PART I
Fundamentals

1 Basic Quantum Mechanics

1.1 MEASUREMENTS AND PROBABILITY

In the beginning of 20th century, it was discovered that the behavior of very small particles, such as electrons, the nuclei of atoms, and molecules, cannot be described by classical mechanics, which had been quite successful in explaining the macroscopic world until then. Nonetheless, it was soon discovered that the description of these phenomena on the atomic scale is possible by the set of laws described by quantum mechanics. Both classical mechanics and quantum mechanics are based on the description of measurements of observable quantities called dynamical variables, such as position, momentum, and energy. Consider an experiment in which we can make three measurements successive in time. Let's denote the first of observable quantities A, the second B, and the third C. We also denote a, b, and c as one of a number of possible results that could come from the measurement of A, B, and C, respectively. Let $P(b\,|\,a)$ be the conditional probability that if the measurement of A results in a, then the measurement of B will result in b. From the elementary probability theory, the conditional probability $P(b\,|\,a)$ can be written as follows:

$$P(b\,|\,a) = \frac{P(a,b)}{P(a)}, \tag{1.1}$$

where $P(a,b)$ is the joint probability that measurements of both A and B will give a and b, simultaneously, and $P(a)$ is the probability that the measurement of A will give the outcome a. For three successive measurements A, B, and C, the conditional probability $P(cb\,|\,a)$ that if the measurement of A results in a, then the measurement of B will result in b, then the measurement of C will result in c is given by:

$$P(cb\,|\,a) = P(c\,|\,b)P(b\,|\,a). \tag{1.2}$$

Engineering Quantum Mechanics, First Edition. Doyeol Ahn, Seoung-Hwan Park.

Moreover, if we sum Equation (1.2) over all the mutually exclusive alternatives for b, we obtain the conditional probability $P(c \mid a)$:

$$P(c \mid a) = \sum_b P(c \mid b) P(b \mid a). \tag{1.3}$$

In classical mechanics, the above relation described by Equation (1.3) is always true. However, it was found that the above relation sometimes fails on the atomic scale, and one needs to modify Equations (1.1) to (1.3) by introducing new complex quantities φ_{ba}, φ_{cb}, and φ_{ca}, called probability amplitudes, which are related to probabilities by [1,2]

$$P(b \mid a) = |\varphi_{ba}|^2, \tag{1.4}$$

and

$$P(c \mid a) = \left| \sum_b \varphi_{cb} \varphi_{ba} \right|^2. \tag{1.5}$$

Equations (1.4) and (1.5) describe the probability of measurement outcome in quantum mechanics. From the mathematical point of view, the probability amplitude is found to be the inner product of vectors in a special kind of vector space called the Hilbert space:

$$\varphi_{ba} = \langle b || a \rangle, \tag{1.6}$$

where $|a\rangle$ is the column vector, called the "ket vector," corresponding to the observable a, and $\langle b|$ is the row vector, called the "bra vector," corresponding to the observable b.

1.2 DIRAC FORMULATION

In quantum mechanics, a physical state corresponding to the observable quantity a is represented by the ket vector, $|a\rangle$, in a complex vector space H with dimension N. For example, when $N = 2$, the ket vector $|a\rangle$ is a column vector given by [1,3]

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \tag{1.7}$$

where a_1 and a_2 are complex numbers. We can also consider the case where the dimension of the vector space is infinite. In this case, the ket vector $|a\rangle$ is represented by a column vector given by

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ . \\ . \\ . \\ a_\infty \end{pmatrix}, \tag{1.8}$$

with complex quantities $a_1, a_2, a_3, \ldots, a_\infty$. From now on, we will denote ket vectors simply as vectors.

If $|a\rangle$ and $|b\rangle$ are vectors in H, and α and β are complex numbers, then the linear superposition of these two vectors $\alpha|a\rangle + \beta|b\rangle$ is also a vector in H. For each vector $|a\rangle$ in H, we can relate a row vector $\langle a|$ called bra vector, which is given by

$$\langle a| = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix}, \text{for } N = 2, \tag{1.9}$$

and

$$\langle a| = \begin{pmatrix} a_1^* & a_2^* & a_3^* \ldots . a_\infty^* \end{pmatrix}, \text{for } N = \infty, \tag{1.10}$$

where * is the complex conjugate. By comparing Equations (1.7) with (1.10), one can see that the ket vector $|a\rangle$ and bra vector $\langle b|$ are related by

$$\langle a| = (|a\rangle)^\dagger, \tag{1.11}$$

where $\dagger$ is the adjoint operation, which is the transposition, followed by the complex conjugation.

The inner product between two vectors $|a\rangle$ and $|b\rangle$ is a complex number $\langle b|a\rangle$, which is given by

$$\langle b|a\rangle = b_1^* a_1 + b_2^* a_2 + \ldots + b_\infty^* a_\infty = \langle a|b\rangle^*. \tag{1.12}$$

The vector space where one can define the inner product relation of Equation (1.12) is called the Hilbert space. The length of the vector $|a\rangle$ is defined by

$$\|\|a\rangle\| = \sqrt{\langle a|a\rangle}, \tag{1.13}$$

and when the vector has the unit length, we call it a normal vector.

The vectors in the Hilbert space H are mapped to different vectors in the Hilbert space H' by the linear transformation $\hat{A}$, which is often called the "linear operator" in quantum mechanics. Mathematically, the act of the linear operator $\hat{A}$ on the vectors of the Hilbert space H is expressed as $\hat{A} : H \to H'$. In most cases, the initial Hilbert space H and the final Hilbert space H' are the same, and unless otherwise specified explicitly, we will assume that is the case. Any two vectors $|a\rangle$ and $|b\rangle$ in H are transformed by $\hat{A}$ as

$$\hat{A}(\alpha|a\rangle + \beta|b\rangle) = \alpha\hat{A}|a\rangle + \beta\hat{A}|b\rangle, \tag{1.14}$$

and

$$\left(\hat{A}\alpha|a\rangle\right)^{\dagger} = \alpha^*\langle a|\hat{A}^{\dagger}, \tag{1.15}$$

where α and β are complex constants. If we set $|c\rangle = \hat{A}|a\rangle$ from Equation (1.11), we obtain $\langle c| = (|c\rangle)^{\dagger} = \langle a|\hat{A}^{\dagger}$, and then, using Equation (1.12), we get

$$\langle b|\hat{A}|a\rangle^* = \langle b|c\rangle^* = \langle c|b\rangle = \langle a|\hat{A}^{\dagger}|b\rangle. \tag{1.16}$$

For a given operator $\hat{A}$, there exists particular set of vectors $\{|a_1\rangle, |a_2\rangle, \ldots, |a_n\rangle, \ldots\}$ called eigenstates, which satisfy

$$\hat{A}|a_1\rangle = a_1|a_1\rangle,\ \hat{A}|a_2\rangle = a_2|a_2\rangle, \ldots,\ \hat{A}|a_n\rangle = a_n|a_n\rangle, \ldots \tag{1.17}$$

Here, the numbers $a_1, a_2, \ldots, a_n, \ldots$ are called eigenvalues. Of the many kinds of operators, one particular type of operator, called the Hermitian operator, plays an important role in quantum mechanics. If $\hat{A}$ is a Hermitian operator, then it satisfies the following properties:

(I) $\hat{A}^{\dagger} = \hat{A}$.

(II) Eigenvalues $a_1, a_2, \ldots, a_n, \ldots$ are real.

(III) Eigenvectors corresponding to different eigenvalues are orthogonal.

(IV) $\sum_n |a_n\rangle\langle a_n| = I$, where I is an identity matrix.

The proof is as follows: From $\hat{A}|a_i\rangle = a_i|a_i\rangle$ and $\hat{A}|a_j\rangle = a_j|a_j\rangle$, we have

$$\langle a_j | \hat{A} = \langle a_j | \hat{A}^\dagger = \left(\hat{A} | a_j \rangle \right)^\dagger = a_j^* \langle a_j |. \tag{1.18}$$

Then, we get

$$\langle a_j | \hat{A} | a_i \rangle = a_i \langle a_j | a_i \rangle, \tag{1.19}$$

and

$$\langle a_j | \hat{A} | a_i \rangle = a_j^* \langle a_j | a_i \rangle. \tag{1.20}$$

Subtracting Equation (1.20) from Equation (1.19), we obtain

$$(a_i - a_j^*) \langle a_j | a_i \rangle = 0. \tag{1.21}$$

When $i \neq j$, we get $\langle a_j | a_i \rangle = 0$, which proves the property (III). On the other hand, if $i = j$, then we have $a_i = a_i^*$, thus giving the property (II). The property (III) dictates that the set of eigenvectors $\{|a_i\rangle\}$ of a Hermitian operator $\hat{A}$ form an orthogonal basis if the state $|a_i\rangle$ is properly normalized—that is, $\langle a_i | a_i \rangle = 1$ and $\langle a_i | a_j \rangle = 0$ for $i \neq j$. Let the Hilbert space spanned by these basis vectors be denoted as H. Then any vector $|\psi\rangle$ that belongs to H can be expressed as

$$|\psi\rangle = \sum_m C_m |a_m\rangle, \tag{1.22}$$

where C_m is an expansion coefficient that can be calculated by taking an inner product between the state vectors $|\psi\rangle$ and $|a_m\rangle$:

$$C_m = \langle a_m | \psi \rangle. \tag{1.23}$$

By substituting Equation (1.23) into Equation (1.22), we obtain

$$\begin{aligned} |\psi\rangle &= \sum_m C_m |a_m\rangle \\ &= \sum_m |a_m\rangle \langle a_m | \psi \rangle \\ &= \left(\sum_m |a_m\rangle \langle a_m | \right) |\psi\rangle \\ &= I |\psi\rangle, \end{aligned} \tag{1.24}$$

which proves the property (IV). It would be handy to memorize that given a chain of vectors or operators, we can insert the identity operator

defined by (IV) in any place at our convenience. For example, the Hermitian operator $\hat{A}$ can be written as

$$\begin{aligned}\hat{A} &= I\,\hat{A}\,I \\ &= \left(\sum_n |a_n\rangle\langle a_n|\right)\hat{A}\left(\sum_m |a_m\rangle\langle a_m|\right) \\ &= \sum_{n,m} |a_n\rangle\langle a_n|\,\hat{A}\,|a_m\rangle\langle a_m| \\ &= \sum_{n,m} |a_n\rangle(a_m\langle a_n|a_m\rangle)\langle a_m| \\ &= \sum_n a_n |a_n\rangle\langle a_n|,\end{aligned} \tag{1.25}$$

which is also called the spectral representation of an operator $\hat{A}$.

Let $\hat{A}$ and $\hat{B}$ be linear operators, and we define $\hat{D}$ as $\hat{D} = \hat{A}\hat{B}$. Moreover, we define $|b\rangle = \hat{B}|a\rangle$ and $|d\rangle = \hat{D}|a\rangle = \hat{A}|b\rangle$. Then, from Equations (1.11) and (1.15), we obtain

$$\begin{aligned}\langle d| &= \langle a|\hat{D}^\dagger \\ &= \langle b|\hat{A}^\dagger \\ &= \langle a|\hat{B}^\dagger\hat{A}^\dagger,\end{aligned} \tag{1.26}$$

or

$$\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger. \tag{1.27}$$

1.3 BRIEF DETOUR TO CLASSICAL MECHANICS

Almost seven decades ago, Dirac made a connection between classical mechanics and quantum mechanics by assuming that the linear operators correspond to the dynamical variables at that time. By "dynamical variables," we mean quantities such as the coordinates and the components of velocity, momentum, and angular momentum of particles, and functions of these quantities, the variables in terms of which classical mechanics is built. Even now, 70 years later, his postulates of quantum mechanics are still valid and perhaps only plausible approaches. Dirac's postulates require that those dynamical variables shall also occur in quantum mechanics, but with the difference that they are now subject to an algebra in which the commutative axiom of multiplication does

not hold. Nonetheless, the dynamical variables of quantum mechanics still have many properties in common with their classical counterparts, and it will still be possible to build up a theory of them closely analogous to the classical theory and form a generalization of it. In this spirit, the transition from classical mechanics to quantum mechanics can be made most conveniently and easily using the Hamiltonian formulation of classical mechanics [4,5].

Classical mechanics is based on the assumption that any physically interesting variable, that is, dynamical variable, can be measured with arbitrary precision and without mutual interference from any other such measurement. On the other hand, quantum mechanics is based on the realization that the measuring process may affect the physical system. The measurement of one variable affects other variables in such a way that it prevents us from knowing what their values might have been. The mathematical formulation of the law of physics that takes this basic idea into account is very different from the mathematical formulation of classical mechanics.

Hamilton's least action principle, which is equivalent to Newton's law, is formulated as follows.

> The laws of physics are such that the time integral over a certain function $L(q_i,\dot{q}_i,t)$, called Lagrangian of the physical system, assumes a minimum.

For mechanical systems, the variables q_i on which the Lagrangian depends on are the coordinates of all independent parts of the system. A system with f degrees of freedom has f coordinates $q_1,q_2,\cdots,q_f$ and the time integral J, which is defined by

$$J=\int_{t_1}^{t_2} L(q_i,\dot{q}_i,t)dt, \tag{1.28}$$

is minimum. In other words, when $\delta q_i=0$ at $t=t_1,t_2$, we get

$$\begin{aligned}\delta J&=\int_{t_1}^{t_2}\delta L(q_i,\dot{q}_i;t)dt\\&=\int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q_i}\delta q_i+\frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\right)dt\\&=\int_{t_1}^{t_2}\left(\frac{\partial L}{\partial q_i}-\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right)\delta q_i dt\\&=0.\end{aligned} \tag{1.29}$$

Equation (1.29) dictates that the Lagrangian satisfies the following Euler equation:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0, \quad i = 1,2,3,\ldots,f. \tag{1.30}$$

The behavior of the physical system is thus completely specified by Euler's equation once the Lagrangian is known. The proper Lagrangian is the one that leads to a description of the physical system that is in agreement with experimental observations.

For example, if we choose $L = T - V = \frac{1}{2}m\dot{x}^2 - V(x)$ for a one-dimensional particle with mass m in the potential field $V(x)$, we obtain

$$\frac{\partial L}{\partial x} = -\frac{\partial V(x)}{\partial x} \text{ and } \frac{\partial L}{\partial \dot{x}} = m\dot{x}. \tag{1.31}$$

Then the Euler equation yields

$$m\ddot{x} = -\frac{\partial V(x)}{\partial x} = F(x), \tag{1.32}$$

which is the famous Newton's first law of mechanics.

For later purpose, we make the following canonical transformation:

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}, \quad H \equiv \sum_i p_i \dot{q}_i - L, \tag{1.33}$$

where H is called the Hamiltonian of the system. Then we obtain the following, Hamilton's equation of motion:

$$\begin{aligned} &\frac{\partial H}{\partial p_i} = \dot{q}, \\ &\dot{p}_i = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i} = \frac{\partial}{\partial q_i}\left(\sum_j p_j \dot{q}_j - H\right) = -\frac{\partial H}{\partial q_i}, \end{aligned} \tag{1.34}$$

or,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{1.35}$$

Here, the Hamiltonian H represents the total energy of the system. For any dynamical variable F that depends on canonical variables (q_i, p_i), the time derivative of F is given by

$$\begin{aligned}\frac{dF}{dt} &= \sum_i \left\{ \frac{\partial F}{\partial q_i}\dot{q}_i + \frac{\partial F}{\partial p_i} \right\} + \frac{\partial F}{\partial t} \\ &= \sum_i \left\{ \frac{\partial F}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q_i} \right\} + \frac{\partial F}{\partial t} \\ &= \{F, H\} + \frac{\partial F}{\partial t},\end{aligned} \tag{1.36}$$

where the Poisson bracket $\{A, B\}$ for dynamical variables A,B is defined by

$$\{A, B\} = \sum_i \left\{ \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right\} = -\{B, A\}. \tag{1.37}$$

Equations (1.36) and (1.37) imply that

$$\frac{dH}{dt} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}, \tag{1.38}$$

which says if H does not explicitly dependents on the time t, the Hamiltonian, the total energy of the system, is conserved. Among many interesting properties of the Poisson bracket, the following relation is especially useful for the latter purpose:

$$\{q_i, p_j\} = \delta_{ij}. \tag{1.39}$$

For a particle moving in a one-dimensional world specified by the coordinate x, the Lagrangian is given by $L = (1/2m)\dot{x}^2 - V(x)$, as before. Then the canonical transformation yields,

$$\begin{aligned} p &= \frac{\partial L}{\partial \dot{x}} = m\dot{x}, \\ H &= p\dot{x} - L = \frac{1}{2}m\dot{x}^2 + V(x) = \frac{p^2}{2m} + V(x). \end{aligned} \tag{1.40}$$

Equation (1.40) allows us to interpret the Hamiltonian H as the total energy of the system and p as the momentum. Hamilton's equation of motion, Equations (1.34) and (1.35), gives

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m},$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial V(x)}{\partial x},$$

Newton's law.

If we have a charged particle in an electromagnetic field, the situation is a bit more complex. The electric field $\vec{E}$ and the magnetic flux density $\vec{B}$ can be expressed by a vector potential $\vec{A}$ and a scalar potential ϕ as

$$\begin{aligned} \vec{E} &= -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t}, \\ \vec{B} &= \vec{\nabla} \times \vec{A}. \end{aligned} \tag{1.41}$$

The divergence of a magnetic flux density is zero, so it can be written as the curl of the vector, the well-known vector potential $\vec{A}$. In static, the curl of the electric field is zero, and it can be written as the gradient of a scalar function. In the time-varying case, the electric field and the magnetic field are related by the following Maxwell's equations:

$$\begin{aligned} \vec{\nabla} \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \cdot \vec{B} &= 0, \\ \vec{\nabla} \cdot \vec{D} &= \rho, \\ \vec{\nabla} \times \vec{H} &= \vec{J} + \frac{\partial \vec{D}}{\partial t}, \end{aligned} \tag{1.42}$$

with $\vec{D} = \varepsilon \vec{E}$ and $\vec{B} = \mu \vec{H}$. Here, $\vec{D}$ is the electric fulx density, $\vec{H}$ is the magnetic field, ρ is the charge density, $\vec{J}$ is the current density, ε is the permittivity, and μ is the permeability. We have used the international system of units (SI units) to write Maxwell's equation. From substituting Equation (1.41) into (1.42), we find that

$$\vec{\nabla} \times \left(\vec{E} + \frac{\partial \vec{A}}{\partial t} \right) = 0.$$

Then it is obvious that we have

$$\vec{E} + \frac{\partial \vec{A}}{\partial t} = -\vec{\nabla}\phi. \tag{1.43}$$

Equation (1.30) implies that the generalized force Q_i is defined by

$$Q_i = -\frac{\partial V}{\partial q_i} + \frac{d}{dt}\left(\frac{\partial V}{\partial \dot{q}_i}\right). \tag{1.44}$$

The force acting on the charged particle, called the Lorentz force, is

$$\vec{F} = e\left\{\vec{E} + \dot{\vec{r}} \times \vec{B}\right\}. \tag{1.45}$$

Substituting Equation (1.41) into Equation (1.45), we obtain

$$\vec{F} = e\left\{-\vec{\nabla}\left(\phi - \dot{\vec{r}} \cdot \vec{A}\right) - \frac{d\vec{A}}{dt}\right\}, \tag{1.46}$$

where we have used the following relation:

$$\dot{\vec{r}} \times (\vec{\nabla} \times \vec{A}) = \vec{\nabla}\left(\dot{\vec{r}} \cdot \vec{A}\right) - \left(\dot{\vec{r}} \cdot \vec{\nabla}\right)\vec{A}.$$

Equations (1.44) and (1.46) indicate that the generalized potential in the case of a charged particle moving in an electromagnetic field is given by

$$V = e\left(\phi - \dot{\vec{r}} \cdot \vec{A}\right), \tag{1.47}$$

and the corresponding Lagrangian is

$$L = \frac{1}{2}m\dot{\vec{r}}^2 + e\dot{\vec{r}} \cdot \vec{A} - e\phi. \tag{1.48}$$

The generalized canonical momentum is then

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = m\dot{x}_i + eA_i, \quad q_i = x_i, \tag{1.49}$$

and the Hamiltonian is given by

$$\begin{aligned} H &= \sum_i p_i \dot{q}_i - L \\ &= \sum_i (m\dot{x}_i + eA_i)\dot{x}_i - \frac{1}{2}m\dot{\vec{r}}^2 - e\dot{\vec{r}} \cdot \vec{A} + e\phi \\ &= \frac{1}{2}m\dot{\vec{r}}^2 + e\phi \\ &= \frac{\left(\vec{p} - e\vec{A}\right)^2}{2m} + e\phi. \end{aligned} \tag{1.50}$$

1.4 A ROAD TO QUANTUM MECHANICS

In classical mechanics, we dealt with functions of the coordinates q_i and momentum p_i such as energy; we describe these quantities collectively as "observable." The term "observable" describes any quantity accessible to the measurement processes. We assume that every physical observable is mathematically represented by a Hermitian operator, and every measurement of the physical observable will result in one of the eigenvalues of the corresponding Hermitian operator. The eigenvector is used to characterize the state of the physical system.

Quantum mechanics assumes that any arbitrary state of the physical system is characterized by a state vector that is not necessarily an eigenvector of any particular Hermitian operator. After a measurement has been performed, the state vector collapses to one of the eigenvectors with an eigenvalue E_n. If we describe the state of the system by a ket vector $|\Psi\rangle$, then we can represent this state vector by $|\Psi\rangle = \sum_n |E_n\rangle\langle E_n|\Psi\rangle$, where $|E_n\rangle$ is an eigenvector of a particular Hermitian operator corresponding to the measurement done on the system. How does $|\Psi\rangle$ relate to possible measurements when the result of a measurement must be one of the eigenvalues $\{E_n\}$? For this, we need the following postulate.

1.4.1 Postulate

The quantity $\langle\Psi|H|\Psi\rangle$ represents the average value of a series of measurements on an ensemble of systems that are all described by the state vector $|\Psi\rangle$ and is given by

$$\langle\Psi|H|\Psi\rangle = \sum_n |\langle E_n|\Psi\rangle|^2 E_n, \tag{1.51}$$

where $P_n = |\langle E_n|\Psi\rangle|^2$ is the probability of obtaining the value of E_n as a result of a measurement.

Previously, we described that in quantum mechanics the dynamical variables of classical mechanics are replaced by corresponding Hermitian operators. In classical mechanics, the dynamics of an observable are described by the Poisson bracket. We would like to extend the Poisson bracket to describe the dynamics of a quantum mechanical operator. The Poisson bracket for the classical observables A, B is defined in Equation (1.37) as

$$\{A,B\} = \sum_i \left\{ \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right\} = -\{B,A\}. \tag{1.37}$$

It is straightforward to show the following properties:

$$\{A+C,B\}=\{A,B\}+\{C,B\}, \tag{1.52a}$$

$$\{A,B+C\}=\{A,B\}+\{A,C\}, \tag{1.52b}$$

$$\{AB,C\}=\{A,C\}B+A\{B,C\}, \tag{1.53a}$$

$$\{A,BC\}=\{A,B\}C+B\{A,C\}. \tag{1.53b}$$

Let us assume that a quantum mechanical Poisson bracket is analogous to a classical one. So we assume that a quantum mechanical Poisson bracket satisfies all the conditions of Equations (1.37), (1.52), and (1.53). We shall denote the quantum mechanical Poisson bracket for operators $\hat{A}$ and $\hat{B}$ as $\left[\hat{A},\hat{B}\right]$. We use these conditions to determine the functional form of a quantum Poisson bracket by evaluating $\left[\hat{A}\hat{B},\hat{C}\hat{D}\right]$ in two different ways from Equation (1.53a,b):

$$\begin{aligned}\left[\hat{A}\hat{B},\hat{C}\hat{D}\right]&=\left[\hat{A},\hat{C}\hat{D}\right]\hat{B}+\hat{A}\left[\hat{B},\hat{C}\hat{D}\right]\\&=\left\{\left[\hat{A},\hat{C}\right]\hat{D}+\hat{C}\left[\hat{A},\hat{D}\right]\right\}\hat{B}+\hat{A}\left\{\left[\hat{B},\hat{C}\right]\hat{D}+\hat{C}\left[\hat{B},\hat{D}\right]\right\}\\&=\left[\hat{A},\hat{C}\right]\hat{D}\hat{B}+\hat{C}\left[\hat{A},\hat{D}\right]\hat{B}+\hat{A}\left[\hat{B},\hat{C}\right]\hat{D}+\hat{A}\hat{C}\left[\hat{B},\hat{D}\right],\end{aligned} \tag{1.54}$$

and

$$\begin{aligned}\left[\hat{A}\hat{B},\hat{C}\hat{D}\right]&=\left[\hat{A}\hat{B},\hat{C}\right]\hat{D}+\hat{C}\left[\hat{A}\hat{B},\hat{D}\right]\\&=\left\{\left[\hat{A},\hat{C}\right]\hat{B}+\hat{A}\left[\hat{B},\hat{C}\right]\right\}\hat{D}+\hat{C}\left\{\left[\hat{A},\hat{D}\right]\hat{B}+\hat{A}\left[\hat{B},\hat{D}\right]\right\}\\&=\left[\hat{A},\hat{C}\right]\hat{B}\hat{D}+\hat{A}\left[\hat{B},\hat{C}\right]\hat{D}+\hat{C}\left[\hat{A},\hat{D}\right]\hat{B}+\hat{C}\hat{A}\left[\hat{B},\hat{D}\right].\end{aligned} \tag{1.55}$$

Equating Equations (1.54) and (1.55), we obtain

$$-\left[\hat{A},\hat{C}\right]\left(\hat{B}\hat{D}-\hat{D}\hat{B}\right)+\left(\hat{A}\hat{C}-\hat{C}\hat{A}\right)\left[\hat{B},\hat{D}\right]=0. \tag{1.56}$$

Since the above condition holds for arbitrary Hermitian operators $\hat{A}$, $\hat{B}$, $\hat{C}$, and $\hat{D}$, we must have

$$\left[\hat{A},\hat{C}\right]=\left(\hat{A}\hat{C}-\hat{C}\hat{A}\right)\text{ and }\left[\hat{B},\hat{D}\right]=\left(\hat{B}\hat{D}-\hat{D}\hat{B}\right). \tag{1.57}$$

From now on, we shall call a quantum Poisson bracket a commutator. We further assume that a commutator or a quantum Poisson bracket is proportional to the corresponding classical Poisson bracket:

$$\left[\hat{A},\hat{B}\right]=i\hbar\{A,B\}, \tag{1.58}$$

where $\hbar$ is Planck's constant divided by 2π. This suggests that quantum mechanics is based on the assumption that the Poisson bracket assumes the same physical meaning and the same numerical values as in classical mechanics. In particular,

$$[\hat{q}_i,\hat{p}_j]=i\hbar\{q_i,p_j\}=i\hbar\delta_{ij}, \tag{1.59}$$

which is the fundamental quantum condition.

The time evolution of a quantum mechanical operator can be obtained from the equation of motion for the classical observable:

$$\frac{dF}{dt}=\frac{\partial F}{\partial t}+\{F,H\}, \tag{1.36}$$

$$\frac{d\hat{F}}{dt}=\frac{\partial\hat{F}}{\partial t}+\frac{1}{i\hbar}\left[\hat{F},\hat{H}\right], \tag{1.60}$$

where $\hat{H}$ is the energy operator corresponding to the classical Hamiltonian. Equation (1.60) is called the equation of motion in the Heisenberg picture. This particular quantum mechanical representation assumes that the operators vary with time, while the state vector $|\Psi\rangle$ is time independent. This picture is formally analogous to classical mechanics, since the equations of motion for the operators closely resemble the corresponding classical equations.

Now, let us study a different picture, called the Schrödinger picture, where the operators are constant in time, while the time variation is expressed by the state vectors. In this picture, the explicit time dependence of an operator still remains. Different quantum mechanical pictures follow from each other by a unitary transformation. From now on, we denote a quantum mechanical operator $\hat{A}$ simply as A when we don't need to distinguish it from the corresponding classical observable. Let us denote the state vector and operator in the new picture by $|\Psi'\rangle$ and A', respectively. Then, they are related to $|\Psi\rangle$ and A of an old picture by

$$|\Psi'\rangle=U|\Psi\rangle,\ A'=UAU^{\dagger} \tag{1.61}$$

and

$$\langle\Psi'|A'|\Psi'\rangle=\langle\Psi|U^{\dagger}UAU^{\dagger}U|\Psi\rangle=\langle\Psi|A|\Psi\rangle, \tag{1.62}$$

since

$$U^{\dagger}U = UU^{\dagger} = I, \tag{1.63}$$

when U is a unitary operator. Equation (1.62) indicates that the unitary transformation does not change the physical content of the theory. Also, we have

$$\begin{aligned}\frac{dA'}{dt} &= \frac{dU}{dt}AU^{\dagger} + U\frac{dA}{dt}U^{\dagger} + UA\frac{dU^{\dagger}}{dt} \\ &= \frac{dU}{dt}AU^{\dagger} + U\frac{\partial A}{\partial t}U^{\dagger} + \frac{1}{i\hbar}U[A,H]U^{\dagger} + UA\frac{dU^{\dagger}}{dt}.\end{aligned} \tag{1.64}$$

If A is not explicitly dependent on time, $\partial A/\partial t = 0$, and the operator A in the Schrödinger picture is time independent except for an explicit time dependence. This implies that

$$\frac{dA'}{dt} - U\frac{\partial A}{\partial t}U^{\dagger} = 0. \tag{1.65}$$

From Equations (1.64) and (1.65), we get

$$\begin{aligned}&\frac{dU}{dt}AU^{\dagger} + \frac{1}{i\hbar}U[A,H]U^{\dagger} + UA\frac{dU^{\dagger}}{dt} \\ &= \frac{dU}{dt}AU^{\dagger} + UA\frac{dU^{\dagger}}{dt} + \frac{1}{i\hbar}U(AH - HA)U \\ &= \frac{dU}{dt}U^{\dagger}A' + A'U\frac{dU^{\dagger}}{dt} + \frac{1}{i\hbar}(A'H' - H'A') \\ &= \left(\frac{dU}{dt}U^{\dagger} - \frac{1}{i\hbar}H'\right)A' + A'\left(U\frac{dU^{\dagger}}{dt} + \frac{1}{i\hbar}H'\right) \\ &= 0.\end{aligned} \tag{1.66}$$

Equation (1.66) should hold for any quantum mechanical operators A' in the Schrödinger picture, and, as a consequence, we have

$$i\hbar\frac{dU}{dt} = H'U. \tag{1.67}$$

Since $|\Psi'\rangle = U|\Psi\rangle$, we obtain the following Schrödinger equation for the state vector

$$i\hbar \frac{d}{dt}|\Psi'\rangle = H'|\Psi'\rangle. \tag{1.68}$$

The Schrödinger picture is perhaps the most widely used because it leads directly to the formulation of wave mechanics. In this picture, eigenvectors of the position operator q are used to represent the state vector of the system. We consider the continuous set of eigenvalues q' of the position operator q given by

$$q|q'\rangle = q'|q\rangle. \tag{1.69}$$

We assume that corresponding eigenvectors $\{|q'\rangle\}$ form a complete set. For simplicity, we consider the one-dimensional case only, but the extension to the higher dimensional case is straightforward. The position representation of the state vector is defined by

$$\Psi(q') = \langle q'|\Psi\rangle. \tag{1.70}$$

From Equation (1.59), the canonical momentum operator p and the position operator q satisfy the following quantum Poisson's bracket or the commutator relation

$$[q, p] = (qp - pq) = i\hbar, \tag{1.71}$$

and

$$(qp - pq)|\Psi\rangle = i\hbar|\Psi\rangle. \tag{1.72}$$

If we take an inner product of Equation (1.72) by the bra vector $\langle q'|$, we obtain

$$\langle q'|(qp - pq)|\Psi\rangle = q'\langle q'|p|\Psi\rangle - \langle q'|pq|\Psi\rangle. \tag{1.73}$$

Also,

$$\langle q'|(qp - pq)|\Psi\rangle = i\hbar\langle q'|\Psi\rangle. \tag{1.74}$$

Equations (1.73) and (1.74) are consistent only if the following condition is satisfied

$$\langle q'|p|\Psi\rangle = -i\hbar\frac{\partial}{\partial q'}\langle q'|\Psi\rangle = -i\hbar\frac{\partial}{\partial q'}\Psi(q'), \tag{1.75}$$

since Equation (1.75) implies

$$\langle q'|pq|\Psi\rangle = -i\hbar\frac{\partial}{\partial q'}(q'\Psi(q')). \tag{1.76}$$

Moreover, we have the following relations:

$$\langle q'|p|q''\rangle = -i\hbar\frac{\partial}{\partial q'}\langle q'|q''\rangle = -i\hbar\frac{\partial}{\partial q'}\delta(q'-q''), \tag{1.77}$$

and

$$I = \int_{-\infty}^{\infty} dq|q\rangle\langle q|. \tag{1.78}$$

Then, we get

$$\begin{aligned}\langle\Phi|\Psi\rangle &= \int_{-\infty}^{\infty} dq\langle\Phi|q\rangle\langle q|\Psi\rangle \\ &= \int_{-\infty}^{\infty} dq\ \Phi^*(q)\Psi(q),\end{aligned} \tag{1.79}$$

$$\begin{aligned}\langle\Phi|p|\Psi\rangle &= \int_{-\infty}^{\infty} dq'\int_{-\infty}^{\infty} dq''\langle\Phi|q'\rangle\langle q'|p|q''\rangle\langle q''|\Psi\rangle \\ &= \int_{-\infty}^{\infty} dq'\int_{-\infty}^{\infty} dq''\Phi^*(q')\left(-i\hbar\frac{\partial}{\partial q'}\delta(q'-q'')\right)\Psi(q'') \\ &= \int_{-\infty}^{\infty} dq'\int_{-\infty}^{\infty} dq''\left(i\hbar\frac{\partial}{\partial q'}\Phi^*(q')\right)\delta(q'-q'')\Psi(q'') \\ &= \int_{-\infty}^{\infty} dq'\left(i\hbar\frac{\partial}{\partial q'}\Phi^*(q')\right)\Psi(q'') \\ &= \int_{-\infty}^{\infty} dq'\Phi^*(q')\left(i\hbar\frac{\partial}{\partial q'}\right)\Psi(q''),\end{aligned} \tag{1.80}$$

and

$$\langle q'|F(q,p)|\Psi\rangle = F\left(q', -i\hbar\frac{\partial}{\partial q'}\right)\Psi(q'). \tag{1.81}$$

As a special case, we consider $F = H$, where H is the Hamiltonian of the system. Then the Schrödinger equation (1.68) becomes

$$i\hbar\frac{\partial}{\partial t}\Psi(q',t) = H(q',-i\hbar\partial/\partial q')\Psi(q',t), \tag{1.82}$$

of the wave mechanics.

As an example, we consider a particle moving in a one-dimensional potential $V(x)$. If we set the position operator as $q' = x$, the classical Hamiltonian is given by Equation (1.40):

$$H = \frac{p^2}{2m} + V(x).$$

Then, the corresponding Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t). \tag{1.83}$$

For three dimensions, we simply replace q' with $\vec{r}$ and $\partial/\partial q'$ with $\vec{\nabla}$. For example, the Schrödinger equation for a charged particle moving in an electromagnetic field is

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \frac{1}{2m}\left(-i\hbar\vec{\nabla} - e\vec{A}(\vec{r},t)\right)^2\Psi(\vec{r},t) + e\phi(\vec{r})\Psi(\vec{r},t). \tag{1.84}$$

When the Hamiltonian H is time independent, the time-dependent Schrödinger equation can be rewritten in time-independent form by trying the solution of the form

$$\Psi(\vec{r},t) = \exp(-iEt/\hbar)\psi_E(\vec{r}) \tag{1.85}$$

into Equation (1.83). Then, we obtain the following time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_E(\vec{r}) + V(\vec{r})\psi_E(\vec{r}) = E\psi_E(\vec{r}), \tag{1.86}$$

where E is the energy of the particle.

One can also consider the eigenvectors of the momentum operator p, which are given by

$$p|p'\rangle = p'|p'\rangle. \tag{1.87}$$

From

$$\langle q'|p|p'\rangle = -i\hbar\frac{\partial}{\partial q'}\langle q'|p'\rangle = p'\langle q'|p'\rangle, \tag{1.88}$$

we get

$$\langle q'|p'\rangle = C\exp(iq'p'/\hbar), \tag{1.89}$$

where C is a normalization constant. If we assume that $\langle p'|p''\rangle = \delta(p'-p'')$, then it is straightforward to calculate the normalization constant, which is given by $1/\sqrt{2\pi\hbar}$. As a consequence, we have

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(ixp/\hbar), \tag{1.90}$$

and

$$\langle \vec{r}|\vec{p}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\exp(i\vec{r}\cdot\vec{p}/\hbar). \tag{1.91}$$

1.5 THE UNCERTAINTY PRINCIPLE

The most remarkable property of quantum mechanics is that the measurements of different dynamical variables are not necessarily independent. This property was first formulated by Heisenberg, and is known as the uncertainty principle. We start with a quantum Poisson bracket for the position and momentum operators q and p,

$$[q,p] = i\hbar.$$

Let $|\Psi\rangle$ be a state vector, and $\bar{q}$ and $\bar{p}$ be the average values of the measurements of q and p, respectively:

$$\bar{q} = \langle\Psi|q|\Psi\rangle,\ \bar{p} = \langle\Psi|p|\Psi\rangle.$$

We now calculate the mean-square deviations of measured values,

$$\begin{aligned}(\Delta q)^2 &= \langle\Psi|(q-\bar{q})^2|\Psi\rangle \\ &= \langle\Psi|q^2|\Psi\rangle - (\langle\Psi|q|\Psi\rangle)^2,\end{aligned} \tag{1.92}$$

and

$$\begin{aligned}(\Delta p)^2 &= \langle\Psi|(p-\bar{p})^2|\Psi\rangle \\ &= \langle\Psi|p^2|\Psi\rangle - (\langle\Psi|p|\Psi\rangle)^2.\end{aligned} \tag{1.93}$$

We also define $\alpha = q - \bar{q}$ and $\beta = p - \bar{p}$, and we get

$$[\alpha,\beta] = [q,p] = i\hbar.$$

Also,

$$(\Delta\alpha)^2 = (\Delta q)^2 \text{ and } (\Delta\beta)^2 = (\Delta p)^2. \tag{1.94}$$

From Equation (1.94), we get

$$\begin{aligned}(\Delta q)^2(\Delta p)^2 &= (\Delta\alpha)^2(\Delta\beta)^2 \\ &= \langle\Psi|\alpha^2|\Psi\rangle\langle\Psi|\beta^2|\Psi\rangle \\ &\geq |\langle\Psi|\alpha\beta|\Psi\rangle|^2,\end{aligned} \tag{1.95}$$

from the Schwarz inequality. Since $\alpha\beta = 1/2(\alpha\beta - \beta\alpha) + 1/2(\alpha\beta + \beta\alpha)$, we also obtain

$$\begin{aligned}|\langle\Psi|\alpha\beta|\Psi\rangle|^2 &= \frac{1}{4}|\langle\Psi|[\alpha,\beta]|\Psi\rangle + \langle\Psi|(\alpha\beta+\beta\alpha)|\Psi\rangle|^2 \\ &\geq \frac{1}{4}|\langle\Psi|[\alpha,\beta]|\Psi\rangle|^2 = \frac{\hbar^2}{4}.\end{aligned} \tag{1.96}$$

Equations (1.95) and (1.96) give Heisenberg's famous uncertainty relation:

$$\Delta q \Delta p \geq \frac{\hbar}{2}. \tag{1.97}$$

1.6 THE HARMONIC OSCILLATOR

The one-dimensional simple harmonic oscillator is perhaps the most important and useful problem in quantum mechanics. The Lagrangian for the harmonic oscillator is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2. \tag{1.98}$$

The canonical momentum is

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}, \tag{1.99}$$

and the Hamiltonian becomes

$$H = p\dot{x} - L = \frac{p^2}{2m} + \frac{1}{2}kx^2. \tag{1.100}$$

The time-independent Schrödinger equation for the harmonic oscillator is then given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi = E\psi, \tag{1.101}$$

with the boundary condition $\psi = 0$ at $x = \pm\infty$. The solution of Equation (1.101) gives the energy eigenvalues of the harmonic oscillator and the eigenfunctions in terms of Hermite polynomials. In this section, we introduce an operator method that is based on the algebraic approach, and is much simpler than solving the Schrödinger directly. We introduce new operators

$$\begin{aligned} a &= \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x + ip), \\ a^\dagger &= \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x + ip), \\ \omega &= \sqrt{\frac{k}{m}}. \end{aligned} \tag{1.102}$$

From

$$aa^\dagger = \frac{1}{2m\hbar\omega}(m\omega x + ip)(m\omega x - ip),$$

$$a^\dagger a = \frac{1}{2m\hbar\omega}(m\omega x - ip)(m\omega x + ip),$$

we obtain

$$aa^\dagger - a^\dagger a = \frac{i}{\hbar}(px - xp) = \frac{i}{\hbar}(-i\hbar) = 1. \tag{1.103}$$

We also have

$$\begin{aligned} x &= \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^{\dagger}\right), \\ p &= i\sqrt{\frac{m\hbar\omega}{2}}\left(a^{\dagger} - a\right). \end{aligned} \tag{1.104}$$

Substituting Equation (1.104) into Equation (1.100), and using Equation (1.103), we get

$$\begin{aligned} H &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \\ &= \frac{(-1)}{2m}\left(\frac{m\omega\hbar}{2}\right)\left(a^{\dagger} - a\right)\left(a^{\dagger} - a\right) + \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}\left(a + a^{\dagger}\right)\left(a + a^{\dagger}\right) \\ &= \frac{\hbar\omega}{2}\left(aa^{\dagger} + a^{\dagger}a\right) \\ &= \hbar\omega\left(a^{\dagger}a + \frac{1}{2}\right). \end{aligned} \tag{1.105}$$

Let's assume that the state is in a particular eigenstate $|E'\rangle$ with eigenvalue E',

$$H|E'\rangle = E'|E'\rangle. \tag{1.106}$$

Now,

$$aH|E'\rangle = aE'|E'\rangle,$$

with $aH = a\hbar\omega\left(a^{\dagger}a + \frac{1}{2}\right)$. From $\left[a, a^{\dagger}\right] = 1$, we get $aa^{\dagger}a = a^{\dagger}aa + a$, and

$$aH|E'\rangle = Ha|E'\rangle + \hbar\omega a|E'\rangle = E'|E'\rangle. \tag{1.107}$$

Equation (1.107) can be rewritten as

$$Ha|E'\rangle = (E' - \hbar\omega)|E'\rangle. \tag{1.108}$$

In other words, if $|E'\rangle$ is an eigenstate of a harmonic oscillator Hamiltonian H with an eigenvalue E', $a|E'\rangle$ is also an eigenstate of H but with different eigenvalue $E' - \hbar\omega$.

By the way,

$$\begin{aligned}\langle E|H|E\rangle &= \hbar\omega\langle E|a^\dagger a|E\rangle + \frac{1}{2}\hbar\omega\langle E|E\rangle \\ &= E\langle E|E\rangle.\end{aligned} \tag{1.109}$$

Since

$$\begin{aligned}\langle E|E\rangle &= \int dq\langle E|q\rangle\langle q|E\rangle \\ &= \int dq|\langle E|q\rangle|^2 \\ &\geq 0,\end{aligned}$$

we have

$$\langle E|a^\dagger a|E\rangle = \int dq|\langle q|a|E\rangle|^2 \geq 0. \tag{1.110}$$

Combining Equations (1.109) and (1.110), the energy eigenvalue E must be a nonnegative number. On the other hand, Equation (1.108) indicates that the operation of an operator a on the energy eigenstate $|E\rangle$ lowers the energy eigenvalue by an amount $\hbar\omega$. Nonetheless, the energy eigenvalue must be always nonnegative, so the reduction of the eigenvalue must be terminated at the ground state $|E_0\rangle$, that is, $a|E_0\rangle = 0$, and as a result, we obtain

$$E_0 = \frac{1}{2}\hbar\omega. \tag{1.111}$$

Likewise,

$$a^\dagger H|E'\rangle = E'a^\dagger|E'\rangle,$$

and after some mathematical manipulations, we get

$$Ha^\dagger|E'\rangle = (E' + \hbar\omega)a^\dagger|E'\rangle. \tag{1.112}$$

This indicates that $a^\dagger|E'\rangle$ is also an eigenstate of H, but with a new eigenvalue $E' + \hbar\omega$. We can see that the operator $a^\dagger$ raises the eigenvalue by the amount of $\hbar\omega$. So if $|E_n\rangle$ is the nth eigenstate, one can generate $|E_n\rangle$ from $|E_0\rangle$ by n successive applications of $a^\dagger$,

$$|E_n\rangle = A_n\left(a^\dagger\right)^n |E_0\rangle, \tag{1.113}$$

where A_n is the normalization factor. The normalization factor A_n is determined from the condition

$$\langle E_n | E_n\rangle = 1$$

with the relations

$$\begin{aligned} a\left(a^\dagger\right)^n &= aa^\dagger\left(a^\dagger\right)^{n-1} \\ &= \left(a^\dagger\right)^{n-1} + a^\dagger a\left(a^\dagger\right)^{n-1} \\ &= \left(a^\dagger\right)^{n-1} + a^\dagger\left[\left(a^\dagger\right)^{n-2} + a^\dagger a\left(a^\dagger\right)^{n-2}\right] \\ &= 2\left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^2 a\left(a^\dagger\right)^{n-2} \\ &= n\left(a^\dagger\right) + \left(a^\dagger\right)^n a \end{aligned} \tag{1.114}$$

and

$$a^n\left(a^\dagger\right)^n = na^{n-1}(a^\dagger)^{n-1} + a^{n-1}(a^\dagger)^n a.$$

Then we obtain

$$\begin{aligned} \langle E_n | E_n\rangle &= A_n^2 \langle E_0 | a^n\left(a^\dagger\right)^n | E_0\rangle \\ &= nA_n^2 \langle E_0 | a^{n-1}\left(a^\dagger\right)^{n-1} | E_0\rangle \\ &= n!\, A_n^2 \langle E_0 | E_0\rangle \\ &= n!\, A_n^2 \\ &= 1. \end{aligned}$$

The normalization factor is

$$A_n = \frac{1}{\sqrt{n!}}$$

and the normalized eigenstate is

$$|E_n\rangle = \frac{\left(a^\dagger\right)^n}{\sqrt{n!}} |E_0\rangle. \tag{1.115}$$

From Equations (1.114) and (1.115), we get

$$\begin{aligned} a|E_n\rangle &= \frac{a(a^\dagger)^n}{\sqrt{n!}}|E_0\rangle \\ &= \frac{n(a^\dagger)^{n-1}}{\sqrt{n!}}|E_0\rangle \\ &= \sqrt{n}\,|E_{n-1}\rangle \end{aligned} \tag{1.116}$$

and

$$\begin{aligned} a^\dagger|E_n\rangle &= \frac{(a^\dagger)^{n+1}}{\sqrt{n!}}|E_0\rangle \\ &= \sqrt{n+1}\,|E_{n+1}\rangle. \end{aligned} \tag{1.117}$$

We call the operator a an annihilation operator because it destroys a single quantum of energy. The operator $a^\dagger$ is called a creation operator since it raises (or creates) a quantum of energy. The operator $a^\dagger a$ is called the number operator because if operating on the state, one can see that its eigenvalue is the number of energy quantum n,

$$a^\dagger a|E_n\rangle = a^\dagger\sqrt{n}\,|E_{n-1}\rangle = n|E_n\rangle. \tag{1.118}$$

The operator method can also be used to determine the wave function of the one-dimensional harmonic oscillator in the coordinate space. Since $a|E_0\rangle = 0$, from Equation (1.102), we have

$$\begin{aligned} \langle x|a|E_0\rangle &= \langle x|\left(\frac{m\omega}{\sqrt{2m\hbar\omega}}x + i\frac{1}{\sqrt{2m\hbar\omega}}p\right)|E_0\rangle \\ &= \sqrt{\frac{m\omega}{2\hbar}}x\langle x|E_0\rangle + \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x}\langle x|E_0\rangle \\ &= 0, \end{aligned} \tag{1.119}$$

where Equations (1.69) and (1.75) are used. If we denote $\psi_0(x) = \langle x|E_0\rangle$, then Equation (1.119) can be rewritten as

$$\frac{d}{dx}\psi_0(x) + \frac{m\omega x}{\hbar}\psi_0(x) = 0. \tag{1.120}$$

Solving the first-order differential equation is straightforward, and the solution is given by

$$\psi_0(x) = A\exp\left(-\frac{m\omega}{2\hbar}x^2\right), \tag{1.121}$$

where A is the normalization constant given by

$$A = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}. \tag{1.122}$$

In order to determine the normalization constant, we have used the condition

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2\, dx = 1, \tag{1.123}$$

and the Gaussian integral

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2) dx = \sqrt{\frac{\pi}{\alpha}}\ , \quad \alpha > 0. \tag{1.124}$$

The excited state wave functions can be obtained by successive application of a creation operator $a^\dagger$ on the state $|E_0\rangle$ and taking an inner product with the bra vector $\langle x|$. For example, the first excited state wave function is

$$\begin{aligned}
\psi_1(x) &= \langle x|a^\dagger|E_0\rangle \\
&= \langle x|\left(\sqrt{\frac{m\omega}{2\hbar}}x - i\frac{p}{\sqrt{2m\omega}}\right)|E_0\rangle \\
&= \sqrt{\frac{m\omega}{2\hbar}}x\psi_0(x) - \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x}\psi_0(x) \\
&= \sqrt{\frac{2m\omega}{\hbar}}x\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right),
\end{aligned} \tag{1.125}$$

and the nth state wave function is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right). \tag{1.126}$$

Here, $H_n(\zeta)$ is the Hermite polynomials, and the first few Hermite polynomials are

$$H_0(\zeta) = 1,\ H_1(\zeta) = 2\zeta,\ H_2(\zeta) = 4\zeta^2 - 2, \cdots \tag{1.127}$$

1.7 ANGULAR MOMENTUM EIGENSTATES

If the potential term $V(\vec{r})$ in the time-independent Schrödinger equation has a spherical symmetry, then the angular momentum $\vec{L} = \vec{r} \times \vec{p}$ is conserved. We need the following mathematical relations to prove the previous statement.

$$\begin{aligned}
\left(\vec{r}\times\vec{\nabla}\right)\cdot\left(\vec{r}\times\vec{\nabla}\right) &= \left\{\left(\vec{r}\times\vec{\nabla}\right)\times\vec{r}\right\}\cdot\vec{\nabla} - \vec{r}\cdot\left\{\left(\vec{r}\times\vec{\nabla}\right)\times\vec{\nabla}\right\} \\
&= \left\{-\vec{r}\left(\vec{\nabla}\cdot\vec{r}\right)+\vec{\nabla}\left(\vec{r}\cdot\vec{r}\right)\right\}\cdot\vec{\nabla} - \vec{r}\cdot\left\{-\vec{r}\left(\vec{\nabla}\cdot\vec{\nabla}\right)+\vec{\nabla}\left(\vec{r}\cdot\vec{\nabla}\right)\right\} \\
&= -3\vec{r}\cdot\vec{\nabla}+\vec{\nabla}\left(r^2\right)\cdot\nabla + r^2\nabla^2 - \left(\vec{r}\cdot\vec{\nabla}\right)\left(\vec{r}\cdot\vec{\nabla}\right) \\
&= -r\frac{\partial}{\partial r} + r^2\nabla^2 - r\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) \\
&= -r^2\frac{\partial^2}{\partial r^2} - 2r\frac{\partial}{\partial r} + r^2\nabla^2.
\end{aligned} \tag{1.128}$$

Here, we used the vector identity

$$\left(\vec{A}\times\vec{B}\right)\times\vec{C} = -\vec{A}\left(\vec{B}\cdot\vec{C}\right)+\vec{B}\left(\vec{C}\cdot\vec{A}\right) \tag{1.129}$$

and

$$\vec{r}\cdot\vec{\nabla} = r\frac{\partial}{\partial r}. \tag{1.130}$$

If we define the orbital angular momentum operator $\vec{L}$ as

$$\vec{L} = -i\hbar\vec{r}\times\vec{\nabla}, \tag{1.131}$$

then, from Equation (1.128), we obtain

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r^2} - \frac{\vec{L}\cdot\vec{L}}{\hbar^2 r^2}. \tag{1.132}$$

The time-independent Schrödinger equation (1.86) becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r^2} - \frac{\vec{L}\cdot\vec{L}}{\hbar^2 r^2}\right)\psi_E(\vec{r}) + V(r)\psi_E(\vec{r}) = E\psi_E(\vec{r}), \tag{1.133}$$

and the Hamiltonian with spherically symmetric potential is given by

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r^2} - \frac{\vec{L}\cdot\vec{L}}{\hbar^2 r^2}\right) + V(r)\ldots \tag{1.134}$$

The angular momentum operator can be written, component-wise, as

$$\begin{aligned} L_x &= \left(-i\hbar\vec{r}\times\vec{\nabla}\right)_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \\ L_y &= \left(-i\hbar\vec{r}\times\vec{\nabla}\right)_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \\ L_z &= \left(-i\hbar\vec{r}\times\vec{\nabla}\right)_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right), \end{aligned} \tag{1.135}$$

and they satisfy the following commutation relations

$$\begin{aligned} [L_y, L_z] &= i\hbar L_x, \\ [L_z, L_x] &= i\hbar L_y, \\ [L_x, L_y] &= i\hbar L_z. \end{aligned} \tag{1.136}$$

Now consider the infinitesimal rotation about the z-axis by an angle θ. The rotated coordinates are given by

$$\begin{aligned} x' &= x\cos\theta + y\sin\theta \approx x + \theta y, \\ y' &= -x\sin\theta + y\cos\theta \approx -\theta x + y, \\ z' &= z. \end{aligned} \tag{1.137}$$

Since the Hamiltonian is invariant under the rotation, we have

$$H\psi_E(x,y,z) = E\psi_E(x,y,z), \tag{1.138}$$

and

$$H\psi_E(x',y',z') = E\psi_E(x',y',z'). \tag{1.139}$$

Also, we have

$$\begin{aligned} \psi_E(x+\theta y, -\theta x + y, z) &= \psi_E(x,y,z) + \theta\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\psi_E(x,y,z) \\ &= \psi_E(x,y,z) - \frac{i\theta}{\hbar}L_z\psi_E(x,y,z). \end{aligned} \tag{1.140}$$

From Equations (1.138) to (1.140), we obtain

$$HL_z\psi_E = L_zH\psi_E,$$

or

$$[H, L_z] = 0. \tag{1.141}$$

In other words, the operators H and L_z share the same set of eigenfunctions. It is straightforward to show that

$$[L_z, L^2] = 0, \tag{1.142}$$

which implies that we can choose a common set of eigenfunctions for the operators H, L_z, L^2. Let's assume that the wave function $\psi_E(x,y,z)$ is given by

$$\psi_E(x,y,z) = R_E(r)Y_\lambda(\theta,\phi), \tag{1.143}$$

where (r,θ,ϕ) is a set of spherical coordinates, and $Y_\lambda(\theta,\phi)$ is a simultaneous eigenfunction of L_z and L^2 such that

$$\begin{aligned} L_zY_{lm}(\theta,\phi) &= m\hbar Y_{lm}(\theta,\phi), \\ L^2Y_{lm}(\theta,\phi) &= l(l+1)\hbar^2Y_{lm}(\theta,\phi), \\ Y_{lm}(\theta,\phi) &= \langle\theta,\phi|lm\rangle. \end{aligned} \tag{1.144}$$

By using the definition of the differential operator $\vec{\nabla}$

$$\begin{aligned} \vec{\nabla} &= \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} \\ &= \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{\partial}{r\partial\theta} + \hat{\phi}\frac{\partial}{r\sin\theta\partial\phi}, \end{aligned} \tag{1.145}$$

we get

$$\begin{aligned} \frac{\partial}{\partial x} &= \hat{x}\cdot\vec{\nabla} \\ &= \sin\theta\cos\phi\frac{\partial}{\partial r} + \cos\theta\cos\phi\frac{\partial}{r\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}, \end{aligned} \tag{1.146}$$

$$\begin{aligned} \frac{\partial}{\partial y} &= \hat{y}\cdot\vec{\nabla} \\ &= \sin\theta\sin\phi\frac{\partial}{\partial r} + \cos\theta\sin\phi\frac{\partial}{r\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}, \end{aligned} \tag{1.147}$$

and

$$\begin{aligned}\frac{\partial}{\partial z} &= \hat{z}\cdot\vec{\nabla} \\ &= \cos\theta\frac{\partial}{\partial r} - \sin\theta\frac{\partial}{r\partial\theta}.\end{aligned} \tag{1.148}$$

Then, by combining Equations (1.135) to (1.148), we obtain

$$\begin{aligned}L_x &= i\hbar\left[\cot\theta\cos\phi\frac{\partial}{\partial\phi} + \sin\phi\frac{\partial}{\partial\theta}\right], \\ L_y &= i\hbar\left[\cot\theta\sin\phi\frac{\partial}{\partial\phi} - \cos\phi\frac{\partial}{\partial\theta}\right], \\ L_z &= -i\hbar\frac{\partial}{\partial\phi}.\end{aligned} \tag{1.149}$$

We also define the ladder operators $L_\pm$ as

$$\begin{aligned}L_\pm &= L_x \pm L_y \\ &= \hbar\exp(\pm i\phi)\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right).\end{aligned} \tag{1.150}$$

Then, we get the following relations among operators:

$$\begin{aligned}[L_z, L_\pm] &= \pm\hbar L_\pm, \\ [L_+, L_-] &= 2\hbar L_z, \\ L_+L_- &= L^2 - L_z^2 + \hbar L_z, \\ L_-L_+ &= L^2 - L_z^2 - \hbar L_z, \\ (L_\pm)^\dagger &= L_\mp.\end{aligned} \tag{1.151}$$

This implies that

$$\begin{aligned}\langle lm|L_+L_-|lm\rangle &= \langle lm|L^2 - L_z^2 + \hbar L_z|lm\rangle \\ &= \hbar^2\big(l(l+1) - m^2 + m\big) \geq 0,\end{aligned}$$

and as a result

$$-l \leq m \leq l+1. \tag{1.152}$$

Similarly, we also have

$$-l \le m \le l, \tag{1.153}$$

from

$$\langle lm | L_- L_+ | lm \rangle \ge 0. \tag{1.154}$$

Also, we have

$$\langle lm | L^2 | lm \rangle = \hbar^2 l(l+1) \ge 0. \tag{1.155}$$

Next, consider $L_\pm |lm\rangle$. From $[L_z, L_\pm] = \pm\hbar L_\pm$, we get

$$\begin{aligned} L_z L_\pm |lm\rangle &= ([L_z,\ L_\pm] + L_\pm L_z)|lm\rangle \\ &= (L_\pm L_z \pm \hbar L_\pm)|lm\rangle \\ &= \hbar(m \pm 1)|lm\rangle. \end{aligned} \tag{1.156}$$

Thus, $L_\pm |lm\rangle$ are eigenstates of L_z with eigenvalues $m \pm 1$:

$$L_\pm |lm\rangle = c_\pm |lm \pm 1\rangle. \tag{1.157}$$

For this reason, we call $L_\pm$ the ladder operators, in particular, the angular momentum-raising and -lowering operators. The normalization constants $c_\pm$ are evaluated with the aid of Equation (1.151):

$$\begin{aligned} |c_\pm|^2 &= \langle lm | L_\mp L_\pm | lm \rangle \\ &= \hbar^2 (l(l+1) - m(m \pm 1)). \end{aligned} \tag{1.158}$$

If we take $c_\pm$ as positive, then we have the following expressions:

$$c_\pm = \hbar \sqrt{l(l+1) - m(m \pm 1)}. \tag{1.159}$$

In order to find the eigenfunction of the orbital angular momentum, we start with

$$\langle \theta, \phi | L_z | lm \rangle = -i\hbar \frac{\partial}{\partial \phi} \langle \theta, \phi | lm \rangle = \hbar m \langle \theta, \phi | lm \rangle, \tag{1.160}$$

which gives

$$\langle \theta, \phi | lm \rangle = e^{im\phi} \langle \theta, 0 | lm \rangle. \tag{1.161}$$

By the way, Equations (1.157) and (1.159) imply that

$$L_+ |ll\rangle = 0, \tag{1.162}$$

Or, from Equation (1.150),

$$\left(\frac{\partial}{\partial\theta} - l\cot\theta\right)\langle\theta,\phi|lm\rangle = 0. \tag{1.163}$$

Since the function $(\sin\theta)^l$ satisfies Equation (1.163), the orbital angular momentum eigenfunction has the following functional form:

$$\begin{aligned} Y_{ll}(\theta,\phi) &= \langle\theta,\phi|ll\rangle \\ &= \alpha e^{il\phi}(\sin\theta)^l. \end{aligned}$$

The normalization constant α is evaluated from the condition

$$\begin{aligned} 1 &= \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)|\alpha|^2 (\sin\theta)^{2l} \\ &= 2\pi|\alpha|^2 \int_{-1}^{1} du\left(1-u^2\right)^l \\ &= 2\pi|\alpha|^2 \frac{2^{2l+1}(l!)^2}{(2l)!(2l+1)}, \end{aligned} \tag{1.164}$$

which gives

$$Y_{ll}(\theta,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(2l)!}{4\pi}}e^{il\phi}(\sin\theta)^l. \tag{1.165}$$

Here, $(-1)^l$ is the conventional phase factor. In order to get $Y_{lm}(\theta,\phi)$, we apply L_- to Equation (1.165) $(l-m)$ times and from Equation (1.157) we obtain

$$Y_{im}(\theta,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}}\left(\frac{d}{d(\cos\theta)}\right)^{l-m}(\sin\theta)^l. \tag{1.166}$$

In mathematical physics, the function $Y_{lm}(\theta,\phi)$ is called as spherical harmonics.

1.8 QUANTIZATION OF ELECTROMAGNETIC FIELDS

There are cases where one needs to treat the electromagnetic field quantum mechanically, such as the spontaneous emission, the Lamb shift, the resonance florescence, and nonclassical light, such as squeezed states. Also, the fluctuation intensity of the laser near the threshold needs to be treated by the quantized electromagnetic fields. The classical electromagnetic fields are governed by Maxwell's equations (1.42). In most treatment of the quantized electromagnetic fields, unbound regions are considered, and vector potentials are used. In many applications, we are primarily considering the interaction between the laser radiation with electrons in atoms or quantum structures, such as the semiconductor quantum dot within the electric-dipole approximation. In such a case, it is convenient to develop the theory in a gauge-invariant form more appropriate for quantum electronics, emphasizing the electric and magnetic fields;

$$\begin{aligned} \vec{\nabla}\times\vec{H} &= \frac{\partial\vec{D}}{\partial t}, \\ \vec{\nabla}\times\vec{E} &= -\frac{\partial\vec{B}}{\partial t}, \\ \vec{\nabla}\cdot\vec{B} &= 0, \\ \vec{\nabla}\cdot\vec{E} &= 0, \end{aligned} \tag{1.167}$$

with $\vec{B}=\mu_0\vec{H}$ and $\vec{D}=\varepsilon_0\vec{E}$. We also take the electric field to have the spatial dependence appropriate for the cavity resonator with propagation axis in the z-direction such that [6]

$$E_x(z,t)=q(t)\left(\frac{2\Omega^2 M}{V\varepsilon_0}\right)^{1/2}\sin Kz \tag{1.168}$$

where V is the cavity volume, $K=\Omega/c$ is the wave number, M is the constant with the dimension of mass, and $q(t)$ is the quantum mechanical variable with the dimension of length. Then, from Maxwell's equations (1.167),

$$\begin{aligned} \vec{\nabla}\times\vec{H} &= -\hat{x}\frac{\partial H_y}{\partial z} \\ &= \hat{x}\varepsilon_0\dot{q}(t)\left(\frac{2\Omega^2 M}{V\varepsilon_0}\right)^{1/2}\sin Kz, \end{aligned} \tag{1.169}$$

we obtain the magnetic field

$$H_y(z,t) = \dot{q}(t)\frac{\varepsilon_0}{K}\left(\frac{2\Omega^2 M}{V\varepsilon_0}\right)^{1/2}\cos Kz. \tag{1.170}$$

The total electromagnetic energy contained in the cavity is then

$$\begin{aligned} H &= \frac{1}{2}\int_V dv\left\{\varepsilon_0 E_x^2 + \mu_0 H_y^2\right\} \\ &= \frac{1}{2}\int_V dv\left\{q^2(t)\frac{2\Omega^2 M}{V}\sin^2 Kz + \dot{q}^2(t)\frac{2M}{V}\cos^2 Kz\right\} \\ &= \frac{p^2(t)}{2M} + \frac{1}{2}M\Omega^2 q^2(t), \end{aligned} \tag{1.171}$$

where we have defined the generalized momentum $p(t) = M\dot{q}(t)$. By comparing Equation (1.105), we see that the total electromagnetic energy inside the cavity is the same as that of the simple harmonic oscillator with mass M and angular frequency Ω. We can now define the creation and annihilation operator for a single mode of electromagnetic field quanta denoted as a photon by

$$\begin{aligned} a(t) &= \frac{1}{\sqrt{2\hbar M\Omega}}(M\Omega q(t) + ip(t)), \\ a^\dagger(t) &= \frac{1}{\sqrt{2\hbar M\Omega}}(M\Omega q(t) - ip(t)). \end{aligned} \tag{1.171}$$

The quantization rule for the photon is then

$$[q,p] = i\hbar, \quad \left[a,a^\dagger\right] = 1. \tag{1.172}$$

We also have

$$a(t) = a(0)\exp(-i\Omega t), \quad a^\dagger(t) = a(0)\exp(-i\Omega t). \tag{1.173}$$

Then, the quantized electric field can be written as

$$E_x(z,t) = \left(a + a^\dagger\right)E_o \sin Kz, \tag{1.174}$$

where E_o is the electric field per photon. The total electromagnetic energy contained in the cavity is

$$H = \hbar\Omega(a\ a + 1/2), \tag{1.175}$$

and the n-photon state in which n photons is defined as $|n\rangle$, where each photon has an energy $\hbar\Omega$. We interpret the vacuum state $|0\rangle$ as a state which contains no photon. Photons are quanta of a single mode of the electromagnetic fields, and are not localized at any particular position within the cavity. Rather, they are spread out over the entire cavity. The quantized electromagnetic fields seem to offer amazingly satisfying accounts of a very wide range of radiative phenomena, and there is no real need to have a corpuscular theory of photons.

When there is more than one mode of electromagnetic fields in the cavity, the electromagnetic fields can be expanded by multi-modes

$$\begin{aligned} \bar{E}(z,t) &= x\sum_n q_n(t)\left(\frac{2\Omega_n^2 M_n}{V\varepsilon_0}\right)^{1/2}\sin K_n z, \\ \bar{H}(z,t) &= y\sum_n \dot{q}_n(t)\frac{\varepsilon_0}{K_n}\left(\frac{2\Omega_n^2 M_n}{V\varepsilon_0}\right)^{1/2}\cos K_n z, \end{aligned} \tag{1.176}$$

with $\Omega_n = n\pi c/L$, $K_n = n\pi/L$, and L is the length of the cavity. The total electromagnetic energy contained in the cavity is

$$H = \frac{1}{2}\sum_n\left(M_n\Omega_n^2 q_n^2 + \frac{p_n^2}{M_n}\right), \tag{1.177}$$

and

$$[q_n, p_{n'}] = i\hbar\delta_{n,n'}, \quad [q_n, q_{n'}] = [p_n, p_{n'}] = 0. \tag{1.178}$$

The annihilation and creation operators for the mode n are

$$\begin{aligned} a_n(t) &= (2\hbar M_n\Omega_n)^{-1/2}(M_n\Omega_n q_n(t) + ip_n(t)), \\ a_n^\dagger(t) &= (2\hbar M_n\Omega_n)^{-1/2}(M_n\Omega_n q_n(t) - ip_n(t)), \end{aligned} \tag{1.179}$$

and a quantized electric field is given by

$$E_x(z,t) = \sum_n\left(a_n + a_n^\dagger\right)E_n\sin K_n z. \tag{1.180}$$

For a mode s, we have

$$a_s^\dagger a_s\,|n_s\rangle = \hbar\Omega_s\,|n_s\rangle.$$

The general eigenstate of H has n_1 photons in the first mode, n_2 in the second, n_s in the sth, and so forth, and can be written as

$$\begin{aligned} |n_1 n_2 \ldots n_s \ldots\rangle &\equiv |\{n_s\}\rangle \\ &= |n_1\rangle |n_2\rangle \ldots |n_s\rangle \ldots \end{aligned} \tag{1.181}$$

The annihilation operator a_s destroys a photon in the n_s mode alone:

$$a_s |n_1 n_2 \ldots n_s \ldots\rangle = \sqrt{n_s}\, |n_1 n_2 \ldots n_s - 1 \ldots\rangle. \tag{1.182}$$

The general state vector for the field is a superposition of these eigenstates:

$$|\psi\rangle = \sum_{n_1, n_2, \ldots n_s, \ldots} C_{n_1 n_2 \ldots n_s \ldots} |n_1 n_2 \ldots n_s \ldots\rangle. \tag{1.183}$$

This state includes the correlations between different field modes and is called an entangled state. The entangled state arises from perturbations such as the atom-field interaction coupled by an electric-dipole interaction.

1.9 PERTURBATION THEORY

In this section, we deal systematically with the technique for calculating the effect of small extra potential, or Hamiltonian H', acting on a system governed mainly by a free Hamiltonian H_0. Suppose for simplicity that our unperturbed Hamiltonian H_0 governs the noninteracting system with

$$H_0 |\Psi_0\rangle = E_0 |\Psi_0\rangle, \tag{1.184}$$

and the corresponding eigenstate is normalized. When the perturbation is applied, we shall need to solve the equation

$$(E - H_0)|\Psi\rangle = H'|\Psi\rangle. \tag{1.185}$$

Provided we make no condition on the normalization of the new eigenstate $|\Psi\rangle$, we may always split it into two terms [3]

$$|\Psi\rangle = |\Psi_0\rangle + |\Phi\rangle, \tag{1.186}$$

where the change due to the perturbation is to be orthogonal to the unperturbed state:

$$\langle \Psi_0 | \Phi \rangle = 0. \tag{1.187}$$

This condition can be expressed by the formal introduction of projection operator P:

$$P = |\Psi_0\rangle\langle\Psi_0|, \tag{1.188}$$

which acts on any quantum state $|\Phi\rangle$ as

$$P|\Phi\rangle = |\Psi_0\rangle\langle\Psi_0|\Phi\rangle.$$

The complementary projection operator is defined as

$$Q = 1 - P. \tag{1.189}$$

The complementary operator is idempotent, that is, $Q^2 = Q$, as in the case of P, and it projects any state upon the manifold in Hilbert space that is orthogonal to $|\Psi_0\rangle$. Then one can see that, from Equations (1.186) and (1.187), one can write

$$Q|\Psi\rangle = |\Phi\rangle. \tag{1.190}$$

Applying the unperturbed Hamiltonian operator to this function, we get

$$\begin{aligned} QH_0|\Phi\rangle &= H_0|\Phi\rangle - |\Psi_0\rangle\langle\Psi_0|H_0|\Phi\rangle \\ &= H_0|\Phi\rangle - E_0|\Psi_0\rangle\langle\Psi_0|\Phi\rangle \\ &= H_0|\Phi\rangle \\ &= H_0 Q|\Phi\rangle, \end{aligned} \tag{1.191}$$

showing that Q commutes with H_0. The one we write

$$(E - H_0)|\Psi\rangle = (E - E_0)|\Psi_0\rangle + (E - H_0)|\Phi\rangle, \tag{1.192}$$

$$Q(E - H_0)|\Psi\rangle = (E - H_0)Q|\Psi\rangle = (E - H_0)|\Phi\rangle, \tag{1.193}$$

and from Equations (1.185) and (1.193), we obtain

$$(E - H_0)|\Phi\rangle = QH'|\Psi\rangle. \tag{1.194}$$

Applying P to Equation (1.185), we get

$$E = E_0 + \langle \Psi_0 | H' | \Psi \rangle. \tag{1.195}$$

Equation (1.194) can also be written as

$$|\Phi\rangle = (E - H_0)^{-1} QH' |\Psi\rangle, \tag{1.196}$$

which implies that there is an operator $(E - H_0)^{-1}$ which is the inverse of $(E - H_0)$. Then, Equations (1.185), (1.186), and (1.192) can be combined into

$$|\Psi\rangle = |\Psi_0\rangle + (E - H_0)^{-1} QH' |\Psi\rangle. \tag{1.197}$$

This is an exact equation, but can only be solved approximately by iteration. Thus

$$\begin{aligned} |\Psi\rangle &= |\Psi_0\rangle + (E - H_0)^{-1} QH' \Big(|\Psi_0\rangle + (E - H_0)^{-1} QH' |\Psi\rangle \Big) \\ &= |\Psi_0\rangle + (E - H_0)^{-1} QH' |\Psi_0\rangle \\ &\quad + (E - H_0)^{-1} QH' (E - H_0)^{-1} QH' |\Psi_0\rangle + \cdots. \end{aligned} \tag{1.198}$$

This series is known as the Brillouin-Wigner perturbation expansion. Let $\{|\Psi_n\rangle\}$ be the complete eigenset of the free Hamiltonian H_0, then we have

$$\sum_n |\Psi_n\rangle\langle\Psi_n| = I, \tag{1.199}$$

and

$$Q|\Psi_n\rangle = |\Psi_n\rangle, \quad n \neq 0. \tag{1.200}$$

Thus from Equations (1.195) to (1.200), we obtain the energy equation (1.195), and represent all states and operators in eigenstates of H_0. We get

$$\begin{aligned} E &= E_0 + \langle\Psi_0|H'|\Psi\rangle \\ &= E_0 + \langle\Psi_0|H'\left(|\Psi_0\rangle + \frac{1}{E - H_0} QH' |\Psi_0\rangle + \cdots \right) \\ &= E_0 + \langle\Psi_0|H'|\Psi_0\rangle + \sum_n \langle\Psi_0|(E - H_0)^{-1} |\Psi_n\rangle\langle\Psi_n| QH' |\Psi_0\rangle + \cdots \\ &= E_0 + \langle\Psi_0|H'|\Psi_0\rangle + \sum_{n \neq 0} \frac{|\langle\Psi_0|H'|\Psi_n\rangle|^2}{E - E_n} + \cdots. \end{aligned} \tag{1.201}$$

The projection operator Q automatically excludes certain matrix elements from the summations in each term of the series. It is an implicit equation to be solved for E. Consider the very simple case where H' couples just two states of nearly equal energy. If the expectation value of H' is zero in each of these states, we get

$$E = E_0 + \frac{|\langle \Psi_0 | H' | \Psi_1 \rangle|^2}{E - E_1} = E_0 + \frac{|H'_{01}|^2}{E - E_1}, \tag{1.202}$$

which has two roots to be obtained from the equation

$$E^2 - (E_0 + E_1)E + E_0 E_1 - |H'_{01}|^2 = 0. \tag{1.203}$$

Note that this is the same as the solution of the determinantal equation for the degenerate or nearly degenerate Rayleigh-Schrödinger perturbation theory, that is

$$\begin{vmatrix} E - E_0 & H'_{01} \\ H'_{10} & E - E_1 \end{vmatrix} = 0. \tag{1.204}$$

PROBLEMS

1. We consider the ket vector $|a\rangle$ represented by a column vector given by

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_\infty \end{pmatrix},$$

with complex quantities $a_1, a_2, a_3, \ldots, a_\infty$, and the bra vector given by $\langle b| = \begin{pmatrix} b_1^* & b_2^* & b_3^* \ldots . b_\infty^* \end{pmatrix}$. The outer product of vectors $|a\rangle$ and $|b\rangle$ is defined by

$$|a\rangle\langle b| = \begin{pmatrix} a_1 b_1^* & a_1 b_2^* & \cdots & a_1 b_\infty^* \\ a_2 b_1^* & a_2 b_2^* & \cdots & a_2 b_\infty^* \\ \vdots & \vdots & \ddots & \vdots \\ a_\infty b_1^* & a_\infty b_2^* & \cdots & a_\infty b_\infty^* \end{pmatrix}.$$

In two-dimensional Hilbert space, the basis vectors are given by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The Pauli operators are defined by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Obtain the spectral representation of Puali operators from Equation (1.25).

2. If A and B are two fixed noncommuting operators, and λ is a parameter, then show that

$$\exp(\lambda A) B \exp(-\lambda A) = B + \lambda[a,b] + \frac{\lambda^2}{2!}[A,[A,B]] + \frac{\lambda^3}{3!}[A,[A,[A,B]]] + \cdots.$$

When $[A,[A,B]] = [B,[A,B]] = 0$, show that

$$\exp(A+B) = \exp(A)\exp(B)\exp\left(-\frac{1}{2}[A,B]\right).$$

Hint: Consider the operator function $f(\lambda) = \exp(\lambda A)\exp(\lambda B)$, and differentiate $f(\lambda)$ with respect to λ to obtain $df(\lambda)/d\lambda = (A + \exp(\lambda A) B \exp(-\lambda A)) f(\lambda)$, and solve the differential equation.

3. In one dimension, the Hamiltonian is given by $\hat{H} = \hat{p}^2/2m + V(\hat{x})$. Let $|E_n\rangle$ be the eigenvector of $\hat{H}$, and E_n be the eigenvalue. Then show that

$$\sum_{n'} |\langle E_{n''}|\hat{x}|E_{n'}\rangle|^2 (E_{n'} - E_{n''}) = \frac{\hbar^2}{2m}.$$

4. In two-dimensional Hilbert space, the basis vectors are given by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

When the Hamiltonian of this two-dimensional system is given by

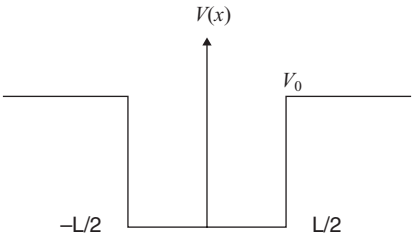

Figure 1.1. Finite potential well.

$$H = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1| + V(|1\rangle\langle 0| + |0\rangle\langle 1|),$$

find eigenvectors and eigenvalues of H.

5. A one-dimensional harmonic oscillator is under the electric field F, and the total Hamiltonian is given by $H = p^2/2m + \frac{1}{2}\omega^2 x^2 - eFx$. Using the perturbation theory equation (1.201), calculate the ground state energy.

6. Find the wave functions and the energy levels of a particle in the potential well given by $V(x) = 0$ if $|x| \le L/2$ and $V(x) = V_0 > 0$ if $|x| > L/2$ (Fig. 1.1).

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