

# Introduction

The fundamentals of nonrelativistic quantum mechanics will be summarized to lay a foundation for understanding more advanced concepts in relativistic quantum mechanics and scattering theory. Dirac's elegant notation is used to highlight the orthogonality and completeness properties of eigenstates of physical observables and to stress the importance of transformation theory through the use of Dirac transformation coefficients and unitary operators. The Schrödinger equation is embedded in a unitary time translation operator, and the Schrödinger, Heisenberg, and Dirac-interaction pictures are reviewed. Notation conventions and units are also discussed in this introductory chapter.

## 1.A Principles of Quantum Mechanics

To begin let us briefly review the principles of nonrelativistic quantum mechanics stated in Dirac notation:

i. A physical system is characterized by a state vector  $|\psi\rangle$  in a normed linear vector space (Hilbert space) with the corresponding coordinate-space wave function  $\psi(x) = \langle x | \psi \rangle$ . The probability density  $|\psi(x)|^2 = \psi^*(x)\psi(x) \geq 0$  of finding the system at  $x$  in state  $|\psi\rangle$  has physical significance. In rigorous terms, it can be shown that the absolute square of the norm  $|\psi|^2 = \langle \psi | \psi \rangle$  has the coordinate-space representation

$$\langle \psi | \psi \rangle = \int dx \langle \psi | x \rangle \langle x | \psi \rangle = \int dx |\psi(x)|^2 \quad (1.1)$$

and can be chosen as unity for a stable system.

ii. Every physical observable is represented by a linear hermitian operator which, under suitable mathematical restrictions, has real eigenvalues. The hamiltonian operator  $H$  with real energy eigenvalues  $E_n$  is a case in point:

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \quad (1.2)$$

where the eigenvectors  $|\psi_n\rangle$  are orthogonal:  $\langle\psi_n|\psi_m\rangle = 0$  if  $E_n \neq E_m$ . The free-particle hamiltonian is  $H = \mathbf{p}^2/2m$ , and the momentum operator has the coordinate-space representation  $\mathbf{p} = -i\hbar\nabla$ .

iii. If two state vectors  $|\psi_1\rangle$  and  $|\psi_2\rangle$  can govern the state of the system, then the superposition principle guarantees that  $|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$  does also. In terms of eigenstates, the superposition principle states that  $|\psi\rangle$  can be represented by the eigenstate expansion

$$|\psi\rangle = \sum_n c_n|\psi_n\rangle, \quad (1.3)$$

where  $c_n = \langle\psi_n|\psi\rangle$ . The discrete eigenstates  $|\psi_n\rangle$  are sometimes written as  $|n\rangle$  in analogy with the continuous basis  $|x\rangle$ . Since these bases are in no way fundamental, expansion theorems like (1.1) and (1.3) can be used to transform the system from one representation to another.

iv. The time development of the state vectors  $|\psi(t)\rangle$  is governed by the Schrödinger equation (Schrödinger 1926)

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle. \quad (1.4)$$

An alternative but equivalent picture is the time development of the operators  $O$ , given by the Heisenberg equation of motion (Heisenberg 1925)

$$i\hbar \frac{dO}{dt} = [O, H] = OH - HO. \quad (1.5)$$

Unless otherwise specified, we shall assume that operators  $O$  and  $H$  do not contain any explicit time dependence.

v. There is an hermitian probability current corresponding to a particle velocity  $\mathbf{p}/m$  with density

$$\mathbf{j}(\mathbf{x}, t) = -\frac{i\hbar}{2m} [\psi^*(\mathbf{x}, t)\nabla\psi(\mathbf{x}, t) - (\nabla\psi^*(\mathbf{x}, t))\psi(\mathbf{x}, t)], \quad (1.6)$$

which can be combined with the probability density  $|\psi(\mathbf{x}, t)|^2$  in a continuity equation

$$\frac{\partial}{\partial t} |\psi(\mathbf{x}, t)|^2 + \nabla \cdot \mathbf{j} = 0. \quad (1.7)$$

This insures that the physical requirement of probability conservation is satisfied.

vi. Spin- $\frac{1}{2}$  fermions (e.g., electrons) must obey the *exclusion principle* (Pauli 1925). This corresponds to a wave function describing the combined state of two electrons which is antisymmetric under interchange of the electrons,

$$\psi_{n_1, n_2}(x_1, x_2) = -\psi_{n_1, n_2}(x_2, x_1). \quad (1.8)$$

The extension of (1.8) to all pairs of half-integer fermions along with the analogous symmetric property for pairs of identical integer-spin bosons (e.g., photons) under interchange is referred to as “the connection between spin and statistics”. Its proof goes beyond the bounds of nonrelativistic quantum mechanics (Pauli 1940), and so we assume it as a basic postulate.

**Connection with Classical Physics.** The foregoing six postulates are sufficient to develop a complete quantum mechanics, the significance of which is clarified by the following principles:

- a. The *correspondence principle* (Bohr 1923) notes that the predictions of quantum mechanics approach the classical limit as either  $\hbar \rightarrow 0$  or the quantum numbers of bound systems become large,  $n \rightarrow \infty$ .
- b. The *uncertainty principle* (Heisenberg 1927) relates the inherent spread of finite wave packets with respect to position or time and in the Fourier-transform variable,  $\Delta x \Delta k \gtrsim 1$ ,  $\Delta t \Delta \omega \gtrsim 1$  (valid for Maxwell waves as well as Schrödinger waves), with the scales set by  $\hbar$  via the de Broglie and Planck relations,  $p = \hbar k$ ,  $E = \hbar \omega$ . This results in the uncertainty products  $\Delta x \Delta p \gtrsim \hbar$ ,  $\Delta t \Delta E \gtrsim \hbar$ .
- c. The *complementarity principle* (Bohr 1928) states that any given experiment can probe either the wave or particle nature of radiation or matter, but not both together.

These principles are linked to the fundamental postulates via the probability interpretation of  $|\psi|^2$ . The significance of  $\psi$  itself, however, as a material “matter wave” as opposed to a statistical measure of the behavior of an ensemble of particles, is a debated question. Nevertheless it is generally accepted that the physical consequence of the theory is to add to classical physics the four purely quantum effects: uncertainty-principle “jittering”, quantum-mechanical “tunneling”, discrete energy levels of bound systems, and “exclusion-principle repulsion” for identical fermions or “symmetrization-induced attraction” for identical bosons.

**Units.** We shall henceforth adhere to the convention (unless otherwise stated) that  $\hbar = c = 1$ . This reduces the three fundamental units of length, time, and mass to only one, e.g., mass. To convert from one form of this basic unit to another, it will be convenient to use  $\hbar = 0.658 \times 10^{-15}$  eV-sec, or  $\hbar c = 1973$  eV-Å = 197.3 MeV-fm, where  $c = 3 \times 10^{10}$  cm/sec. We shall also use rationalized electromagnetic units, so that the dimensionless fine-structure constant is  $\alpha = e^2/4\pi = 1/137$ . See Appendix I.

## 1.B Angular-Momentum Expansions

**Transformation Coefficients.** Given the postulates of Section 1.A, it is useful to condense many of the results of nonrelativistic quantum mechanics in terms of the transformation coefficients  $c_n$  in (1.3). Consider, for example, the hermitian orbital-angular-momentum operator  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ , with eigenstates

$|lm\rangle$  satisfying

$$L^2 |lm\rangle = l(l+1) |lm\rangle, \quad (1.9)$$

$$L_3 |lm\rangle = m |lm\rangle \quad (1.10)$$

for nonnegative integers  $l$ , where the  $2l+1$  integral values of  $m$  range from  $-l$  to  $l$ . These eigenstates obey the formal completeness relation

$$\sum_{l,m} |lm\rangle \langle lm| = 1 \quad (1.11)$$

in Hilbert space, which means that

$$\langle a|b\rangle = \sum_{l,m} \langle a|lm\rangle \langle lm|b\rangle. \quad (1.12)$$

They are also orthonormal,

$$\langle l'm'|lm\rangle = \delta_{l'l} \delta_{m'm}, \quad (1.13)$$

which is equivalent to the solid-angle integral ( $\hat{\mathbf{r}} \cdot \hat{\mathbf{r}} = 1$ )

$$\delta_{l'l} \delta_{m'm} = \int d\Omega_r \langle l'm'|\hat{\mathbf{r}}\rangle \langle \hat{\mathbf{r}}|lm\rangle = \int d\Omega_r Y_l^{m'*}(\hat{\mathbf{r}}) Y_l^m(\hat{\mathbf{r}}), \quad (1.14)$$

where the surface spherical harmonic  $Y_l^m(\hat{\mathbf{r}})$  can be chosen to correspond to the transformation coefficient  $\langle \hat{\mathbf{r}}|lm\rangle$ ,

$$Y_l^m(\hat{\mathbf{r}}) = \langle \hat{\mathbf{r}}|lm\rangle. \quad (1.15)$$

We shall henceforth follow the CSR phase convention (Condon and Shortley 1951, Rose 1957)  $Y_l^{m*} = (-)^m Y_l^{-m}$  with  $Y_l^{\pm 1} = \mp (3/8\pi)^{1/2} \hat{\mathbf{r}} \cdot (\hat{\mathbf{x}} \pm i\hat{\mathbf{y}})$  and  $Y_1^0 = (3/4\pi)^{1/2} \hat{\mathbf{r}} \cdot \hat{\mathbf{z}}$ . These transformation coefficients then satisfy the addition theorem for spherical harmonics (a group-theory derivation of which is given in Chapter 2),

$$\sum_m \langle \hat{\mathbf{r}}|lm\rangle \langle lm|\hat{\mathbf{r}}'\rangle = \sum_m Y_l^{m*}(\hat{\mathbf{r}}') Y_l^m(\hat{\mathbf{r}}) = \frac{2l+1}{4\pi} P_l(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}}), \quad (1.16)$$

where  $P_l(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}})$  is the usual Legendre polynomial and is a function of only the direction cosine  $\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}} = \cos \theta$ .

The utility of such transformation coefficients arises from the following fact. Given just a few of them, such as (1.15) along with [the phase  $i^l$  in (1.18)] will be explained in Chapter 6]

$$\langle \hat{\mathbf{p}}|lm\rangle = Y_l^m(\hat{\mathbf{p}}), \quad (1.17)$$

$$\langle \mathbf{r}|r'lm\rangle = i^l Y_l^m(\hat{\mathbf{r}}) \delta(r' - r)/r, \quad (1.18)$$

$$\langle \mathbf{p}|p'lm\rangle = Y_l^m(\hat{\mathbf{p}}) \delta(p' - p)/p, \quad (1.19)$$

$$\langle r'l'm'|p'lm\rangle = 4\pi p r j_l(pr) \delta_{l'l} \delta_{m'm}, \quad (1.20)$$

where  $j_l(pr)$  is the usual spherical Bessel function, a whole host of familiar angular-momentum expansion theorems can be read off, e.g.,

$$\begin{aligned}\delta^2(\hat{\mathbf{r}}' - \hat{\mathbf{r}}) &= \langle \hat{\mathbf{r}}' | \hat{\mathbf{r}} \rangle = \sum_{l,m} \langle \hat{\mathbf{r}}' | lm \rangle \langle lm | \hat{\mathbf{r}} \rangle \\ &= (4\pi)^{-1} \sum_l (2l+1) P_l(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}}),\end{aligned}\quad (1.21)$$

$$\begin{aligned}\delta^3(\mathbf{r}' - \mathbf{r}) &= \langle \mathbf{r}' | \mathbf{r} \rangle = \sum_{l,m} \int \langle \mathbf{r}' | r'' lm \rangle dr'' \langle r'' lm | \mathbf{r} \rangle \\ &= \frac{\delta(r' - r)}{4\pi r^2} \sum_l (2l+1) P_l(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}}),\end{aligned}\quad (1.22)$$

$$\begin{aligned}e^{i\mathbf{p} \cdot \mathbf{r}} &= \langle \mathbf{r} | \mathbf{p} \rangle = \sum_{l'm'm'} \iint \langle \mathbf{r} | r'' lm \rangle dr'' \langle r'' lm | p'' l' m' \rangle \\ &\quad \times dp'' \langle p'' l' m' | \mathbf{p} \rangle \\ &= \sum_l (2l+1) i^l j_l(pr) P_l(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}).\end{aligned}\quad (1.23)$$

In practice the knowledge of (1.21)–(1.23) serves to define (1.15) and (1.17)–(1.20). The latter coefficients are then a useful tool with which to study other angular-momentum expansions, as we shall shortly demonstrate.

**Normalization.** As an aside it should be noted that (1.20) and (1.23) define our normalization convention. The factor  $(2\pi)^3$  in the delta-function representation

$$\int d^3r e^{i\mathbf{p} \cdot \mathbf{r}} = (2\pi)^3 \delta^3(\mathbf{p}) \quad (1.24)$$

appears only in momentum space with our conventions, i.e.,

$$\langle \mathbf{r}' | \mathbf{r} \rangle = \delta^3(\mathbf{r}' - \mathbf{r}), \quad \langle \mathbf{p}' | \mathbf{p} \rangle = (2\pi)^3 \delta^3(\mathbf{p}' - \mathbf{p}). \quad (1.25)$$

To streamline the notation a bit, we parallel the convention  $\hbar = h/2\pi$  and define

$$\delta^3(\mathbf{p}) \equiv (2\pi)^3 \delta^3(\mathbf{p}), \quad d^3p \equiv d^3p/(2\pi)^3, \quad (1.26a)$$

for then

$$\int d^3p \delta^3(\mathbf{p}) = \int d^3p \delta^3(\mathbf{p}) = 1. \quad (1.26b)$$

A similar convention will be used in  $n$  dimensions, with the crossed notation referring to an appropriate factor of  $(2\pi)^n$  associated with  $\delta^n(\mathbf{p})$  and  $d^n p$ .

This notation becomes extremely useful if we also normalize plane-wave solutions for a free particle of momentum  $p$  in a box of volume  $V$ ,

$$\langle \mathbf{r} | \psi_{\mathbf{p}} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{p} \cdot \mathbf{r}}, \quad (1.27)$$

for then the probability of the particle being somewhere in the box is unity. We can, of course, identify (1.27) with (1.23) by setting  $V = 1$ . The advantage of using (1.27) will be apparent when calculating physical rates, lifetimes, or cross sections. The normalization volume  $V$  cancels out of the quantity of physical interest; any unphysical quantity will vanish or become infinitely large as  $V \rightarrow \infty$ . If we had employed the continuum normalization with periodic boundary conditions, then  $V \rightarrow (2\pi)^3$ , and typical scattering amplitudes would contain as many as 12 powers of  $2\pi$ , sometimes a bewildering situation indeed! Use of box normalization goes a long way toward “keeping the factors of  $2\pi$  straight”. One further modification, covariant box normalization, will be useful for relativistic particles. It will be discussed in Chapters 3–5 and used extensively in the latter part of this book.

**Selection Rules.** Returning to the discussion of angular-momentum transformation coefficients, we observe that if the hamiltonian is independent of  $L$  or depends only upon  $L^2$ , then (1.5) implies

$$i \frac{d\mathbf{L}}{dt} = [\mathbf{L}, H] = 0, \quad (1.28)$$

i.e.,  $\mathbf{L}$  is conserved. As a consequence of (1.28) we have

$$0 = \langle l'm | [H, L^2] | lm \rangle = [l'(l' + 1) - l(l + 1)] \langle l'm | H | lm \rangle,$$

$$0 = \langle l'm' | [H, L_3] | lm \rangle = (m' - m) \langle l'm' | H | lm \rangle,$$

which leads to the angular-momentum selection rule

$$\langle l'm' | H | lm \rangle \propto \delta_{l'l} \delta_{m'm}. \quad (1.29)$$

The scattering operator  $S$ , called the  $S$ -matrix, is the scattering analog to  $H$  in the sense that energy conservation (magnitude of momentum conservation in the one-body nonrelativistic scattering case) and angular-momentum conservation lead to a selection rule similar to (1.29):

$$\langle p'l'm' | S | plm \rangle = S_l(p) \delta(p' - p) \delta_{l'l} \delta_{m'm}. \quad (1.30)$$

We shall have much more to say about the  $S$ -matrix later. Note now that the “reduced matrix element”  $S_l(p)$  is independent of the  $L_3$  eigenvalue  $m$ ; this will be verified in Section 2.C. For the moment we may treat (1.30) as another transformation coefficient like (1.15) or (1.17)–(1.20) and thus compute (suppressing summation indices and integrals)

$$\begin{aligned} \langle \mathbf{p}' | S | \mathbf{p} \rangle &= \sum \langle \mathbf{p}' | p'l'm' \rangle \langle p'l'm' | S | plm \rangle \langle plm | \mathbf{p} \rangle \\ &= \frac{(2\pi)^3 \delta(p' - p)}{4\pi p^2} \sum_l (2l + 1) S_l(p) P_l(\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}). \end{aligned} \quad (1.31)$$

The factor  $(2\pi)^3$  in (1.31) is consistent with our momentum normalization. When  $S_l(p)$  is expressed as a phase  $\exp(2i\delta_l(p))$ , the relation (1.31) is referred to as the partial-wave or phase-shift expansion. It is hoped that the reader

appreciates the transparent simplicity of (1.31) when the transformation-coefficient technique is applied. A similar pattern is valid for other operator eigenfunction expansions.

## 1.C Unitary Operators and Transformation Theory

While no mention of unitary operators was made in the postulates of quantum mechanics in Section 1.A, they nevertheless play a significant role in the theory. If two observers view the state of a quantum system as  $|\psi\rangle$  and  $|\psi'\rangle$ , respectively, then they must of necessity measure the same quantum probability. The “off-diagonal” version of this statement is that for  $|\psi\rangle$  and  $|\psi'\rangle$  to have the same probability overlap to the respective states  $\langle\phi|$  and  $\langle\phi'|$ , then

$$|\langle\phi'|\psi'\rangle|^2 = |\langle\phi|\psi\rangle|^2. \quad (1.32)$$

**Unitary Operators.** There are two solutions of (1.32), the obvious one being

$$\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle. \quad (1.33)$$

This leads naturally to a unitary operator  $U = U^{\dagger-1}$  (where the adjoint operation  $\dagger$  corresponds to transposition and complex conjugation of finite-dimensional matrices) which transforms the state  $|\psi\rangle$  to the state  $|\psi'\rangle$  as

$$|\psi'\rangle = U|\psi\rangle. \quad (1.34)$$

The relation (1.33) then follows from (1.34), the unitary property of  $U$ , and the adjoint property

$$\langle\phi'| = \langle U\phi| = \langle\phi|U^\dagger. \quad (1.35)$$

The latter is linked to the linearity of  $U$ ,

$$U|\alpha_1\psi_1 + \alpha_2\psi_2\rangle = \alpha_1 U|\psi_1\rangle + \alpha_2 U|\psi_2\rangle, \quad (1.36)$$

where  $\alpha_{1,2}$  are complex numbers.

**Antiunitary Operators.** The second solution of (1.32) is

$$\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle^* \quad (1.37a)$$

$$= \langle\psi|\phi\rangle. \quad (1.37b)$$

The solution of (1.37a) is

$$|\psi'\rangle = A|\psi\rangle, \quad (1.38)$$

where  $A$  is again unitary,  $A^\dagger A = I$ , but now “antilinear”, satisfying instead of (1.36),

$$A|\alpha_1\psi_1 + \alpha_2\psi_2\rangle = \alpha_1^* A|\psi_1\rangle + \alpha_2^* A|\psi_2\rangle. \quad (1.39)$$

The antilinear analog of (1.35), consistent with the solution (1.37a), is

$$\langle\phi'| = \langle A\phi| = \langle\phi|.A^\dagger, \quad (1.40)$$

where  $A$  operating to the left corresponds to

$$\langle \phi | .A | \psi \rangle = \langle A^\dagger \phi | \psi \rangle^* \quad (1.41)$$

and the dot in  $.A$  is sometimes omitted. In effect we can replace the unitary-antilinear operator  $A$  (henceforth referred to as antiunitary) by a purely unitary operator  $U$  (now meaning unitary-linear) and a complex conjugation operator  $K$ , i.e.,  $A = UK$ . It is also possible to define an antiunitary operator in a slightly different manner, following the form (1.37b) rather than (1.37a), but we shall not pursue this possibility in detail.

**Transformations.** The *active* interpretation of (1.34) or (1.38), without reference to any observers, is that  $U$  (or  $A$ ) represents the physical transformation which converts  $|\psi\rangle$  to  $|\psi'\rangle$ . As such,  $U$  (or  $A$ ) is the primary quantity of interest in transformation theory. In particular, we can investigate the action of  $U$  (or  $A$ ) on operators by generalizing (1.33) and (1.37a) to

$$\langle \phi' | O' | \psi' \rangle = \langle \phi | O | \psi \rangle \quad (1.42)$$

for unitary transformations and

$$\langle \phi' | O' | \psi' \rangle = \langle \phi | O | \psi \rangle^* \quad (1.43)$$

for antiunitary transformations. Owing to the properties (1.35) and (1.40), (1.42) and (1.43) imply the same operator behavior

$$U^\dagger O' U = O, \quad A^\dagger O' A = O. \quad (1.44)$$

The unitary property of both  $U$  and  $A$  then leads to

$$O' = U O U^{-1}, \quad O' = A O A^{-1} \quad (1.45)$$

in the two cases, both equations taking the form of similarity transformations from  $O$  to  $O'$ . It may be recalled that such similarity transformations as (1.45) leave the form of operator equations unchanged except in the case of complex numbers in the latter equation because the antilinearity of  $A$  means complex conjugation of "c-numbers", as in (1.39). For example, the commutation relation  $[X, Y] = iZ$  would become  $[X', Y'] = -iZ'$ , for antiunitary transformations. A case in point would be the behavior of the commutator  $[x, p_x] = i$  under various transformations, thus determining the unitary or antiunitary nature of those transformations.

Next, consider the case where the operator  $O$  is left invariant by the transformation, i.e.,  $O' = O$  in (1.45). One may then conclude that

$$[U, O] = 0. \quad (1.46)$$

However antiunitary operators will not obey (1.46), because, as we shall see, invariance under an antiunitary operation will not mean  $O' = O$ .

**Infinitesimal Generators.** Let us now consider in more detail unitary (unitary-linear) transformations dependent upon a small parameter  $\varepsilon$  and

evolving continuously from the identity. In this case we may write

$$U_\varepsilon = 1 - i\varepsilon G, \quad (1.47)$$

where  $G$  is called the *infinitesimal generator* of the transformation. Clearly a unitary  $U_\varepsilon = U_\varepsilon^\dagger^{-1}$  implies an hermitian  $G = G^\dagger$ . Applying (1.47) to the operator transformation  $O' = UOU^\dagger$  leads to

$$O' = O - i\varepsilon[G, O], \quad (1.48)$$

so that if  $G$  commutes with  $O$ , then  $O$  is left unchanged by the transformation,  $O' = O$ . If  $O$  as well as  $G$  is hermitian, both operators could be physical observables and  $[G, O] = 0$  would then imply that  $G$  and  $O$  are simultaneously measurable.

For noninfinitesimal unitary transformations ( $\varepsilon \rightarrow \lambda$ ), (1.47) can be exponentiated:

$$U_\lambda = e^{-i\lambda G}. \quad (1.49)$$

By use of the operator Taylor series expansion

$$\begin{aligned} e^{-i\lambda G} O e^{i\lambda G} &= O - i\lambda[G, O] + \frac{(-i\lambda)^2}{2!} [G, [G, O]] \\ &+ \frac{(-i\lambda)^3}{3!} [G, [G, [G, O]]] + \dots, \end{aligned} \quad (1.50)$$

which follows by differentiating the left-hand side of (1.50) with respect to  $\lambda$ , the form  $U_\lambda O U_\lambda^\dagger$  can be evaluated and  $O'$  is thus generalized from (1.48) to (1.50) for noninfinitesimal values of the parameter  $\lambda$ .

## 1.D Translations in Time

**Time-Translation Operator.** The dynamical development of states governed by the Schrödinger equation can be recast in the form of a unitary transformation. For time-dependent states ( $\partial_t = \partial/\partial t$ )

$$(i\partial_t - H)|\psi(t)\rangle = 0, \quad (1.51)$$

a time translation of  $|\psi(t)\rangle$  means, according to (1.34), that we may define a time-translation operator by

$$|\psi(t')\rangle = U(t', t)|\psi(t)\rangle, \quad (1.52)$$

where  $U(t', t)$  is unitary,  $U^{-1} = U^\dagger$ . Moreover  $U$  obeys the fundamental "closure" property,

$$U(t', t) = U(t', t'')U(t'', t), \quad (1.53)$$

stating that two successive time translations constitute a time translation. In order to determine the explicit form of  $U$ , one notes from (1.52) that

$U(t, t) = 1$ . For  $t' = t + \delta t$ , it is therefore clear that  $U(t'; t)$  evolves continuously from the identity, and following (1.47), one writes

$$U(t + \delta t, t) = 1 - iH \delta t, \quad (1.54)$$

where the infinitesimal parameter  $\delta t$  in (1.54) is required by (1.53). Then the infinitesimal generator of time translations can be identified as the hamiltonian of (1.51). In fact, (1.54) indicates that  $U$  itself satisfies a Schrödinger equation

$$(i\partial_t - H)U(t, t_0) = 0. \quad (1.55)$$

To proceed further, one must make a dynamical assumption concerning  $H$ . If the physical states are isolated between observations, then  $H$  is independent of  $t$  and (1.54) can be exponentiated to

$$U(t', t) = e^{-i(t'-t)H}. \quad (1.56a)$$

If instead the system is not isolated between observations, then  $H$  may be explicitly time dependent. In this case the differential equation (1.55) and the boundary condition  $U(t_0, t_0) = 1$  can be combined into an integral equation

$$U(t, t_0) = 1 - i \int_{t_0}^t dt' H(t')U(t', t_0),$$

which can be iterated successively (plug  $U = 1$  into the integral to approximate  $U$ , etc.) to form the time-ordered infinite series ( $t_1 \geq t_2 \geq \dots \geq t_n$ )

$$U(t', t) = 1 + \sum_{n=1}^{\infty} (-i)^n \int_t^{t'} dt_1 \int_t^{t_1} dt_2 \cdots \int_t^{t_{n-1}} dt_n H(t_1)H(t_2) \cdots H(t_n). \quad (1.56b)$$

Clearly (1.56b) becomes (1.56a) if  $H$  is time independent; alternatively if  $H(t)$  commutes with  $H(t')$ , then the upper limits  $t_1, \dots, t_n$  in (1.56b) can be extended to  $t'$  (accompanied by a factor of  $1/n!$  due to a change of integration regions—see Chapter 7), leading to

$$U(t', t) = \exp \left( -i \int_t^{t'} dt'' H(t'') \right). \quad (1.56c)$$

Then again (1.56a) follows as a special case of (1.56c).

**Time-Development Pictures.** The above formulation of time development makes no mention of the time dependence of observable operators (other than  $H$ ). The time evolution of states  $|\psi(t)\rangle_S$ , combined with time-independent observables  $O_S$ , is referred to as the Schrödinger picture. An alternative but equivalent dynamical scheme, called the Heisenberg picture, involves stationary states  $|\psi\rangle_H$  along with observables  $O_H(t)$  which change with time according to the Heisenberg equation of motion (1.5). More

specifically we may choose

$$|\psi(t)\rangle_S = |\psi(t)\rangle, \quad |\psi\rangle_H = |\psi(t_0)\rangle \quad (1.57a)$$

$$O_S = O(t_0), \quad O_H(t) = O(t), \quad (1.57b)$$

with  $t_0$  a fixed time ( $t = t_0$ ). These two pictures are related by

$$|\psi\rangle_H = U^{-1}(t, t_0)|\psi(t)\rangle_S \quad (1.58a)$$

$$\langle\psi_H|O_H(t)|\psi_H\rangle = \langle\psi_S(t)|O_S|\psi_S(t)\rangle, \quad (1.58b)$$

where (1.58a) follows from (1.52), and (1.58b) is in the spirit of (1.42). Combining (1.58a) and (1.58b) leads to the similarity transformation relating the observables in the two pictures,

$$O_H(t) = U^{-1}(t, t_0)O_S U(t, t_0). \quad (1.59)$$

**Interaction Picture.** There is a third picture, called the Dirac or interaction picture, which makes use of the decomposition  $H = H_0 + V$  with observables  $O_I(t)$  dynamically driven by  $H_0$  and states  $|\psi(t)\rangle_I$  driven by  $V$ . In particular one defines

$$|\psi(t)\rangle_I = e^{iH_0 t} |\psi(t)\rangle, \quad (1.60)$$

which removes the  $e^{-iH_0 t}$  dependence from  $|\psi(t)\rangle_I$ . Given (1.51),  $|\psi(t)\rangle_I$  satisfies a Schrödinger equation driven only by  $V$ ,

$$(i\partial_t - V_I(t))|\psi(t)\rangle_I = 0 \quad (1.61)$$

with  $V_I$  in turn driven only by  $H_0$ ,

$$V_I(t) = e^{iH_0 t} V e^{-iH_0 t} \quad (1.62)$$

[note that the general identity (1.50) may be applied to (1.62)]. In fact (1.62) is one example of the general similarity transformation relating any observable in the interaction and Schrödinger pictures ( $V_S = V$ ), obtained from (1.60) and the connection between matrix elements in the two pictures,

$$\langle\psi_I(t)|O_I(t)|\psi_I(t)\rangle = \langle\psi_S(t)|O_S|\psi_S(t)\rangle. \quad (1.63)$$

Finally, we may define a unitary time translation operator in the interaction picture,  $U_I(t', t)$  [similar in nature to the Schrödinger-picture operator  $U_S(t', t) = U(t', t)$ ]:

$$|\psi(t')\rangle_I = U_I(t', t)|\psi(t)\rangle_I. \quad (1.64)$$

Like (1.61),  $U_I$  obeys

$$(i\partial_t - V_I(t))U_I(t, t_0) = 0, \quad (1.65)$$

which, like (1.56b), can be iterated to the general time-ordered form

$$U_I(t', t) = 1 + \sum_{n=1}^{\infty} (-i)^n \int_t^{t'} dt_1 \int_t^{t_1} dt_2 \cdots \int_t^{t_{n-1}} dt_n V_I(t_1)V_I(t_2) \cdots V_I(t_n). \quad (1.66)$$

The interaction picture will play a fundamental role in the general formulation of the scattering problem discussed in Chapter 7. Even earlier in Chapter 6, however, we will make frequent use of the scattering operator

$$S_I = U_I(t' = \infty, t = -\infty). \quad (1.67)$$

This is a form of the  $S$ -matrix which explicitly shows, as in (1.66), that  $S$  contains all the dynamics of the hamiltonian. For systems with no hamiltonian defined, which is usually the case in elementary-particle physics,  $S$  continues to describe the dynamics of the interaction.

The material presented in this chapter is intended only as a brief review of the fundamentals of quantum mechanics needed as a basis for this book. For a more detailed exposition of this subject, the reader is referred to Pauli (1933), Ludwig (1954), Kramers (1957), Mandl (1957), Dirac (1958), Landau and Lifshitz (1958), Messiah (1962), Feynman et al. (1965), Gottfried (1966), Tomanaga (1966), Matthews (1968), Schiff (1968), Merzbacher (1970), Gasiorowicz (1974), and Mathews and Venkatesan (1976).