 = \frac{3}{7}, \tag{3.171}$$

$$P(a_3) = \left| \frac{1}{\sqrt{7}} \langle \phi_3 | \phi_3 \rangle \right|^2 = \frac{1}{7}, \qquad P(a_4) = \left| \frac{1}{\sqrt{7}} \langle \phi_4 | \phi_4 \rangle \right|^2 = \frac{1}{7}. \tag{3.172}$$

(c) An energy measurement that yields $4\mathcal{E}_0$ implies that the system is left in the state $|\phi_2\rangle$. A measurement of the observable A immediately afterwards leads to

$$\langle \phi_2 | \hat{A} | \phi_2 \rangle = 3a_0 \langle \phi_2 | \phi_2 \rangle = 3a_0. \tag{3.173}$$

Problem 3.5

(a) Assuming that the system of Problem 3.4 is initially in the state $|\phi_3\rangle$, what values for the energy and the observable A will be obtained if we measure: (i)H first then A, (ii) A first then H?

(b) Compare the results obtained in (i) and (ii) and infer whether $\hat{H}$ and $\hat{A}$ are compatible. Calculate $[\hat{H},\ \hat{A}]|\phi_3\rangle$.

Solution

(a) (i) The measurement of H first then A is represented by $\hat{A}\hat{H}|\phi_3\rangle$. Using the relations $\hat{H}|\phi_n\rangle = n^2\mathcal{E}_0|\phi_n\rangle$ and $\hat{A}|\phi_n\rangle = na_0|\phi_{n+1}\rangle$, we have

$$\hat{A}\hat{H}|\phi_3\rangle = 9\mathcal{E}_0\hat{A}|\phi_3\rangle = 27\mathcal{E}_0 a_0|\phi_4\rangle. \tag{3.174}$$

(ii) Measuring A first and then H, we will obtain

$$\hat{H}\hat{A}|\phi_3\rangle = 3a_0\hat{H}|\phi_4\rangle = 48\mathcal{E}_0 a_0|\phi_4\rangle. \tag{3.175}$$

(b) Equations (3.174) and (3.175) show that the actions of $\hat{A}\hat{H}$ and $\hat{H}\hat{A}$ yield different results. This means that $\hat{H}$ and $\hat{A}$ do not commute; hence they are not compatible. We can thus write

$$[\hat{H},\ \hat{A}]|\phi_3\rangle = (48-27)\mathcal{E}_0 a_0|\phi_4\rangle = 17\mathcal{E}_0 a_0|\phi_4\rangle. \tag{3.176}$$

Problem 3.6
Consider a physical system whose Hamiltonian H and initial state $|\psi_0\rangle$ are given by

$$H = \mathcal{E}\begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad |\psi_0\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 1-i \\ 1-i \\ 1 \end{pmatrix},$$

where $\mathcal{E}$ has the dimensions of energy.

(a) What values will we obtain when measuring the energy and with what probabilities?

(b) Calculate $\langle \hat{H}\rangle$, the expectation value of the Hamiltonian.

Solution

(a) The results of the energy measurement are given by the eigenvalues of H. A diagonalization of H yields a nondegenerate eigenenergy $E_1 = \mathcal{E}$ and a doubly degenerate value $E_2 = E_3 = -\mathcal{E}$ whose respective eigenvectors are given by

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}, \qquad |\phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \\ 0 \end{pmatrix}, \qquad |\phi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}; \tag{3.177}$$

these eigenvectors are orthogonal since H is Hermitian. Note that the initial state $|\psi_0\rangle$ can be written in terms of $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ as follows:

$$|\psi_0\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 1-i \\ 1-i \\ 1 \end{pmatrix} = \sqrt{\frac{2}{5}}|\phi_1\rangle + \sqrt{\frac{2}{5}}|\phi_2\rangle + \frac{1}{\sqrt{5}}|\phi_3\rangle. \tag{3.178}$$

Since $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ are orthonormal, the probability of measuring $E_1 = \mathcal{E}$ is given by

$$P_1(E_1) = |\langle\phi_1|\psi_0\rangle|^2 = \left|\sqrt{\frac{2}{5}}\langle\phi_1|\phi_1\rangle\right|^2 = \frac{2}{5}. \tag{3.179}$$

Now, since the other eigenvalue is doubly degenerate, $E_2 = E_3 = -\mathcal{E}$, the probability of measuring $-\mathcal{E}$ can be obtained from (3.3):

$$P_2(E_2) = |\langle\phi_2|\psi_0\rangle|^2 + |\langle\phi_3|\psi_0\rangle|^2 = \frac{2}{5} + \frac{1}{5} = \frac{3}{5}. \tag{3.180}$$

(b) From (3.179) and (3.180), we have

$$\langle \hat{H}\rangle = P_1 E_1 + P_2 E_2 = \frac{2}{5}\mathcal{E} - \frac{3}{5}\mathcal{E} = -\frac{1}{5}\mathcal{E}. \tag{3.181}$$

We can obtain the same result by calculating the expectation value of $\hat{H}$ with respect to $|\psi_0\rangle$. Since $\langle\psi_0|\psi_0\rangle = 1$, we have $\langle\hat{H}\rangle = \langle\psi_0|\hat{H}|\psi_0\rangle/\langle\psi_0|\psi_0\rangle = \langle\psi_0|\hat{H}|\psi_0\rangle$:

$$\langle \hat{H}\rangle = \langle\psi_0|\hat{H}|\psi_0\rangle = \frac{\mathcal{E}}{5}\begin{pmatrix} 1+i & 1+i & 1 \end{pmatrix}\begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1-i \\ 1-i \\ 1 \end{pmatrix} = -\frac{1}{5}\mathcal{E}. \tag{3.182}$$

Problem 3.7
Consider a system whose Hamiltonian H and an operator A are given by the matrices

$$H = \mathcal{E}_0 \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad A = a \begin{pmatrix} 0 & 4 & 0 \\ 4 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

where $\mathcal{E}_0$ has the dimensions of energy.

(a) If we measure the energy, what values will we obtain?

(b) Suppose that when we measure the energy, we obtain a value of $-\mathcal{E}_0$. Immediately afterwards, we measure A. What values will we obtain for A and what are the probabilities corresponding to each value?

(c) Calculate the uncertainty ΔA.

Solution

(a) The possible energies are given by the eigenvalues of H. A diagonalization of H yields three nondegenerate eigenenergies $E_1 = 0$, $E_2 = -\mathcal{E}_0$, and $E_3 = 2\mathcal{E}_0$. The respective eigenvectors are

$$|\phi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \qquad |\phi_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad |\phi_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}; \tag{3.183}$$

these eigenvectors are orthonormal.

(b) If a measurement of the energy yields $-\mathcal{E}_0$, this means that the system is left in the state $|\phi_2\rangle$. When we measure the next observable, A, the system is in the state $|\phi_2\rangle$. The result we obtain for A is given by any of the eigenvalues of A. A diagonalization of A yields three nondegenerate values: $a_1 = -\sqrt{17}a$, $a_2 = 0$, and $a_3 = \sqrt{17}a$; their respective eigenvectors are given by

$$|a_1\rangle = \frac{1}{\sqrt{34}} \begin{pmatrix} 4 \\ -\sqrt{17} \\ 1 \end{pmatrix}, \qquad |a_2\rangle = \frac{1}{\sqrt{17}} \begin{pmatrix} 1 \\ 0 \\ -4 \end{pmatrix}, \qquad |a_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 4 \\ \sqrt{17} \\ 1 \end{pmatrix}. \tag{3.184}$$

Thus, when measuring A on a system which is in the state $|\phi_2\rangle$, the probability of finding $-\sqrt{17}a$ is given by

$$P_1(a_1) = |\langle a_1|\phi_2\rangle|^2 = \left| \frac{1}{\sqrt{34}} \begin{pmatrix} 4 & -\sqrt{17} & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{34}. \tag{3.185}$$

Similarly, the probabilities of measuring 0 and $\sqrt{17}a$ are

$$P_2(a_2) = |\langle a_2|\phi_2\rangle|^2 = \left| \frac{1}{\sqrt{17}} \begin{pmatrix} 1 & 0 & -4 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \frac{16}{17}, \tag{3.186}$$

$$P_3(a_3) = |\langle a_3|\phi_2\rangle|^2 = \left| \frac{1}{\sqrt{34}} \begin{pmatrix} 4 & \sqrt{17} & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{34}. \tag{3.187}$$

(c) Since the system, when measuring A is in the state $|\phi_2\rangle$, the uncertainty ΔA is given by $\Delta A = \sqrt{\langle\phi_2|A^2|\phi_2\rangle - \langle\phi_2|A|\phi_2\rangle^2}$, where

$$\langle\phi_2|A|\phi_2\rangle = a\begin{pmatrix} 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 4 & 0 \\ 4 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0, \tag{3.188}$$

$$\langle\phi_2|A^2|\phi_2\rangle = a^2\begin{pmatrix} 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 4 & 0 \\ 4 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 4 & 0 \\ 4 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = a^2. \tag{3.189}$$

Thus we have $\Delta A = a$.

Problem 3.8

Consider a system whose state and two observables are given by

$$|\psi(t)\rangle = \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}, \qquad A = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(a) What is the probability that a measurement of A at time t yields -1?

(b) Let us carry out a set of two measurements where B is measured first and then, immediately afterwards, A is measured. Find the probability of obtaining a value of 0 for B and a value of 1 for A.

(c) Now we measure A first then, immediately afterwards, B. Find the probability of obtaining a value of 1 for A and a value of 0 for B.

(d) Compare the results of (b) and (c). Explain.

(e) Which among the sets of operators $\{\hat{A}\}$, $\{\hat{B}\}$, and $\{\hat{A}, \hat{B}\}$ form a complete set of commuting operators (CSCO)?

Solution

(a) A measurement of A yields any of the eigenvalues of A which are given by $a_1 = -1$, $a_2 = 0$, $a_3 = 1$; the respective (normalized) eigenstates are

$$|a_1\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix}, \qquad |a_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \qquad |a_3\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}. \tag{3.190}$$

The probability of obtaining $a_1 = -1$ is

$$P(-1) = \frac{|\langle a_1|\psi(t)\rangle|^2}{\langle\psi(t)|\psi(t)\rangle} = \frac{1}{6}\left|\frac{1}{2}\begin{pmatrix} -1 & \sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}\right|^2 = \frac{1}{3}, \tag{3.191}$$

where we have used the fact that $\langle\psi(t)|\psi(t)\rangle = \begin{pmatrix} -1 & 2 & 1 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix} = 6$.

(b) A measurement of B yields a value which is equal to any of the eigenvalues of B: $b_1 = -1$, $b_2 = 0$, and $b_3 = 1$; their corresponding eigenvectors are

$$|b_1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |b_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{3.192}$$

Since the system was in the state $|\psi(t)\rangle$, the probability of obtaining the value $b_2 = 0$ for B is

$$P(b_2) = \frac{|\langle b_2|\psi(t)\rangle|^2}{\langle\psi(t)|\psi(t)\rangle} = \frac{1}{6}\left|\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}\right|^2 = \frac{2}{3}. \tag{3.193}$$

We deal now with the measurement of the other observable, A. The observables A and B do not have common eigenstates, since they do not commute. After measuring B (the result is $b_2 = 0$), the system is left, according to Postulate 3, in a state $|\phi\rangle$ which can be found by projecting $|\psi(t)\rangle$ onto $|b_2\rangle$:

$$|\phi\rangle = |b_2\rangle\langle b_2|\psi(t)\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}. \tag{3.194}$$

The probability of finding 1 when we measure A is given by

$$P(a_3) = \frac{|\langle a_3|\phi\rangle|^2}{\langle\phi|\phi\rangle} = \frac{1}{4}\left|\frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}\right|^2 = \frac{1}{2}, \tag{3.195}$$

since $\langle\phi|\phi\rangle = 4$. In summary, when measuring B then A, the probability of finding a value of 0 for B and 1 for A is given by the product of the probabilities (3.193) and (3.195):

$$P(b_2, a_3) = P(b_2)P(a_3) = \frac{2}{3}\frac{1}{2} = \frac{1}{3}. \tag{3.196}$$

(c) Next we measure A first then B. Since the system is in the state $|\psi(t)\rangle$, the probability of measuring $a_3 = 1$ for A is given by

$$P'(a_3) = \frac{|\langle a_3|\psi(t)\rangle|^2}{\langle\psi(t)|\psi(t)\rangle} = \frac{1}{6}\left|\frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}\right|^2 = \frac{1}{3}, \tag{3.197}$$

where we have used the expression (3.190) for $|a_3\rangle$.

We then proceed to the measurement of B. The state of the system just after measuring A (with a value $a_3 = 1$) is given by a projection of $|\psi(t)\rangle$ onto $|a_3\rangle$:

$$|\chi\rangle = |a_3\rangle\langle a_3|\psi(t)\rangle = \frac{1}{4}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}\begin{pmatrix} 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix} = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}. \tag{3.198}$$

So the probability of finding a value of $b_2 = 0$ when measuring B is given by

$$P'(b_2) = \frac{|\langle b_2|\chi\rangle|^2}{\langle\chi|\chi\rangle} = \frac{1}{2}\left|\frac{\sqrt{2}}{2}\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}\right|^2 = \frac{1}{2}, \tag{3.199}$$

since $\langle\chi|\chi\rangle = 2$.

So when measuring A then B, the probability of finding a value of 1 for A and 0 for B is given by the product of the probabilities (3.199) and (3.197):

$$P(a_3, b_2) = P'(a_3)P'(b_2) = \frac{1}{3}\frac{1}{2} = \frac{1}{6}. \tag{3.200}$$

(d) The probabilities $P(b_2, a_3)$ and $P(a_3, b_2)$, as shown in (3.196) and (3.200), are different. This is expected, since A and B do not commute. The result of the successive measurements of A and B therefore depends on the order in which they are carried out. The probability of obtaining 0 for B then 1 for A is equal to $\frac{1}{3}$. On the other hand, the probability of obtaining 1 for A then 0 for B is equal to $\frac{1}{6}$. However, if the observables A and B commute, the result of the measurements will not depend on the order in which they are carried out (this idea is illustrated in the following solved problem).

(e) As stated in the text, any operator with non-degenerate eigenvalues constitutes, all by itself, a CSCO. Hence each of $\{\hat{A}\}$ and $\{\hat{B}\}$ forms a CSCO, since their eigenvalues are not degenerate. However, the set $\{\hat{A}, \hat{B}\}$ does not form a CSCO since the opertators $\{\hat{A}\}$ and $\{\hat{B}\}$ do not commute.

Problem 3.9

Consider a system whose state and two observables A and B are given by

$$|\psi(t)\rangle = \frac{1}{6}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix}, \qquad A = \frac{1}{\sqrt{2}}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

(a) We perform a measurement where A is measured first and then, immediately afterwards, B is measured. Find the probability of obtaining a value of 0 for A and a value of 1 for B.

(b) Now we measure B first then, immediately afterwards, A. Find the probability of obtaining a value of 1 for B and a value of 0 for A.

(c) Compare the results of (b) and (c). Explain.

(d) Which among the sets of operators $\{\hat{A}\}$, $\{\hat{B}\}$, and $\{\hat{A}, \hat{B}\}$ form a complete set of commuting operators (CSCO)?

Solution

(a) A measurement of A yields any of the eigenvalues of A which are given by $a_1 = 0$ (not degenerate) and $a_2 = a_3 = 2$ (doubly degenerate); the respective (normalized) eigenstates are

$$|a_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}, \qquad |a_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}, \qquad |a_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{3.201}$$

The probability that a measurement of A yields $a_1 = 0$ is given by

$$P(a_1) = \frac{|\langle a_1|\psi(t)\rangle|^2}{\langle\psi(t)|\psi(t)\rangle} = \frac{36}{17}\left|\frac{1}{\sqrt{2}}\frac{1}{6}\begin{pmatrix} 0 & i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix}\right|^2 = \frac{8}{17}, \tag{3.202}$$

where we have used the fact that $\langle\psi(t)|\psi(t)\rangle = \frac{1}{36}\begin{pmatrix} 1 & 0 & 4 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix} = \frac{17}{36}$.

Since the system was initially in the state $|\psi(t)\rangle$, after a measurement of A yields $a_1 = 0$, the system is left, as mentioned in Postulate 3, in the following state:

$$|\phi\rangle = |a_1\rangle\langle a_1|\psi(t)\rangle = \frac{1}{2}\frac{1}{6}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}\begin{pmatrix} 0 & i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}. \tag{3.203}$$

As for the measurement of B, we obtain any of the eigenvalues $b_1 = -1$, $b_2 = b_3 = 1$; their corresponding eigenvectors are

$$|b_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}, \qquad |b_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}, \qquad |b_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{3.204}$$

Since the system is now in the state $|\phi\rangle$, the probability of obtaining the (doubly degenerate) value $b_2 = b_3 = 1$ for B is

$$\begin{aligned} P(b_2) &= \frac{|\langle b_2|\phi\rangle|^2}{\langle\phi|\phi\rangle} + \frac{|\langle b_3|\phi\rangle|^2}{\langle\phi|\phi\rangle} \\ &= \frac{1}{2}\left|\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & i & 1 \end{pmatrix}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}\right|^2 + \frac{1}{2}\left|\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}\right|^2 \\ &= 1. \end{aligned} \tag{3.205}$$

The reason $P(b_2) = 1$ is because the new state $|\phi\rangle$ is an eigenstate of B; in fact $|\phi\rangle = \sqrt{2}/3|b_2\rangle$.

In sum, when measuring A then B, the probability of finding a value of 0 for A and 1 for B is given by the product of the probabilities (3.202) and (3.205):

$$P(a_1, b_2) = P(a_1)P(b_2) = \frac{8}{17}. \tag{3.206}$$

(b) Next we measure B first then A. Since the system is in the state $|\psi(t)\rangle$ and since the value $b_2 = b_3 = 1$ is doubly degenerate, the probability of measuring 1 for B is given by

$$\begin{aligned} P'(b_2) &= \frac{|\langle b_2|\psi(t)\rangle|^2}{\langle\psi(t)|\psi(t)\rangle} + \frac{|\langle b_3|\psi(t)\rangle|^2}{\langle\psi(t)|\psi(t)\rangle} \\ &= \frac{36}{17}\frac{1}{36}\left[\left|\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix}\right|^2 + \left|\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix}\right|^2\right] \\ &= \frac{9}{17}. \end{aligned} \tag{3.207}$$

We now proceed to the measurement of A. The state of the system immediately after measuring B (with a value $b_2 = b_3 = 1$) is given by a projection of $|\psi(t)\rangle$ onto $|b_2\rangle$, and $|b_3\rangle$

$$\begin{aligned} |\chi\rangle &= |b_2\rangle\langle b_2|\psi(t)\rangle + |b_3\rangle\langle b_3|\psi(t)\rangle \\ &= \frac{1}{12}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}\begin{pmatrix} 0 & i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix} + \frac{1}{6}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix} \\ &= \frac{1}{6}\begin{pmatrix} 1 \\ -2i \\ 2i \end{pmatrix}. \end{aligned} \tag{3.208}$$

So the probability of finding a value of $a_1 = 0$ when measuring A is given by

$$P'(a_1) = \frac{|\langle a_1|\chi\rangle|^2}{\langle\chi|\chi\rangle} = \frac{36}{9}\left|\frac{1}{6\sqrt{2}}\begin{pmatrix} 0 & i & 1 \end{pmatrix}\begin{pmatrix} 1 \\ -2i \\ 2i \end{pmatrix}\right|^2 = \frac{8}{9}, \tag{3.209}$$

since $\langle\chi|\chi\rangle = \frac{9}{36}$.

Therefore, when measuring B then A, the probability of finding a value of 1 for B and 0 for A is given by the product of the probabilities (3.207) and (3.209):

$$P(b_2, a_3) = P'(b_2)P'(a_1) = \frac{9}{17}\frac{8}{9} = \frac{8}{17}. \tag{3.210}$$

(c) The probabilities $P(a_1, b_2)$ and $P(b_2, a_1)$, as shown in (3.206) and (3.210), are equal. This is expected since A and B do commute. The result of the successive measurements of A and B does not depend on the order in which they are carried out.

(d) Neither $\{\hat{A}\}$ nor $\{\hat{B}\}$ forms a CSCO since their eigenvalues are degenerate. The set $\{\hat{A}, \hat{B}\}$, however, does form a CSCO since the opertators $\{\hat{A}\}$ and $\{\hat{B}\}$ commute. The set of eigenstates that are common to $\{\hat{A}, \hat{B}\}$ are given by

$$|a_2,\ b_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}, \qquad |a_1,\ b_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}, \qquad |a_3,\ b_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{3.211}$$

Problem 3.10

Consider a physical system which has a number of observables that are represented by the following matrices:

$$A = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 2 & 1 \end{pmatrix},\ B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 3 \\ 0 & 3 & 0 \end{pmatrix},\ C = \begin{pmatrix} 0 & 3 & 0 \\ 3 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix},\ D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

(a) Find the results of the measurements of these observables.

(b) Which among these observables are compatible? Give a basis of eigenvectors common to these observables.

(c) Which among the sets of operators $\{\hat{A}\}$, $\{\hat{B}\}$, $\{\hat{C}\}$, $\{\hat{D}\}$ and their various combinations, such as $\{\hat{A}, \hat{B}\}$, $\{\hat{A}, \hat{C}\}$, $\{\hat{B}, \hat{C}\}$, $\{\hat{A}, \hat{D}\}$, $\{\hat{A}, \hat{B}, \hat{C}\}$, form a complete set of commuting operators (CSCO)?

Solution

(a) The measurements of A, B, C and D yield $a_1 = -1$, $a_2 = 3$, $a_3 = 5$, $b_1 = -3$, $b_2 = 1$, $b_3 = 3$, $c_1 = -1/\sqrt{2}$, $c_2 = 0$, $c_3 = 1/\sqrt{2}$, $d_1 = -1$, $d_2 = d_3 = 1$; the respective eigenvectors of A, B, C and D are

$$|a_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, \qquad |a_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \qquad |a_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \tag{3.212}$$

$$|b_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, \qquad |b_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |b_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \tag{3.213}$$

$$|c_1\rangle = \frac{1}{\sqrt{26}}\begin{pmatrix} 3 \\ -\sqrt{13} \\ 2 \end{pmatrix}, \quad |c_2\rangle = \frac{1}{\sqrt{13}}\begin{pmatrix} 2 \\ 0 \\ -3 \end{pmatrix}, \quad |c_3\rangle = \frac{1}{\sqrt{26}}\begin{pmatrix} 3 \\ \sqrt{13} \\ 2 \end{pmatrix}, \tag{3.214}$$

$$|d_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}, \qquad |d_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |d_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix}. \tag{3.215}$$

(b) We can verify that, among the observables A, B, C, and D, only A and B are compatible, since the matrices A and B commute; the rest do not commute with one another (neither A nor B commutes with C or D; C and D do not commute).

From (3.212) and (3.213) we see that the three states $|a_1, b_1\rangle$, $|a_2, b_3\rangle$, $|a_3, b_2\rangle$,

$$|a_1, b_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, \qquad |a_2, b_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \qquad |a_3, b_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \tag{3.216}$$

form a common, complete basis for A and B, since $\hat{A}|a_n, b_m\rangle = a_n|a_n, b_m\rangle$ and $\hat{B}|a_n, b_m\rangle = b_m|a_n, b_m\rangle$.

(c) First, since the eigenvalues of the operators $\{\hat{A}\}$, $\{\hat{B}\}$, and $\{\hat{C}\}$ are all nondegenerate, each one of $\{\hat{A}\}$, $\{\hat{B}\}$, and $\{\hat{C}\}$ forms separately a CSCO. Additionally, since two eigenvalues of $\{\hat{D}\}$ are degenerate ($d_2 = d_3 = 1$), the operator $\{\hat{D}\}$ does not form a CSCO.

Now, among the various combinations $\{\hat{A}, \hat{B}\}$, $\{\hat{A}, \hat{C}\}$, $\{\hat{B}, \hat{C}\}$, $\{\hat{A}, \hat{D}\}$, and $\{\hat{A}, \hat{B}, \hat{C}\}$, only $\{\hat{A}, \hat{B}\}$ forms a CSCO, because $\{\hat{A}\}$ and $\{\hat{B}\}$ are the only operators that commute; the set of their joint eigenvectors are given by $|a_1, b_1\rangle$, $|a_2, b_3\rangle$, $|a_3, b_2\rangle$.

Problem 3.11

Consider a system whose initial state $|\psi(0)\rangle$ and Hamiltonian are given by

$$|\psi(0)\rangle = \frac{1}{5}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}, \qquad H = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 5 \\ 0 & 5 & 0 \end{pmatrix}.$$

(a) If a measurement of the energy is carried out, what values would we obtain and with what probabilities?

(b) Find the state of the system at a later time t; you may need to expand $|\psi(0)\rangle$ in terms of the eigenvectors of H.

(c) Find the total energy of the system at time $t = 0$ and any later time t; are these values different?

(d) Does $\{\hat{H}\}$ form a complete set of commuting operators?

Solution

(a) A measurement of the energy yields the values $E_1 = -5$, $E_2 = 3$, $E_3 = 5$; the respective (orthonormal) eigenvectors of these values are

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, \qquad |\phi_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\phi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}. \tag{3.217}$$

The probabilities of finding the values $E_1 = -5$, $E_2 = 3$, $E_3 = 5$ are given by

$$P(E_1) = |\langle\phi_1|\psi(0)\rangle|^2 = \left|\frac{1}{5\sqrt{2}}\begin{pmatrix} 0 & -1 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}\right|^2 = \frac{8}{25}, \tag{3.218}$$

$$P(E_2) = |\langle\phi_2|\psi(0)\rangle|^2 = \left|\frac{1}{5}\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}\right|^2 = \frac{9}{25}, \tag{3.219}$$

$$P(E_3) = |\langle\phi_3|\psi(0)\rangle|^2 = \left|\frac{1}{5\sqrt{2}}\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix}\right|^2 = \frac{8}{25}. \tag{3.220}$$

(b) To find $|\psi(t)\rangle$ we need to expand $|\psi(0)\rangle$ in terms of the eigenvectors (3.217):

$$|\psi(0)\rangle = \frac{1}{5}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix} = \frac{2\sqrt{2}}{5}|\phi_1\rangle + \frac{3}{5}|\phi_2\rangle + \frac{2\sqrt{2}}{5}|\phi_3\rangle; \tag{3.221}$$

hence

$$|\psi(t)\rangle = \frac{2\sqrt{2}}{5}e^{-iE_1t}|\phi_1\rangle + \frac{3}{5}e^{-iE_2t}|\phi_2\rangle + \frac{2\sqrt{2}}{5}e^{-iE_3t}|\phi_3\rangle = \frac{1}{5}\begin{pmatrix} 3e^{-3it} \\ -4i\sin 5t \\ 4\cos 5t \end{pmatrix}. \tag{3.222}$$

(c) We can calculate the energy at time $t = 0$ in three quite different ways. The first method uses the bra-ket notation. Since $\langle\psi(0)|\psi(0)\rangle = 1$, $\langle\phi_n)|\phi_m\rangle = \delta_{nm}$ and since $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$, we have

$$\begin{aligned} E(0) = \langle\psi(0)|\hat{H}|\psi(0)\rangle &= \frac{8}{25}\langle\phi_1|\hat{H}|\phi_1\rangle + \frac{9}{25}\langle\phi_2|\hat{H}|\phi_2\rangle + \frac{8}{25}\langle\phi_3|\hat{H}|\phi_3\rangle \\ &= \frac{8}{25}(-5) + \frac{9}{25}(3) + \frac{8}{25}(5) = \frac{27}{25}. \end{aligned} \tag{3.223}$$

The second method uses matrix algebra:

$$E(0) = \langle\psi(0)|\hat{H}|\psi(0)\rangle = \frac{1}{25}\begin{pmatrix} 3 & 0 & 4 \end{pmatrix}\begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 5 \\ 0 & 5 & 0 \end{pmatrix}\begin{pmatrix} 3 \\ 0 \\ 4 \end{pmatrix} = \frac{27}{25}. \tag{3.224}$$

The third method uses the probabilities:

$$E(0) = \sum_{n=1}^{2} P(E_n)E_n = \frac{8}{25}(-5) + \frac{9}{25}(3) + \frac{8}{25}(5) = \frac{27}{25}. \tag{3.225}$$

The energy at a time t is

$$\begin{aligned} E(t) = \langle\psi(t)|\hat{H}|\psi(t)\rangle &= \frac{8}{25}e^{iE_1t}e^{-iE_1t}\langle\phi_1|\hat{H}|\phi_1\rangle + \frac{9}{25}e^{iE_2t}e^{-iE_2t}\langle\phi_2|\hat{H}|\phi_2\rangle \\ &+ \frac{8}{25}e^{iE_3t}e^{-iE_3t}\langle\phi_3|\hat{H}|\phi_3\rangle = \frac{8}{25}(-5) + \frac{9}{25}(3) + \frac{8}{25}(5) = \frac{27}{25} = E(0). \end{aligned} \tag{3.226}$$

As expected, $E(t) = E(0)$ since $d\langle \hat{H} \rangle / dt = 0$.

(d) Since none of the eigenvalues of $\hat{H}$ is degenerate, the eigenvectors $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ form a compete (orthonormal) basis. Thus $\{\hat{H}\}$ forms a complete set of commuting operators.

Problem 3.12

(a) Calculate the Poisson bracket between the x and y components of the classical orbital angular momentum.

(b) Calculate the commutator between the x and y components of the orbital angular momentum operator.

(c) Compare the results obtained in (a) and (b).

Solution

(a) Using the definition (3.113) we can write the Poisson bracket $\{l_x, l_y\}$ as

$$\{l_x, l_y\} = \sum_{j=1}^{3} \left(\frac{\partial l_x}{\partial q_j} \frac{\partial l_y}{\partial p_j} - \frac{\partial l_x}{\partial p_j} \frac{\partial l_y}{\partial q_j} \right), \tag{3.227}$$

where $q_1 = x$, $q_2 = y$, $q_3 = z$, $p_1 = p_x$, $p_2 = p_y$, and $p_3 = p_z$. Since $l_x = yp_z - zp_y$, $l_y = zp_x - xp_z$, $l_z = xp_y - yp_x$, the only partial derivatives that survive are $\partial l_x / \partial z = -p_y$, $\partial l_y / \partial p_z = -x$, $\partial l_x / \partial p_z = y$, and $\partial l_y / \partial z = p_x$. Thus, we have

$$\{l_x, l_y\} = \frac{\partial l_x}{\partial z} \frac{\partial l_y}{\partial p_z} - \frac{\partial l_x}{\partial p_z} \frac{\partial l_y}{\partial z} = xp_y - yp_x = l_z. \tag{3.228}$$

(b) The components of $\hat{\vec{L}}$ are listed in (3.26) to (3.28): $\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y$, $\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z$, and $\hat{L}_Z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x$. Since $\hat{X}$, $\hat{Y}$, and $\hat{Z}$ mutually commute and so do $\hat{P}_x$, $\hat{P}_y$, and $\hat{P}_z$, we have

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y,\ \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] \\
&= [\hat{Y}\hat{P}_z, \hat{Z}\hat{P}_x] - [\hat{Y}\hat{P}_z, \hat{X}\hat{P}_z] - [\hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x] + [\hat{Z}\hat{P}_y, \hat{X}\hat{P}_z] \\
&= \hat{Y}[\hat{P}_z, \hat{Z}]\hat{P}_x + \hat{X}[\hat{Z}, \hat{P}_z]\hat{P}_y = i\hbar(\hat{X}\hat{P}_y - \hat{Y}\hat{P}_x) \\
&= i\hbar \hat{L}_z.
\end{aligned} \tag{3.229}$$

(c) A comparison of (3.228) and (3.229) shows that

$$\{l_x, l_y\} = l_z \longrightarrow [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z. \tag{3.230}$$

Problem 3.13

Consider a charged oscillator, of positive charge q and mass m, which is subject to an oscillating electric field $E_0 \cos \omega t$; the particle's Hamiltonian is $\hat{H} = P^2/(2m) + k\hat{X}^2/2 + qE_0\hat{X} \cos \omega t$.

(a) Calculate $d\langle \hat{X} \rangle / dt$, $d\langle \hat{P} \rangle / dt$, $d\langle \hat{H} \rangle / dt$.

(b) Solve the equation for $d\langle \hat{X} \rangle / dt$ and obtain $\langle \hat{X} \rangle(t)$ such that $\langle \hat{X} \rangle(0) = x_0$.

Solution

(a) Since the position operator $\hat{X}$ does not depend explicitly on time (i.e., $\partial\hat{X}/\partial t = 0$), equation (3.88) yields

$$\frac{d}{dt}\langle\hat{X}\rangle = \frac{1}{i\hbar}\langle[\hat{X}, \hat{H}]\rangle = \frac{1}{i\hbar}\langle\left[\hat{X}, \frac{P^2}{2m}\right]\rangle = \frac{\langle\hat{P}\rangle}{m}. \tag{3.231}$$

Now, since $[\hat{P}, \hat{X}] = -i\hbar$, $[\hat{P}, \hat{X}^2] = -2i\hbar\hat{X}$ and $\partial\hat{P}/\partial t = 0$, we have

$$\frac{d}{dt}\langle\hat{P}\rangle = \frac{1}{i\hbar}\langle[\hat{P}, \hat{H}]\rangle = \frac{1}{i\hbar}\langle\left[\hat{P}, \frac{1}{2}k\hat{X}^2 + qE_0\hat{X}\cos\omega t\right]\rangle = -k\langle\hat{X}\rangle - qE_0\cos\omega t, \tag{3.232}$$

$$\frac{d}{dt}\langle\hat{H}\rangle = \frac{1}{i\hbar}\langle[\hat{H}, \hat{H}]\rangle + \langle\frac{\partial\hat{H}}{\partial t}\rangle = \langle\frac{\partial\hat{H}}{\partial t}\rangle = -qE_0\omega\langle\hat{X}\rangle\sin\omega t. \tag{3.233}$$

(b) To find $\langle\hat{X}\rangle$ we need to take a time derivative of (3.231) and then make use of (3.232):

$$\frac{d^2}{dt^2}\langle\hat{X}\rangle = \frac{1}{m}\frac{d}{dt}\langle\hat{P}\rangle = -\frac{k}{m}\langle\hat{X}\rangle - \frac{qE_0}{m}\cos\omega t. \tag{3.234}$$

The solution of this equation is

$$\langle\hat{X}\rangle(t) = \langle\hat{X}\rangle(0)\cos\left(\sqrt{\frac{k}{m}}t\right) - \frac{qE_0}{m\omega}\sin\omega t + A, \tag{3.235}$$

where A is a constant which can be determined from the initial conditions; since $\langle\hat{X}\rangle(0) = x_0$ we have $A = 0$, and hence

$$\langle\hat{X}\rangle(t) = x_0\cos\left(\sqrt{\frac{k}{m}}t\right) - \frac{qE_0}{m\omega}\sin\omega t. \tag{3.236}$$

Problem 3.14

Consider a one-dimensional free particle of mass m whose position and momentum at time $t = 0$ are given by x_0 and p_0, respectively.

(a) Calculate $\langle\hat{P}\rangle(t)$ and show that $\langle\hat{X}\rangle(t) = p_0 t^2/m + x_0$.

(b) Show that $d\langle\hat{X}^2\rangle/dt = 2\langle\hat{P}\hat{X}\rangle/m + i\hbar/m$ and $d\langle\hat{P}^2\rangle/dt = 0$.

(c) Show that the position and momentum fluctuations are related by $d^2(\Delta x)^2/dt^2 = 2(\Delta p)^2/m^2$ and that the solution to this equation is given by $(\Delta x)^2 = (\Delta p)_0^2 t^2/m^2 + (\Delta x)_0^2$ where $(\Delta x)_0$ and $(\Delta p)_0$ are the initial fluctuations.

Solution

(a) From the Ehrenfest equations $d\langle\hat{P}\rangle/dt = \langle[\hat{P}, \hat{V}(x,t)]\rangle/i\hbar$ as shown in (3.134), and since for a free particle $\hat{V}(x,t) = 0$, we see that $d\langle\hat{P}\rangle/dt = 0$. As expected this leads to $\langle\hat{P}\rangle(t) = p_0$, since the linear momentum of a free particle is conserved. Inserting $\langle\hat{P}\rangle = p_0$ into Ehrenfest's other equation $d\langle\hat{X}\rangle/dt = \langle\hat{P}\rangle/m$ (see (3.132)), we obtain

$$\frac{d\langle\hat{X}\rangle}{dt} = \frac{1}{m}p_0. \tag{3.237}$$

The solution of this equation with the initial condition $\langle\hat{X}\rangle(0) = x_0$ is

$$\langle\hat{X}\rangle(t) = \frac{p_0}{m}t + x_0. \tag{3.238}$$

(b) First, the proof of $d\langle\hat{P}^2\rangle/dt = 0$ is straightforward. Since $[\hat{P}^2, \hat{H}] = [\hat{P}^2, \hat{P}^2/2m] = 0$ and $\partial\hat{P}^2/\partial t = 0$ (the momentum operator does not depend on time), (3.124) yields

$$\frac{d}{dt}\langle\hat{P}^2\rangle = \frac{1}{i\hbar}\langle[\hat{P}^2, \hat{H}]\rangle + \langle\frac{\partial\hat{P}^2}{\partial t}\rangle = 0. \tag{3.239}$$

For $d\langle\hat{X}^2\rangle/dt$ we have

$$\frac{d}{dt}\langle\hat{X}^2\rangle = \frac{1}{i\hbar}\langle[\hat{X}^2, \hat{H}]\rangle = \frac{1}{2im\hbar}\langle[\hat{X}^2, \hat{P}^2]\rangle, \tag{3.240}$$

since $\partial\hat{X}^2/\partial t = 0$. Using $[\hat{X}, \hat{P}] = i\hbar$, we obtain

$$\begin{aligned}
[\hat{X}^2, \hat{P}^2] &= \hat{P}[\hat{X}^2, \hat{P}] + [\hat{X}^2, \hat{P}]\hat{P} \\
&= \hat{P}\hat{X}[\hat{X}, \hat{P}] + \hat{P}[\hat{X}, \hat{P}]\hat{X} + \hat{X}[\hat{X}, \hat{P}]\hat{P} + [\hat{X}, \hat{P}]\hat{X}\hat{P} \\
&= 2i\hbar(\hat{P}\hat{X} + \hat{X}\hat{P}) = 2i\hbar(2\hat{P}\hat{X} + i\hbar);
\end{aligned} \tag{3.241}$$

hence

$$\frac{d}{dt}\langle\hat{X}^2\rangle = \frac{2}{m}\langle\hat{P}\hat{X}\rangle + \frac{i\hbar}{m}. \tag{3.242}$$

(c) As the position fluctuation is given by $(\Delta x)^2 = \langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2$, we have

$$\frac{d(\Delta x)^2}{dt} = \frac{d\langle\hat{X}^2\rangle}{dt} - 2\langle\hat{X}\rangle\frac{d\langle\hat{X}\rangle}{dt} = \frac{2}{m}\langle\hat{P}\hat{X}\rangle + \frac{i\hbar}{m} - \frac{2}{m}\langle\hat{X}\rangle\langle\hat{P}\rangle. \tag{3.243}$$

In deriving this expression we have used (3.242) and $d\langle\hat{X}\rangle/dt = \langle\hat{P}\rangle/m$. Now, since $d(\langle\hat{X}\rangle\langle\hat{P}\rangle)/dt = \langle\hat{P}\rangle d\langle\hat{X}\rangle/dt = \langle\hat{P}\rangle^2/m$ and

$$\frac{d\langle\hat{P}\hat{X}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{P}\hat{X},\ \hat{H}]\rangle = \frac{1}{2im\hbar}\langle[\hat{P}\hat{X},\ \hat{P}^2]\rangle = \frac{1}{m}\langle\hat{P}^2\rangle, \tag{3.244}$$

we can write the second time derivative of (3.243) as follows:

$$\frac{d^2(\Delta x)^2}{dt^2} = \frac{2}{m}\left(\frac{d\langle\hat{P}\hat{X}\rangle}{dt} - \frac{d\langle\hat{X}\rangle\langle\hat{P}\rangle}{dt}\right) = \frac{2}{m^2}\left(\langle\hat{P}^2\rangle - \langle\hat{P}\rangle^2\right) = \frac{2}{m^2}(\Delta p)_0^2, \tag{3.245}$$

where $(\Delta p)_0^2 = \langle\hat{P}^2\rangle - \langle\hat{P}\rangle^2 = \langle\hat{P}^2\rangle_0 - \langle\hat{P}\rangle_0^2$; the momentum of the free particle is a constant of the motion. We can verify that the solution of the differential equation (3.245) is given by

$$(\Delta x)^2 = \frac{1}{m^2}(\Delta p)_0^2 t^2 + (\Delta x)_0^2. \tag{3.246}$$

This fluctuation is similar to the spreading of a Gaussian wave packet we derived in Chapter 1.

3.10 Exercises

Exercise 3.1
A particle in an infinite potential box with walls at $x = 0$ and $x = a$ (i.e., the potential is infinite for $x < 0$ and $x > a$ and zero in between) has the following wave function at some initial time:

$$\psi(x) = \frac{1}{\sqrt{5a}} \sin\left(\frac{\pi x}{a}\right) + \frac{2}{\sqrt{5a}} \sin\left(\frac{3\pi x}{a}\right).$$

(a) Find the possible results of the measurement of the system's energy and the corresponding probabilities.

(b) Find the form of the wave function after such a measurement.

(c) If the energy is measured again immediately afterwards, what are the relative probabilities of the possible outcomes?

Exercise 3.2
Let $\psi_n(x)$ denote the orthonormal stationary states of a system corresponding to the energy E_n. Suppose that the normalized wave function of the system at time $t = 0$ is $\psi(x, 0)$ and suppose that a measurement of the energy yields the value E_1 with probability 1/2, E_2 with probability 3/8, and E_3 with probability 1/8.

(a) Write the most general expansion for $\psi(x, 0)$ consistent with this information.

(b) What is the expansion for the wave function of the system at time t, $\psi(x, t)$?

(c) Show that the expectation value of the Hamiltonian does not change with time.

Exercise 3.3
Consider a neutron which is confined to an infinite potential well of width $a = 8$ fm. At time $t = 0$ the neutron is assumed to be in the state

$$\Psi(x, 0) = \sqrt{\frac{4}{7a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{7a}} \sin\left(\frac{2\pi x}{a}\right) + \sqrt{\frac{8}{7a}} \sin\left(\frac{3\pi x}{a}\right).$$

(a) If an energy measurement is carried out on the system, what are the values that will be found for the energy and with what probabilities? Express your answer in MeV (the mass of the neutron is $mc^2 \simeq 939$ MeV, $\hbar c \simeq 197$ MeV fm).

(b) If this measurement is repeated on many identical systems, what is the average value of the energy that will be found? Again, express your answer in MeV.

(c) Using the uncertainty principle, estimate the order of magnitude of the neutron's speed in this well as a function of the speed of light c.

Exercise 3.4
Consider the dimensionless harmonic oscillator Hamiltonian

$$\hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2, \qquad \text{with} \quad \hat{P} = -i\frac{d}{dx}.$$

(a) Show that the two wave functions $\psi_0(x) = e^{-x^2/2}$ and $\psi_1(x) = xe^{-x^2/2}$ are eigenfunctions of $\hat{H}$ with eigenvalues $1/2$ and $3/2$, respectively.

(b) Find the value of the coefficient α such that $\psi_2(x) = \left(1 + \alpha x^2\right) e^{-x^2/2}$ is orthogonal to $\psi_0(x)$. Then show that $\psi_2(x)$ is an eigenfunction of $\hat{H}$ with eigenvalue $5/2$.

Exercise 3.5

Consider that the wave function of a dimensionless harmonic oscillator, whose Hamiltonian is $\hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2$, is given at time $t = 0$ by

$$\psi(x, 0) = \frac{1}{\sqrt{8\pi}}\phi_0(x) + \frac{1}{\sqrt{18\pi}}\phi_2(x) = \frac{1}{\sqrt{8\pi}}e^{-x^2/2} + \frac{1}{\sqrt{18\pi}}\left(1 - 2x^2\right)e^{-x^2/2}.$$

(a) Find the expression of the oscillator's wave function at any later time t.

(b) Calculate the probability P_0 to find the system in an eigenstate of energy $1/2$ and the probability P_2 of finding the system in an eigenstate of energy $5/2$.

(c) Calculate the probability density, $\rho(x, t)$, and the current density, $\vec{J}(x, t)$.

(d) Verify that the probability is conserved; that is, show that $\partial\rho/\partial t + \vec{\nabla} \cdot \vec{J}(x, t) = 0$.

Exercise 3.6

A particle of mass m, in an infinite potential well of length a, has the following initial wave function at $t = 0$:

$$\psi(x, 0) = \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right), \tag{3.247}$$

and an energy spectrum $E_n = -\hbar^2\pi^2 n^2/(2ma^2)$.

Find $\psi(x, t)$ at any later time t, then calculate $\frac{\partial\rho}{\partial t}$ and the probability current density vector $\vec{J}(x, t)$ and verify that $\frac{\partial\rho}{\partial t} + \vec{\nabla} \cdot \vec{J}(x, t) = 0$. Recall that $\rho = \psi^*(x, t)\psi(x, t)$ and $\vec{J}(x, t) = \frac{i\hbar}{2m}\left(\psi(x, t)\vec{\nabla}\psi^*(x, t) - \psi^*(x, t)\vec{\nabla}\psi(x, t)\right)$.

Exercise 3.7

Consider a system whose initial state at $t = 0$ is given in terms of a complete and orthonormal set of three vectors: $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ as follows: $|\psi(0)\rangle = 1/\sqrt{3}|\phi_1\rangle + A|\phi_2\rangle + 1/\sqrt{6}|\phi_3\rangle$, where A is a real constant.

(a) Find A so that $|\psi(0)\rangle$ is normalized.

(b) If the energies corresponding to $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ are given by E_1, E_2, and E_3, respectively, write down the state of the system $|\psi(t)\rangle$ at any later time t.

(c) Determine the probability of finding the system at a time t in the state $|\phi_3\rangle$.

Exercise 3.8

The components of the initial state $|\psi_i\rangle$ of a quantum system are given in a complete and orthonormal basis of three states $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ by

$$\langle\phi_1|\psi_i\rangle = \frac{i}{\sqrt{3}}, \quad \langle\phi_2|\psi_i\rangle = \sqrt{\frac{2}{3}}, \quad \langle\phi_3|\psi_i\rangle = 0.$$

Calculate the probability of finding the system in a state $|\psi_f\rangle$ whose components are given in the same basis by

$$\langle\phi_1|\psi_f\rangle = \frac{1+i}{\sqrt{3}}, \quad \langle\phi_2|\psi_f\rangle = \frac{1}{\sqrt{6}}, \quad \langle\phi_3|\psi_f\rangle = \frac{1}{\sqrt{6}}.$$

Exercise 3.9

(a) Evaluate the Poisson bracket $\left\{x^2, p^2\right\}$.

(b) Express the commutator $\left[\hat{X}^2, \hat{P}^2\right]$ in terms of $\hat{X}\hat{P}$ plus a constant in $\hbar^2$.

(c) Find the classical limit of $\left[\hat{x}^2, \hat{p}^2\right]$ for this expression and then compare it with the result of part (a).

Exercise 3.10

A particle bound in a one-dimensional potential has a wave function

$$\psi(x) = \begin{cases} Ae^{5ikx}\cos(3\pi x/a), & -a/2 \le x \le a/2, \\ 0, & |x| > a/2. \end{cases}$$

(a) Calculate the constant A so that $\psi(x)$ is normalized.

(b) Calculate the probability of finding the particle between $x = 0$ and $x = a/4$.

Exercise 3.11

(a) Show that any component of the momentum operator of a particle is compatible with its kinetic energy operator.

(b) Show that the momentum operator is compatible with the Hamiltonian operator only if the potential operator is constant in space coordinates.

Exercise 3.12

Consider a physical system whose Hamiltonian H and an operator A are given by

$$H = \mathcal{E}_0 \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad A = a_0 \begin{pmatrix} 5 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix},$$

where $\mathcal{E}_0$ has the dimensions of energy.

(a) Do H and A commute? If yes, give a basis of eigenvectors common to H and A.

(b) Which among the sets of operators $\{\hat{H}\}$, $\{\hat{A}\}$, $\{\hat{H}, \hat{A}\}$, $\{\hat{H}^2, \hat{A}\}$ form a complete set of commuting operators (CSCO)?

Exercise 3.13

Show that the momentum and the total energy can be measured simultaneously only when the potential is constant everywhere.

Exercise 3.14

The initial state of a system is given in terms of four orthonormal energy eigenfunctions $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, and $|\phi_4\rangle$ as follows:

$$|\psi_0\rangle = |\psi(t=0)\rangle = \frac{1}{\sqrt{3}}|\phi_1\rangle + \frac{1}{2}|\phi_2\rangle + \frac{1}{\sqrt{6}}|\phi_3\rangle + \frac{1}{2}|\phi_4\rangle.$$

(a) If the four kets $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, and $|\phi_4\rangle$ are eigenvectors to the Hamiltonian $\hat{H}$ with energies E_1, E_2, E_3, and E_4, respectively, find the state $|\psi(t)\rangle$ at any later time t.

(b) What are the possible results of measuring the energy of this system and with what probability will they occur?

(c) Find the expectation value of the system's Hamiltonian at $t = 0$ and $t = 10\,\text{s}$.

Exercise 3.15
The complete set expansion of an initial wave function $\psi(x,0)$ of a system in terms of orthonormal energy eigenfunctions $\phi_n(x)$ of the system has three terms, $n = 1, 2, 3$. The measurement of energy on the system represented by $\psi(x,0)$ gives three values, E_1 and E_2 with probability $1/4$ and E_3 with probability $1/2$.

(a) Write down $\psi(x,0)$ in terms of $\phi_1(x)$, $\phi_2(x)$, and $\phi_3(x)$.

(b) Find $\psi(x,0)$ at any later time t, i.e., find $\psi(x,t)$.

Exercise 3.16
Consider a system whose Hamiltonian H and an operator A are given by the matrices

$$H = \mathcal{E}_0 \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 2i \\ 0 & -2i & 0 \end{pmatrix}, \quad A = a_0 \begin{pmatrix} 0 & -i & 0 \\ i & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

(a) If we measure energy, what values will we obtain?

(b) Suppose that when we measure energy, we obtain a value of $\sqrt{5}\mathcal{E}_0$. Immediately afterwards, we measure A. What values will we obtain for A and what are the probabilities corresponding to each value?

(c) Calculate the expectation value $\langle A \rangle$.

Exercise 3.17
Consider a physical system whose Hamiltonian and initial state are given by

$$H = \mathcal{E}_0 \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad |\psi_0\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix},$$

where $\mathcal{E}_0$ has the dimensions of energy.

(a) What values will we obtain when measuring the energy and with what probabilities?

(b) Calculate the expectation value of the Hamiltonian $\langle \hat{H} \rangle$.

Exercise 3.18
Consider a system whose state $|\psi(t)\rangle$ and two observables A and B are given by

$$|\psi(t)\rangle = \begin{pmatrix} 5 \\ 1 \\ 3 \end{pmatrix}, \qquad A = \frac{1}{\sqrt{2}} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

(a) We perform a measurement where A is measured first and then B immediately afterwards. Find the probability of obtaining a value of $\sqrt{2}$ for A and a value of -1 for B.

(b) Now we measure B first and then A immediately afterwards. Find the probability of obtaining a value of -1 for B and a value of $\sqrt{2}$ for A.

(c) Compare the results of (a) and (b). Explain.

Exercise 3.19
Consider a system whose state $|\psi(t)\rangle$ and two observables A and B are given by

$$|\psi(t)\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} -i \\ 2 \\ 0 \end{pmatrix}, \qquad A = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 1 \\ -i & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 0 \end{pmatrix}.$$

(a) Are A and B compatible? Which among the sets of operators $\{\hat{A}\}$, $\{\hat{B}\}$, and $\{\hat{A}, \hat{B}\}$ form a complete set of commuting operators?

(b) Measuring A first and then B immediately afterwards, find the probability of obtaining a value of -1 for A and a value of 3 for B.

(c) Now, measuring B first then A immediately afterwards, find the probability of obtaining 3 for B and -1 for A. Compare this result with the probability obtained in (b).

Exercise 3.20
Consider a physical system which has a number of observables that are represented by the following matrices:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & i \\ -1 & -i & 4 \end{pmatrix}, \quad C = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix}.$$

(a) Find the results of the measurements of the compatible observables.

(b) Which among these observables are compatible? Give a basis of eigenvectors common to these observables.

(c) Which among the sets of operators $\{\hat{A}\}$, $\{\hat{B}\}$, $\{\hat{C}\}$, $\{\hat{A}, \hat{B}\}$, $\{\hat{A}, \hat{C}\}$, $\{\hat{B}, \hat{C}\}$ form a complete set of commuting operators?

Exercise 3.21
Consider a system which is initially in a state $|\psi(0)\rangle$ and having a Hamiltonian $\hat{H}$, where

$$|\psi(0)\rangle = \begin{pmatrix} 4-i \\ -2+5i \\ 3+2i \end{pmatrix}, \qquad H = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 3 & 3 \\ 0 & 3 & 0 \end{pmatrix}.$$

(a) If a measurement of H is carried out, what values will we obtain and with what probabilities?

(b) Find the state of the system at a later time t; you may need to expand $|\psi(0)\rangle$ in terms of the eigenvectors of H.

(c) Find the total energy of the system at time $t = 0$ and any later time t; are these values different?

(d) Does $\hat{H}$ form a complete set of commuting operators?

Exercise 3.22
Consider a particle which moves in a scalar potential $V(\vec{r}) = V_x(x) + V_y(y) + V_z(z)$.

(a) Show that the Hamiltonian of this particle can be written as $\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z$, where $\hat{H}_x = p_x^2/(2m) + V_x(x)$, and so on.

(b) Do $\hat{H}_x$, $\hat{H}_y$, and $\hat{H}_z$ form a complete set of commuting operators?

Exercise 3.23
Consider a system whose Hamiltonian is $H = \mathcal{E}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, where $\mathcal{E}$ is a real constant with the dimensions of energy.

(a) Find the eigenenergies, E_1 and E_2, of H.

(b) If the system is initially (i.e., $t = 0$) in the state $|\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, find the probability so that a measurement of energy at $t = 0$ yields: (i) E_1, and (ii) E_2.

(c) Find the average value of the energy $\langle \hat{H} \rangle$ and the energy uncertainty $\sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}$.
(d) Find the state $|\psi(t)\rangle$.

Exercise 3.24
Prove the relation

$$\frac{d}{dt}\langle \hat{A}\hat{B} \rangle = \langle \frac{\partial \hat{A}}{\partial t}\hat{B} \rangle + \langle \hat{A}\frac{\partial \hat{B}}{\partial t} \rangle + \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}]\hat{B} \rangle + \frac{1}{i\hbar}\langle \hat{A}[\hat{B}, \hat{H}] \rangle.$$

Exercise 3.25
Consider a particle of mass m which moves under the influence of gravity; the particle's Hamiltonian is $\hat{H} = \hat{P}_z^2/(2m) - mg\hat{Z}$, where g is the acceleration due to gravity, $g = 9.8\,\mathrm{m\,s^{-2}}$.
(a) Calculate $d\langle \hat{Z} \rangle/dt$, $d\langle \hat{P}_z \rangle/dt$, $d\langle \hat{H} \rangle/dt$.
(b) Solve the equation $d\langle \hat{Z} \rangle/dt$ and obtain $\langle \hat{Z} \rangle(t)$, such that $\langle \hat{Z} \rangle(0) = h$ and $\langle \hat{P}_z \rangle(0) = 0$. Compare the result with the classical relation $z(t) = -\frac{1}{2}gt^2 + h$.

Exercise 3.26
Calculate $d\langle \hat{X} \rangle/dt$, $d\langle \hat{P}_x \rangle/dt$, $d\langle \hat{H} \rangle/dt$ for a particle with $\hat{H} = \hat{P}_x^2/(2m) + \frac{1}{2}m\omega^2\hat{X}^2 + V_0\hat{X}^3$.

Exercise 3.27
Consider a system whose initial state at $t = 0$ is given in terms of a complete and orthonormal set of four vectors $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, $|\phi_4\rangle$ as follows:

$$|\psi(0)\rangle = \frac{A}{\sqrt{12}}|\phi_1\rangle + \frac{1}{\sqrt{6}}|\phi_2\rangle + \frac{2}{\sqrt{12}}|\phi_3\rangle + \frac{1}{2}|\phi_4\rangle,$$

where A is a real constant.
(a) Find A so that $|\psi(0)\rangle$ is normalized.
(b) If the energies corresponding to $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, $|\phi_4\rangle$ are given by E_1, E_2, E_3, and E_4, respectively, write down the state of the system $|\psi(t)\rangle$ at any later time t.
(c) Determine the probability of finding the system at a time t in the state $|\phi_2\rangle$.