Chapter 7

Unitary Dynamics

7.1 The Schrödinger Equation

The equations of motion of classical Hamiltonian dynamics are of the form

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}, \tag{7.1}$$

where x_1, x_2, etc. are the (generalized) coordinates, p_1, p_2, etc. their conjugate momenta, and $H(x_1, p_1, x_2, p_2, \ldots)$ is the Hamiltonian function on the classical phase space.

In the case of a particle moving in one dimension, there is only a single coordinate x and a single momentum p, and the Hamiltonian is the total energy

$$H = p^2/2m + V(x), \tag{7.2}$$

with $V(x)$ the potential energy. The two equations of motion are then:

$$dx/dt = p/m, \quad dp/dt = -dV/dx. \tag{7.3}$$

For a harmonic oscillator $V(x)$ is $\frac{1}{2}Kx^2$, and the general solution of (7.3) is given in (2.1), where $\omega = \sqrt{K/m}$.

The set of equations (7.1) is deterministic in that there is a unique trajectory or orbit $\gamma(t)$ in the phase space as a function of time which passes through γ_0 at $t = 0$. Of course, the orbit is also determined by giving the point in phase space through which it passes at some time other than $t = 0$. The orbit for a harmonic oscillator is an ellipse in the phase plane; see Fig. 2.1 on page 9.

The quantum analog of (7.1) is *Schrödinger's equation*, which in Dirac notation can be written as

$$i\hbar \frac{d}{dt}|\psi_t\rangle = H|\psi_t\rangle, \tag{7.4}$$

where H is the quantum Hamiltonian for the system, a Hermitian operator which may itself depend upon the time. This is a linear equation, so that if $|\phi_t\rangle$ and $|\omega_t\rangle$ are any two solutions, the linear combination

$$|\chi_t\rangle = \alpha|\phi_t\rangle + \beta|\omega_t\rangle \tag{7.5}$$

is also a solution, where α and β are arbitrary (time-independent) constants. Equation (7.4) is deterministic in the same sense as (7.1): a given $|\psi_0\rangle$ at $t = 0$ gives rise to a unique solution $|\psi_t\rangle$ for all values of t. The result is a *unitary dynamics* for the quantum system in a sense made precise in Sec. 7.3 below.

The Hamiltonian H in (7.4) must be an operator defined on the Hilbert space $\mathcal{H}$ of the system one is interested in. This will be true for an *isolated system*, one which does not interact with anything else—imagine something inside a completely impermeable box. It will also be true if the interaction of the system with the outside world can be approximated by an operator acting only on $\mathcal{H}$. For example, the system may be located in an external magnetic field which is effectively "classical", that is, does not have to be assigned its own quantum mechanical degrees of freedom, and thus enters the Hamiltonian H simply as a parameter.

One is sometimes interested in the dynamics of an *open* (in contrast to isolated) subsystem $\mathcal{A}$ of a composite system $\mathcal{A} \otimes \mathcal{B}$ when there is a significant interaction between $\mathcal{A}$ and $\mathcal{B}$. Of course (7.4) can be applied to the total composite system, assuming that it is isolated. However, there is no comparable equation for the subsystem $\mathcal{A}$, as it cannot, at least in general, be described by its own wave function, and its dynamical evolution is influenced by that of the other subsystem $\mathcal{B}$, often referred to as the *environment* of $\mathcal{A}$. Constructing dynamical equations for open subsystems is a topic which lies outside the scope of this book, although Ch. 15 on density matrices provides some preliminary hints on how to think about open subsystems.

For a particle in one dimension moving in a potential $V(x)$, (7.4) is equivalent to the partial differential equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi \tag{7.6}$$

for a wavepacket $\psi(x,t)$ which depends upon the time as well as the position variable x. The Hamiltonian in this case is the linear differential operator

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{7.7}$$

In general it is much more difficult to find solutions to (7.6) than it is to integrate (7.3). A formal solution to (7.6) for a harmonic oscillator is given in (7.23) below.

One way to think about (7.4) is to choose an orthonormal basis $\{|j\rangle, j = 1, 2, \ldots\}$ of the Hilbert space $\mathcal{H}$ which is *independent of the time t*. Then (7.4) is equivalent to a set of ordinary differential equations, one for each j:

$$i\hbar\frac{d}{dt}\langle j|\psi_t\rangle = \langle j|H|\psi_t\rangle. \tag{7.8}$$

This is a somewhat less abstract than (7.4), because both $\langle j|\psi_t\rangle$ and $\langle j|H|\psi_t\rangle$ are simply complex numbers which depend upon t, thus complex-valued functions of the time. By writing $|\psi_t\rangle$ as a linear combination of the basis vectors,

$$|\psi_t\rangle = \sum_j |j\rangle\langle j|\psi_t\rangle = \sum_j c_j(t)|j\rangle, \tag{7.9}$$

with time-dependent coefficients $c_j(t)$, and expressing the right side of (7.8) in the form

$$\langle j|H|\psi_t\rangle = \sum_k \langle j|H|k\rangle\langle k|\psi_t\rangle, \tag{7.10}$$

one finds that the Schrödinger equation is equivalent to a collection of coupled linear differential equations

$$i\hbar\, dc_j/dt = \sum_k \langle j|H|k\rangle c_k \tag{7.11}$$

for the $c_j(t)$. The operator H, and therefore also its matrix elements, can be a function of the time, but it must be a Hermitian operator at every time, i.e., for any j and k,

$$\langle j|H(t)|k\rangle = \langle k|H(t)|j\rangle^*. \tag{7.12}$$

When $\mathcal{H}$ is two-dimensional, (7.11) has the form

$$\begin{aligned} i\hbar\, dc_1/dt &= \langle 1|H|1\rangle c_1 + \langle 1|H|2\rangle c_2, \\ i\hbar\, dc_2/dt &= \langle 2|H|1\rangle c_1 + \langle 2|H|2\rangle c_2. \end{aligned} \tag{7.13}$$

These are linear equations, and if H, and thus its matrix elements, is independent of time, one can find the general solution by diagonalizing the matrix of coefficients on the right side. Let us assume that this has already been done, since we earlier made no assumptions about the basis $\{|j\rangle\}$, apart from the fact that it is independent of time. That is, assume that

$$H = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|, \tag{7.14}$$

so that the off-diagonal terms $\langle 1|H|2\rangle$ and $\langle 2|H|1\rangle$ in (7.13) vanish, while the diagonal terms are E_1 and E_2. Then the general solution of (7.13) is of the form

$$c_1(t) = b_1 e^{-iE_1 t/\hbar}, \quad c_2(t) = b_2 e^{-iE_2 t/\hbar}, \tag{7.15}$$

where b_1 and b_2 are arbitrary (complex) constants.

The precession of the spin angular momentum of a spin-half particle placed in a constant magnetic field is an example of a two-level system with a time-independent Hamiltonian. If the magnetic field is $\boldsymbol{B} = (B_x, B_y, B_z)$, the Hamiltonian is

$$H = -\gamma(B_x S_x + B_y S_y + B_z S_z), \tag{7.16}$$

where the spin operators S_x, etc., are defined in the manner indicated in (5.30), and γ is the gyromagnetic ratio of the particle in suitable units. This Hamiltonian will be diagonal in the basis $|w^+\rangle$, $|w^-\rangle$, see (4.14), where w is in the direction of the magnetic field $\boldsymbol{B}$.

The preceding example has an obvious generalization to the case in which a time-independent Hamiltonian is diagonal in an orthonormal basis $\{|e_n\rangle\}$:

$$H = \sum_n E_n |e_n\rangle\langle e_n|. \tag{7.17}$$

Then a general solution of Schrödinger's equation has the form

$$|\psi_t\rangle = \sum_n b_n e^{-iE_n t/\hbar} |e_n\rangle, \tag{7.18}$$

where the b_n are complex constants. One can check this by evaluating the time derivative

$$i\hbar\frac{d}{dt}|\psi_t\rangle = \sum_n b_n E_n e^{-iE_n t/\hbar}|e_n\rangle, \tag{7.19}$$

and verifying that it is equal to $H|\psi_t\rangle$. An alternative way of writing (7.18) is

$$|\psi_t\rangle = \exp\bigl(-itH/\hbar\bigr)\,|\psi_0\rangle, \tag{7.20}$$

where $|\psi_0\rangle$ is $|\psi_t\rangle$ when $t = 0$. The operator $\exp\bigl(-itH/\hbar\bigr)$ is defined in the manner indicated in Sec. 3.10, see (3.97). It can be written down explicitly as

$$\exp\bigl(-itH/\hbar\bigr) = \sum e^{-iE_n t/\hbar}|e_n\rangle\langle e_n|. \tag{7.21}$$

In the case of a harmonic oscillator, with

$$E_n = (n + 1/2)\hbar\omega \tag{7.22}$$

the energy and $|\phi_n\rangle$ the eigenstate of the n'th level, (7.18) is equivalent to

$$\psi(x,t) = (e^{-i\omega t/2})\sum_n b_n e^{-in\omega t}\phi_n(x), \tag{7.23}$$

where $\phi_n(x)$ is the position wave function corresponding to the ket $|\phi_n\rangle$.

A particular case of (7.18) is that in which $b_n = \delta_{np}$, that is, all except one of the b_n vanish, so that

$$|\psi_t\rangle = e^{-iE_p t/\hbar}|e_p\rangle. \tag{7.24}$$

The only time dependence comes in the phase factor, but since two states which differ by a phase factor have exactly the same physical significance, a quantum state with a precisely defined energy, known as a *stationary state*, represents a physical situation which is completely independent of time. By contrast, a classical system with a precisely defined energy will typically have a non-trivial time dependence; e.g., a harmonic oscillator tracing out an ellipse in the classical phase plane.

The inner product $\langle\omega_t|\psi_t\rangle$ of any two solutions of Schrödinger's equation in independent of time. Thus $|\psi_t\rangle$ satisfies (7.8), while the complex conjugate of this equation with ψ_t replaced by ω_t is

$$-i\hbar\frac{d}{dt}\langle\omega_t|j\rangle = \langle\omega_t|H|j\rangle, \tag{7.25}$$

where $H^\dagger$ on the right side has been replaced with H, since the Hamiltonian (which could depend upon the time) is Hermitian. Using (7.8) along with (7.25), one arrives at the result

$$\begin{aligned} i\hbar\frac{d}{dt}\langle\omega_t|\psi_t\rangle &= i\hbar\sum_j \frac{d}{dt}\langle\omega_t|j\rangle\langle j|\psi_t\rangle \\ &= \sum_j \langle\omega_t|j\rangle\langle j|H|\psi_t\rangle - \sum_j \langle\omega_t|H|j\rangle\langle j|\psi_t\rangle = 0, \end{aligned} \tag{7.26}$$

since both of the last two sums are equal to $\langle\omega_t|H|\psi_t\rangle$. This means, in particular, that the norm $\|\psi_t\|$ of a solution $|\psi_t\rangle$ of Schrödinger's equation is independent of time, since it is the square root of the inner product of the ket with itself.

The fact that the Schrödinger equation preserves inner products and norms means that its action on the ket vectors in the Hilbert space is analogous to rigidly rotating a collection of vectors in ordinary three-dimensional space about the origin. If one thinks of these vectors as arrows directed outwards from the origin, the rotation will leave the lengths of the vectors and the angles between them, and hence the dot product of any two of them, unchanged, in the same way that inner products of vectors in the Hilbert space are left unchanged by the Schrödinger equation. An operator on the Hilbert space which leaves inner products unchanged is called an *isometry*. If, in addition, it maps the space onto itself, it is a *unitary operator*. Some important properties of unitary operators are stated in the next section, and we shall return to the topic of time development in Sec. 7.3.

7.2 Unitary Operators

An operator U on a Hilbert space $\mathcal{H}$ is said to be *unitary* provided (i) it is an isometry, and (ii) it maps $\mathcal{H}$ onto itself. An isometry preserves inner products, so condition (i) is equivalent to

$$\big(U|\omega\rangle\big)^\dagger U|\phi\rangle = \langle\omega|U^\dagger U|\phi\rangle \tag{7.27}$$

for any pair of kets $|\omega\rangle$ and $|\phi\rangle$ in $\mathcal{H}$, and this in turn will be true if and only if

$$U^\dagger U = I. \tag{7.28}$$

Condition (ii) means that given any $|\eta\rangle$ in $\mathcal{H}$, there is some $|\psi\rangle$ in $\mathcal{H}$ such that $|\eta\rangle = U|\psi\rangle$. This will be the case if, in addition to (7.28),

$$UU^\dagger = I. \tag{7.29}$$

The two equalities (7.28) and (7.29) tell us that $U^\dagger$ is the same as the *inverse* U^{-1} of the operator U. For a finite-dimensional Hilbert space, condition (ii) for a unitary operator is automatically satisfied in the case of an isometry, so (7.28) implies (7.29), and vice versa, and it suffices to check one or the other in order to show that U is unitary.

If U is unitary, then so is $U^\dagger$. In addition, the operator product of two or more unitary operators is a unitary operator. This follows at once from (7.28) and (7.29). and the rule giving the adjoint of a product of operators, (3.32). Thus if both U and V satisfy (7.28), so does their product,

$$(UV)^\dagger UV = V^\dagger U^\dagger UV = V^\dagger IV = I, \tag{7.30}$$

and the same is true for (7.29).

A second, equivalent definition of a unitary operator is the following: Let $\{|j\rangle\}$ be some orthonormal basis of $\mathcal{H}$. Then U is unitary if and only if $\{U|j\rangle\}$ is also an orthonormal basis. If $\mathcal{H}$ is of finite dimension, one need only check that $\{U|j\rangle\}$ is an orthonormal collection, for then it will also be an orthonormal basis, given that $\{|j\rangle\}$ is such a basis.

The matrix $\{\langle j|U|k\rangle\}$ of a unitary operator in an orthonormal basis can be thought of as a collection of column vectors which are normalized and mutually orthogonal, a result which follows at once from (7.28) and the usual rule for matrix multiplication. Similarly, (7.29) tells one that the row vectors which make up this matrix are normalized and mutually orthogonal. Any 2×2 unitary matrix can be written in the form

$$e^{i\phi}\begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}, \tag{7.31}$$

where α and β are complex numbers satisfying

$$|\alpha|^2 + |\beta|^2 = 1, \tag{7.32}$$

and ϕ is an arbitrary phase. It is obvious from (7.32) that the two column vectors making up this matrix are normalized, and their orthogonality is easily checked. The same is true of the two row vectors.

Given a unitary operator, one can find an orthonormal basis $\{|u_j\rangle\}$ in which it can be written in diagonal form

$$U = \sum_j \lambda_j |u_j\rangle\langle u_j|, \tag{7.33}$$

where the eigenvalues λ_j of U are complex numbers with $|\lambda_j| = 1$. Just as Hermitian operators can be thought of as somewhat analogous to real numbers, since their eigenvalues are real, unitary operators are analogous to complex numbers of unit modulus. (In an infinite-dimensional space the sum in (7.33) may have to be replaced by an appropriate integral.) As in the case of Hermitian operators, Sec. 3.7, if some of the eigenvalues in (7.33) are degenerate, the sum can be rewritten in the form

$$U = \sum_k \lambda'_k S_k, \tag{7.34}$$

where the S_k are projectors which form a decomposition of the identity, and $\lambda'_k \neq \lambda'_l$ for $k \neq l$.

All operators in a collection $\{U, V, W, \ldots\}$ of unitary operators which *commute* with each other can be simultaneously diagonalized using a single orthonormal basis. That is, there is some basis $\{|u_j\rangle\}$ in which U, V, W, and so forth can be expressed using the same collection of dyads $|u_j\rangle\langle u_j|$, as in (7.33), but with different eigenvalues for the different operators. If one writes down expressions of the form (7.34) for V, W, etc., the decompositions of the identity need not be identical with the $\{S_j\}$, appropriate for U, but the different decompositions will all be compatible in the sense that the projectors will all commute with one another.

7.3 Time Development Operators

Consider integrating Schrödinger's equation from time $t = 0$ to $t = \tau$ starting from an arbitrary initial state $|\psi_0\rangle$. Because the equation is linear, the dependence of the state $|\psi_\tau\rangle$ at time τ upon the initial state $|\psi_0\rangle$ can be written in the form

$$|\psi_\tau\rangle = T(\tau, 0)|\psi_0\rangle, \tag{7.35}$$

where $T(\tau, 0)$ is a linear operator. And because Schrödinger's equation preserves inner products, (7.26), $T(\tau, 0)$ is an isometry. In addition, it maps $\mathcal{H}$ onto itself, because if $|\eta\rangle$ is any ket in $\mathcal{H}$, we can treat it as a "final" condition at time τ and integrate Schrödinger's equation backwards to time 0 in order to obtain a ket $|\zeta\rangle$ such that $|\eta\rangle = T(\tau, 0)|\zeta\rangle$. Therefore $T(\tau, 0)$ is a unitary operator, since it satisfies the conditions given Sec. 7.2.

Of course there is nothing special about the times 0 and τ, and the same argument could be applied equally well to the integration of Schrödinger's equation between two arbitrary times t' and t, where t can be earlier or later than t'. That is to say, there is a collection of unitary *time development operators* $T(t, t')$, labeled by the two times t and t', such that if $|\psi_t\rangle$ is any solution of Schrödinger's equation, then

$$|\psi_t\rangle = T(t, t')|\psi_{t'}\rangle. \tag{7.36}$$

These time development operators satisfy a set of fairly obvious conditions. First, if t' is equal to t,

$$T(t, t) = I. \tag{7.37}$$

Next, since

$$|\psi_t\rangle = T(t, t'')|\psi_{t''}\rangle = T(t, t')|\psi_{t'}\rangle = T(t, t')T(t', t'')|\psi_{t''}\rangle, \tag{7.38}$$

it follows that

$$T(t, t')T(t', t'') = T(t, t'') \tag{7.39}$$

for any three times t, t', t''. In particular, if we set $t'' = t$ in this expression and use (7.37), the result is

$$T(t, t')T(t', t) = I. \tag{7.40}$$

Since $T(t, t')$ is a unitary operator, this tells us that

$$T(t', t) = T(t, t')^\dagger = T(t, t')^{-1}. \tag{7.41}$$

Thus the adjoint of a time-development operator, which is the same as its inverse, is obtained by interchanging its two arguments.

If one applies the dagger operation to (7.36), see (3.33), the result is:

$$\langle\psi_t| = \langle\psi_{t'}|T(t, t')^\dagger = \langle\psi_{t'}|T(t', t). \tag{7.42}$$

Consequently, the projectors $[\psi_t]$ and $[\psi_{t'}]$ onto the rays containing $|\psi_t\rangle$ and $|\psi_{t'}\rangle$ are related by

$$[\psi_t] = |\psi_t\rangle\langle\psi_t| = T(t, t')|\psi_{t'}\rangle\langle\psi_{t'}|T(t', t) = T(t, t')[\psi_{t'}]T(t', t). \tag{7.43}$$

This formula can be generalized to the case in which $P_{t'}$ is any projector onto some subspace $\mathcal{P}_{t'}$ of the Hilbert space. Then P_t defined by

$$P_t = T(t, t')P_{t'}T(t', t) \tag{7.44}$$

is a projector onto a subspace $\mathcal{P}_t$ with the property that if $|\psi_{t'}\rangle$ is any ket in $\mathcal{P}_{t'}$, its image $T(t, t')|\psi_{t'}\rangle$ under the time translation operator lies in $\mathcal{P}_t$, and $\mathcal{P}_t$ is composed of kets of this form. That is to say, the same unitary dynamics which "moves" one ket onto another through (7.36) "moves" subspaces in the manner indicated in (7.44). The difference is that only a single T operator is needed to move kets, while two are necessary in order to move a projector.

Since $|\psi_t\rangle$ in (7.36) satisfies Schrödinger's equation (7.4), it follows that

$$i\hbar\frac{\partial T(t,t')}{\partial t} = H(t)T(t,t'), \tag{7.45}$$

where one can write H in place of $H(t)$ if the Hamiltonian is independent of time. There is a similar equation in which the first argument of $T(t,t')$ is held fixed,

$$-i\hbar\frac{\partial T(t,t')}{\partial t'} = T(t,t')H(t'), \tag{7.46}$$

obtained by taking the adjoint of (7.45) with the help of (7.41), and then interchanging t and t'. Given a time-independent orthonormal basis $\{|j\rangle\}$, (7.45) is equivalent to a set of coupled ordinary differential equations for the matrix elements of $T(t,t')$,

$$i\hbar\frac{\partial}{\partial t}\langle j|T(t,t')|k\rangle = \sum_m \langle j|H(t)|m\rangle\langle m|T(t,t')|k\rangle, \tag{7.47}$$

and one can write down an analogous expression corresponding to (7.46)

Obtaining explicit forms for the time development operators is in general a very difficult task, since it is equivalent to integrating the Schrödinger equation for all possible initial conditions. However, if the Hamiltonian is independent of time, one can write

$$T(t,t') = \exp[-i(t-t')H/\hbar] = \sum_n e^{-iE_n(t-t')/\hbar}|e_n\rangle\langle e_n|, \tag{7.48}$$

where the E_n and $|e_n\rangle$ are the eigenvalues and eigenfunctions of H, (7.17). Thus when the Hamiltonian is independent of time, $T(t,t')$ depends only on the difference $t-t'$ of its two arguments.

7.4 Toy Models

The unitary dynamics of most quantum systems is quite complicated and difficult to understand. Among the few exceptions are: trivial dynamics, in which $T(t',t) = I$ independent of t and t'; a spin-half particle in a constant magnetic field with Hamiltonian (7.16); and the harmonic oscillator, which has a simple time dependence because its energy levels have a uniform spacing, (7.22). Even a particle moving in one dimension in the potential $V(x) = 0$ represents a non-trivial dynamical problem in quantum theory. Though one can write down closed-form solutions, they tend to be a bit messy, especially in comparison with the simple trajectory $x = x_0 + (p_0/m)t$ and $p = p_0$ in the classical phase space.

In order to gain some intuitive understanding of quantum dynamics, it is important to have simple model systems whose properties can be worked out explicitly with very little effort "on the back of an envelope", but which allow more complicated behavior than occurs in the case of a spin half particle or a harmonic oscillator. We want to be able to discuss interference effects, measurements, radioactive decay, and so forth. For this purpose toy models resembling the one introduced in Sec. 2.5, where a particle can be located at one of a finite number of discrete sites, turn out to be particularly useful. The key to obtaining simple dynamics in a toy model is to make *time* (like space) a *discrete variable.* Thus we shall assume that the time t takes on only integer values: $-1, 0, 1, 2$, etc. These could, in principle, be integer multiples of some very short interval of time, say 10^{-50} seconds, so discretization is not, by itself, much of a limitation (or simplification).

Though it is not essential, in many cases one can assume that $T(t, t')$ depends only on the time difference $t - t'$; this is the toy analog of a time-independent Hamiltonian. Then one can write

$$T(t, t') = T^{t-t'}, \tag{7.49}$$

where the symbol T *without any arguments* will represent a unitary operator on the (usually finite-dimensional) Hilbert space of the toy model. The strategy for constructing a useful toy model is to make T a very simple operator, as in the examples discussed below. Because t takes integer values, $T(t, t')$ is given by integer powers of the operator T, and can be calculated by applying T several times in a row. To be sure, these powers can be negative, but that is not so bad, because we will be able to choose T in such a way that its inverse $T^{-1} = T^\dagger$ is also a very simple operator.

As a first example, consider the model introduced in Sec. 2.5 with a particle located at one of $M = M_a + M_b + 1$ sites placed in a one-dimensional line and labeled with an integer m in the interval

$$-M_a \le m \le M_b, \tag{7.50}$$

where M_a and M_b are large integers. This becomes a *hopping model* if the time development operator T is set equal to the *shift operator* S defined by:

$$S|m\rangle = |m+1\rangle, \quad S|M_b\rangle = |-M_a\rangle. \tag{7.51}$$

That is, during a single time step the particle hops one space to the right, but when it comes to the maximum value of m it hops to the minimum value. Thus the dynamics has a "periodic boundary condition", and one may prefer to imagine the successive sites as located not on a line but on a large circle, so that the one labeled M_b is just to the left of the one labeled $-M_a$. One must check that $T = S$ is unitary, and this is easily done. The collection of kets $\{|m\rangle\}$ forms an orthonormal basis of the Hilbert space, and the collection $\{S|m\rangle\}$, since it consists of precisely the same elements, is also an orthonormal basis. Thus the criterion in the second definition in Sec. 7.2 is satisfied, and S is unitary.

To make the hopping model a bit more interesting, let us add a detector, a second particle which can be at only one of the two sites $n = 0$ or 1 indicated in Fig. 7.1. The Hilbert space $\mathcal{H}$ for this system is, as noted in Sec. 6.3, a tensor product $\mathcal{M} \otimes \mathcal{N}$ of an M-dimensional space $\mathcal{M}$ for the first particle and a two-dimensional space $\mathcal{N}$ for the detector, and the $2M$ kets $\{|m, n\rangle\}$ form an orthonormal basis. What makes the detector act like a detector is a choice for the unitary dynamics in which the time-development operator is

$$T = SR, \tag{7.52}$$

where $S = S \otimes I$, using the notation of Sec. 6.4, is the extension to $\mathcal{M} \otimes \mathcal{N}$ of the shift operator defined earlier on $\mathcal{M}$ using (7.51), and R is defined by

$$\begin{aligned} R|m, n\rangle &= |m, n\rangle \text{ for } m \ne 2, \\ R|2, n\rangle &= |2, 1-n\rangle. \end{aligned} \tag{7.53}$$

Thus R does nothing at all unless the particle is at $m = 2$, in which case it "flips" the detector from $n = 0$ to $n = 1$ and vice versa. That R is unitary follows from the fact that the collection of kets $\{R|m,n\rangle\}$ is identical to the collection $\{|m,n\rangle\}$, as all that R does is interchange two of them, and is thus an orthonormal basis of $\mathcal{H}$. The extended operator $S \otimes I$ satisfies (7.28) when S satisfies this condition, so it is unitary. The unitarity of $T = SR$ is then a consequence of the fact that the product of unitary operators is unitary, as noted in Sec. 7.2. (While it is not hard to show directly that T is unitary, the strategy of writing it as a product of other unitary operators is useful in more complicated cases, which is why we have used it here.) The action of $T = SR$ on the combined system of particle plus detector is as follows. At each time step the particle hops from m to $m+1$ (except when it makes the big jump from M_b to $-M_a$). The detector remains at $n = 0$ or at $n = 1$, wherever it happens to be, except during a time step in which the particle hops from 2 to 3, when the detector hops from n to $1 - n$, that is, from 0 to 1 or 1 to 0.

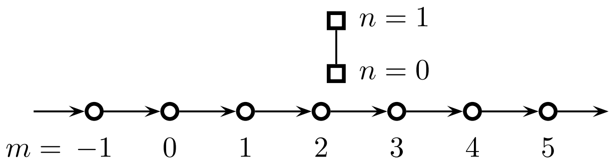

Figure 7.1: Toy model of particle with detector.

What justifies calling the detector a detector? Let us use a notation in which $\mapsto$ denotes the action of T in the sense that

$$|\psi\rangle \mapsto T|\psi\rangle \mapsto T^2|\psi\rangle \mapsto \cdots . \tag{7.54}$$

Suppose that the particle starts off at $m = 0$ and the detector is in the state $n = 0$, "ready to detect the particle", at $t = 0$. The initial state of the combined system of particle plus detector develops in time according to

$$|0,0\rangle \mapsto |1,0\rangle \mapsto |2,0\rangle \mapsto |3,1\rangle \mapsto |4,1\rangle \mapsto \cdots . \tag{7.55}$$

That is to say, during the time step from $t = 2$ to $t = 3$, in which the particle hops from $m = 2$ to $m = 3$, the detector moves from $n = 0$ "ready" to $n = 1$, "have detected the particle," and it continues in the "have detected" state at later times. Not all later times, since the particle will eventually hop from $M_b > 0$ to $-M_a < 0$, and then m will increase until, eventually, the particle will pass by the detector a second time and "untrigger" it. But by making M_a or M_b large compared with the times we are interested in, we can ignore this possibility. More sophisticated models of detectors are certainly possible, and some of these will be introduced in later chapters. However, the essential spirit of the toy model approach is to use the simplest possibility which provides some physical intuition. The detector in Fig. 7.1 is perfectly adequate for many purposes, and will be used repeatedly in later chapters.

It is worth noting that the measurement of the particle's position (or its passing the position of the detector) in this way does *not* influence the motion of the particle: in the absence of the detector one would have the same sequence of positions m as a function of time as those in (7.55). But is it not the case that *any* quantum measurement perturbs the measured system? One of the benefits of introducing toy models is that they make it possible to study this and other pieces of quantum folklore in specific situations. In later chapters we will explore the issue of perturbations produced by measurements in more detail. For the present it is enough to note that quantum measurement apparatus can be designed so that it does not perturb certain properties, even though it may perturb other properties.

Another example of a toy model is the one in Fig. 7.2, which can be used to illustrate the process of radioactive decay. Consider alpha decay, and adopt the picture in which an alpha particle is rattling around inside a nucleus until it eventually tunnels out through the Coulomb barrier. One knows that this is a fairly good description of the escape process, even though it is bad nuclear physics if taken too literally. However, the unitary time development of a particle tunneling through a potential barrier is not easy to compute; one needs WKB formulas and other approximations.

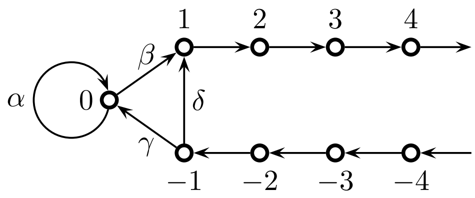

Figure 7.2: Toy model for alpha decay.

By contrast, the unitary time development of the toy model in Fig. 7.2, which is a slight modification of the hopping model (without a detector) introduced earlier, can be worked out very easily. The different sites represent possible locations of the alpha particle, with the $m = 0$ site inside the nucleus, and the other sites outside the nucleus. At each time step, the particle at $m = 0$ can either stay put, with amplitude α, or escape to $m = 1$, with amplitude β. Once it reaches $m = 1$, it hops to $m = 2$ at the next time step, and then on to $m = 3$, etc. Eventually it will hop from $m = +M_b$ to $m = -M_a$ and begin its journey back towards the nucleus, but we will assume that M_b is so large that we never have to consider the return process. (One could make M_a and M_b infinite, at the price of introducing an infinite-dimensional Hilbert space.) The time development operator is $T = S_a$, where

$$\begin{aligned} S_a|m\rangle &= |m+1\rangle \text{ for } m \neq 0, -1, M_b, \quad S_a|M_b\rangle = |-M_a\rangle, \\ S_a|0\rangle &= \alpha|0\rangle + \beta|1\rangle, \quad S_a|-1\rangle = \gamma|0\rangle + \delta|1\rangle. \end{aligned} \tag{7.56}$$

Thus S_a is identical to the simple shift S of (7.51), except when applied to the two kets $|0\rangle$ and $|-1\rangle$.

The operator S_a is unitary if the complex constants $\alpha, \beta, \gamma, \delta$ form a unitary matrix

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}. \tag{7.57}$$

If we use the criterion, Sec. 7.2, that the row vectors are normalized and mutually orthogonal, the conditions for unitarity can be written in the form:

$$|\alpha|^2 + |\beta|^2 = 1 = |\gamma|^2 + |\delta|^2, \quad \alpha^*\gamma + \beta^*\delta = 0. \tag{7.58}$$

That S_a is unitary when (7.58) is satisfied can be seen from the fact that it maps the orthonormal basis $\{|m\rangle\}$ into an orthonormal collection of vectors, which, since the Hilbert space is finite, must itself be an orthonormal basis. In particular, S_a applied to $|0\rangle$ and to $|-1\rangle$ yields two normalized vectors which are mutually orthogonal to each other, a result ensured by (7.58).

Note how the requirement of unitarity leads to the non-trivial consequence that if the action of the shift operator S on $|0\rangle$ is modified so that the particle can either hop or remain in place during one time step, there must be an additional modification of S someplace else. In this example the other modification occurs at $|-1\rangle$, which is a fairly natural place to put it. The fact that $|\gamma| = |\beta|$ means that if there is an amplitude for the alpha particle to escape from the nucleus, there is also an amplitude for an alpha particle approaching the nucleus along the $m < 0$ sites to be captured at $m = 0$, rather than simply being scattered to $m = 1$. As one might expect, $|\beta|^2$ is the probability that the alpha particle will escape during a particular time step, and $|\alpha|^2$ the probability that it will remain in the nucleus. However, showing that this is so requires additional developments of the theory found in the following chapters; see Secs. 9.5 and 12.4.

The unitary time development of an initial state $|0\rangle$ at $t = 0$, corresponding to the alpha particle being inside the nucleus, is easily worked out. Using the $\mapsto$ notation of (7.54), one has:

$$\begin{aligned} |0\rangle &\mapsto \alpha|0\rangle + \beta|1\rangle \mapsto \alpha^2|0\rangle + \alpha\beta|1\rangle + \beta|2\rangle \\ &\mapsto \alpha^3|0\rangle + \alpha^2\beta|1\rangle + \alpha\beta|2\rangle + \beta|3\rangle \mapsto \cdots, \end{aligned} \tag{7.59}$$

so that for any time $t > 0$,

$$|\psi_t\rangle = T^t|0\rangle = \alpha^t|0\rangle + \alpha^{t-1}\beta|1\rangle + \alpha^{t-2}\beta|2\rangle + \cdots + \beta|t\rangle. \tag{7.60}$$

The magnitude of the coefficient of $|0\rangle$ decreases exponentially with time. The rest of the time development can be thought of in the following way. An “initial wave” reaches site m at $t = m$. Thereafter, the coefficient of $|m\rangle$ decreases exponentially. That is, the wave function is spreading out and, at the same time, its amplitude is decreasing. These features are physically correct in that they will also emerge from a more sophisticated model of the decay process. Even though not every detail of the toy model is realistic, it nonetheless provides a good beginning for understanding some of the quantum physics of radioactive and other decay processes.