TABLE 2.2. The Quantized Energies of a Bouncing Ball in Units of $(mg^2\hbar^2/2)^{1/3}$

n	WKB	Exact
1	2.320	2.338
2	4.082	4.088
3	5.517	5.521
4	6.784	6.787
5	7.942	7.944
6	9.021	9.023
7	10.039	10.040
8	11.008	11.009
9	11.935	11.936
10	12.828	12.829

as

$$E_n = \left(\frac{\lambda_n}{2^{1/3}}\right)\left(mg^2\hbar^2\right)^{1/3}. \tag{2.4.53}$$

The two approaches are compared numerically in Table 2.2 for the first 10 energy levels. We see that agreement is excellent even for small values of n and essentially exact for $n \simeq 10$.

The quantum-theoretical treatment of a bouncing ball may appear to have little to do with the real world. It turns out, however, that a potential of type (2.4.45) is actually of practical interest in studying the energy spectrum of a quark-antiquark bound system, called **quarkonium**. To go from a bouncing ball to a quarkonium, the x in (2.4.45) is replaced by the quark-antiquark separation distance r. The analogue of the downward gravitational force mg is a constant (that is, r-independent) force believed to be operative between a quark and an antiquark. This force is empirically estimated to be in the neighborhood of

$$1\ \text{GeV/fm} \simeq 1.6\times 10^5\ \text{N}, \tag{2.4.54}$$

which corresponds to about 16 tons. This contrasts with the gravitational force of 0.98 N on a ball of 0.1 kg.

2.5. PROPAGATORS AND FEYNMAN PATH INTEGRALS

Propagators in Wave Mechanics

In Section 2.1 we showed how the most general time-evolution problem with a time-independent Hamiltonian can be solved once we expand the initial ket in terms of the eigenkets of an observable that commutes with H. Let us translate this statement into the language of wave mechanics. We start with

$$\begin{aligned}|\alpha, t_0; t\rangle &= \exp\left[\frac{-iH(t-t_0)}{\hbar}\right]|\alpha, t_0\rangle \\ &= \sum_{a'} |a'\rangle\langle a'|\alpha, t_0\rangle \exp\left[\frac{-iE_{a'}(t-t_0)}{\hbar}\right].\end{aligned} \tag{2.5.1}$$

Multiplying both sides by $\langle \mathbf{x}'|$ on the left, we have

$$\langle \mathbf{x}'|\alpha, t_0; t\rangle = \sum_{a'} \langle \mathbf{x}'|a'\rangle\langle a'|\alpha, t_0\rangle \exp\left[\frac{-iE_{a'}(t-t_0)}{\hbar}\right], \tag{2.5.2}$$

which is of the form

$$\psi(\mathbf{x}', t) = \sum_{a'} c_{a'}(t_0) u_{a'}(\mathbf{x}') \exp\left[\frac{-iE_{a'}(t-t_0)}{\hbar}\right], \tag{2.5.3}$$

with

$$u_{a'}(\mathbf{x}') = \langle \mathbf{x}'|a'\rangle \tag{2.5.4}$$

standing for the eigenfunction of operator A with eigenvalue a'. Note also that

$$\langle a'|\alpha, t_0\rangle = \int d^3x' \langle a'|\mathbf{x}'\rangle\langle \mathbf{x}'|\alpha, t_0\rangle, \tag{2.5.5}$$

which we recognize as the usual rule in wave mechanics for getting the expansion coefficients of the initial state:

$$c_{a'}(t_0) = \int d^3x' u_{a'}^*(\mathbf{x}') \psi(\mathbf{x}', t_0). \tag{2.5.6}$$

All this should be straightforward and familiar. Now (2.5.2) together with (2.5.5) can also be visualized as some kind of integral operator acting on the initial wave function to yield the final wave function:

$$\psi(\mathbf{x}'', t) = \int d^3x' K(\mathbf{x}'', t; \mathbf{x}', t_0) \psi(\mathbf{x}', t_0). \tag{2.5.7}$$

Here the kernel of the integral operator, known as the **propagator** in wave mechanics, is given by

$$K(\mathbf{x}'', t; \mathbf{x}', t_0) = \sum_{a'} \langle \mathbf{x}''|a'\rangle\langle a'|\mathbf{x}'\rangle \exp\left[\frac{-iE_{a'}(t-t_0)}{\hbar}\right]. \tag{2.5.8}$$

In any given problem the propagator depends only on the potential and is independent of the initial wave function. It can be constructed once the energy eigenfunctions and their eigenvalues are given.

Clearly, the time evolution of the wave function is completely predicted if $K(\mathbf{x}'', t; \mathbf{x}', t_0)$ is known and $\psi(\mathbf{x}', t_0)$ is given initially. In this sense Schrödinger's wave mechanics is a *perfectly causal theory*. The time development of a wave function subjected to some potential is as "deterministic" as anything else in classical mechanics *provided that the system is left undisturbed*. The only peculiar feature, if any, is that when a measurement intervenes, the wave function changes abruptly, in an uncontrollable way, into one of the eigenfunctions of the observable being measured.

There are two properties of the propagator worth recording here. First, for $t > t_0$, $K(\mathbf{x}'', t; \mathbf{x}', t_0)$ satisfies Schrödinger's time-dependent wave equation in the variables $\mathbf{x}''$ and t, with $\mathbf{x}'$ and t_0 fixed. This is evident from (2.5.8) because $\langle \mathbf{x}''|a'\rangle \exp[-iE_{a'}(t-t_0)/\hbar]$, being the wave function corresponding to $\mathscr{U}(t, t_0)|a'\rangle$, satisfies the wave equation. Second,

$$\lim_{t \to t_0} K(\mathbf{x}'', t; \mathbf{x}', t_0) = \delta^3(\mathbf{x}'' - \mathbf{x}'), \tag{2.5.9}$$

which is also obvious; as $t \to t_0$, because of the completeness of $\{|a'\rangle\}$, sum (2.5.8) just reduces to $\langle \mathbf{x}''|\mathbf{x}'\rangle$.

Because of these two properties, the propagator (2.5.8), regarded as a function of $\mathbf{x}''$, is simply the wave function at t of a particle which was localized *precisely* at $\mathbf{x}'$ at some earlier time t_0. Indeed, this interpretation follows, perhaps more elegantly, from noting that (2.5.8) can also be written as

$$K(\mathbf{x}'', t; \mathbf{x}', t_0) = \langle \mathbf{x}''|\exp\left[\frac{-iH(t-t_0)}{\hbar}\right]|\mathbf{x}'\rangle, \tag{2.5.10}$$

where the time-evolution operator acting on $|\mathbf{x}'\rangle$ is just the state ket at t of a system that was localized precisely at $\mathbf{x}'$ at time t_0 ($< t$). If we wish to solve a more general problem where the initial wave function extends over a finite region of space, all we have to do is multiply $\psi(\mathbf{x}', t_0)$ by the propagator $K(\mathbf{x}'', t; \mathbf{x}', t_0)$ and integrate over all space (that is, over $\mathbf{x}'$). In this manner we can add the various contributions from different positions ($\mathbf{x}'$). This situation is analogous to one in electrostatics; if we wish to find the electrostatic potential due to a general charge distribution $\rho(\mathbf{x}')$, we first solve the point-charge problem, multiply the point-charge solution with the charge distribution, and integrate:

$$\phi(\mathbf{x}) = \int d^3x' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}. \tag{2.5.11}$$

The reader familiar with the theory of the Green's functions must have recognized by this time that the propagator is simply the Green's function for the time-dependent wave equation satisfying

$$\left[-\left(\frac{\hbar^2}{2m}\right)\nabla''^2 + V(\mathbf{x}'') - i\hbar\frac{\partial}{\partial t}\right]K(\mathbf{x}'', t; \mathbf{x}', t_0) = -i\hbar\delta^3(\mathbf{x}'' - \mathbf{x}')\delta(t - t_0) \tag{2.5.12}$$

with the boundary condition

$$K(\mathbf{x}'', t; \mathbf{x}', t_0) = 0, \quad \text{for } t < t_0. \tag{2.5.13}$$

The delta function $\delta(t - t_0)$ is needed on the right-hand side of (2.5.12) because K varies discontinuously at $t = t_0$.

The particular form of the propagator is, of course, dependent on the particular potential to which the particle is subjected. Consider, as an example, a free particle in one dimension. The obvious observable that commutes with H is momentum; $|p'\rangle$ is a simultaneous eigenket of the operators p and H:

$$p|p'\rangle = p'|p'\rangle \qquad H|p'\rangle = \left(\frac{p'^2}{2m}\right)|p'\rangle. \tag{2.5.14}$$

The momentum eigenfunction is just the transformation function of Section 1.7 [see (1.7.32)] which is of the plane-wave form. Combining everything, we have

$$K(x'', t; x', t_0) = \left(\frac{1}{2\pi\hbar}\right)\int_{-\infty}^{\infty} dp' \exp\left[\frac{ip'(x''-x')}{\hbar} - \frac{ip'^2(t-t_0)}{2m\hbar}\right]. \tag{2.5.15}$$

The integral can be evaluated by completing the square in the exponent. Here we simply record the result:

$$K(x'', t; x', t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\exp\left[\frac{im(x''-x')^2}{2\hbar(t-t_0)}\right]. \tag{2.5.16}$$

This expression may be used, for example, to study how a Gaussian wave packet spreads out as a function of time.

For the simple harmonic oscillator, where the wave function of an energy eigenstate is given by

$$u_n(x)\exp\left(\frac{-iE_n t}{\hbar}\right) = \left(\frac{1}{2^{n/2}\sqrt{n!}}\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(\frac{-m\omega x^2}{2\hbar}\right)$$
$$\times H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)\exp\left[-i\omega\left(n+\frac{1}{2}\right)t\right], \tag{2.5.17}$$

the propagator is given by

$$K(x'', t; x', t_0) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin[\omega(t-t_0)]}}\exp\left[\left\{\frac{im\omega}{2\hbar\sin[\omega(t-t_0)]}\right\}\right.$$
$$\left.\times\left\{(x''^2+x'^2)\cos[\omega(t-t_0)] - 2x''x'\right\}\right]. \tag{2.5.18}$$

One way to prove this is to use

$$\left(\frac{1}{\sqrt{1-\zeta^2}}\right)\exp\left[\frac{-(\xi^2+\eta^2-2\xi\eta\zeta)}{(1-\zeta^2)}\right]$$
$$=\exp\left[-(\xi^2+\eta^2)\right]\sum_{n=0}\left(\frac{\zeta^n}{2^n n!}\right)H_n(\xi)H_n(\eta), \qquad (2.5.19)$$

which is found in books on special functions (Morse and Feshbach 1953, 786). It can also be obtained using the a, $a^\dagger$ operator method (Saxon 1968, 144–45) or, alternatively, the path-integral method to be described later. Notice that (2.5.18) is a periodic function of t with angular frequency ω, the classical oscillator frequency. This means, among other things, that a particle initially localized precisely at x' will return to its original position with certainty at $2\pi/\omega$ ($4\pi/\omega$, and so forth) later.

Certain space and time integrals derivable from $K(\mathbf{x}'', t; \mathbf{x}', t_0)$ are of considerable interest. Without loss of generality we set $t_0 = 0$ in the following. The first integral we consider is obtained by setting $\mathbf{x}'' = \mathbf{x}'$ and integrating over all space. We have

$$G(t) \equiv \int d^3x' K(\mathbf{x}', t; \mathbf{x}', 0)$$
$$= \int d^3x' \sum_{a'} |\langle \mathbf{x}' | a' \rangle|^2 \exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$
$$= \sum_{a'} \exp\left(\frac{-iE_{a'}t}{\hbar}\right). \qquad (2.5.20)$$

This result is anticipated; recalling (2.5.10),we observe that setting $\mathbf{x}' = \mathbf{x}''$ and integrating are equivalent to taking the trace of the time-evolution operator in the $\mathbf{x}$-representation. But the trace is independent of representations; it can be evaluated more readily using the $\{|a'\rangle\}$ basis where the time-evolution operator is diagonal, which immediately leads to the last line of (2.5.20). Now we see that (2.5.20) is just the "sum over states," reminiscent of the partition function in statistical mechanics. In fact, if we analytically continue in the t variable and make t purely imaginary, with β defined by

$$\beta = \frac{it}{\hbar} \qquad (2.5.21)$$

real and positive, we can identify (2.5.20) with the partition function itself:

$$Z = \sum_{a'} \exp(-\beta E_{a'}). \qquad (2.5.22)$$

For this reason some of the techniques encountered in studying propagators in quantum mechanics are also useful in statistical mechanics.

Next, let us consider the Laplace-Fourier transform of $G(t)$:

$$\begin{aligned}\tilde{G}(E) &\equiv -i\int_0^\infty dt G(t)\exp(iEt/\hbar)/\hbar \\ &= -i\int_0^\infty dt \sum_{a'} \exp(-iE_{a'}t/\hbar)\exp(iEt/\hbar)/\hbar. \qquad (2.5.23)\end{aligned}$$

The integrand here oscillates indefinitely. But we can make the integral meaningful by letting E acquire a small positive imaginary part:

$$E \to E + i\varepsilon. \qquad (2.5.24)$$

We then obtain, in the limit $\varepsilon \to 0$,

$$\tilde{G}(E) = \sum_{a'} \frac{1}{E - E_{a'}}. \qquad (2.5.25)$$

Observe now that the complete energy spectrum is exhibited as simple poles of $\tilde{G}(E)$ in the complex E-plane. If we wish to know the energy spectrum of a physical system, it is sufficient to study the analytic properties of $\tilde{G}(E)$.

Propagator as a Transition Amplitude

To gain further insight into the physical meaning of the propagator, we wish to relate it to the concept of transition amplitudes introduced in Section 2.2. But first, recall that the wave function which is the inner product of the fixed position bra $\langle \mathbf{x}'|$ with the moving state ket $|\alpha, t_0; t\rangle$ can also be regarded as the inner product of the Heisenberg-picture position bra $\langle \mathbf{x}', t|$, which moves "oppositely" with time, with the Heisenberg-picture state ket $|\alpha, t_0\rangle$, which is fixed in time. Likewise, the propagator can also be written as

$$\begin{aligned}K(\mathbf{x}'', t; \mathbf{x}', t_0) &= \sum_{a'} \langle \mathbf{x}''|a'\rangle\langle a'|\mathbf{x}'\rangle \exp\left[\frac{-iE_{a'}(t-t_0)}{\hbar}\right] \\ &= \sum_{a'} \langle \mathbf{x}''|\exp\left(\frac{-iHt}{\hbar}\right)|a'\rangle\langle a'|\exp\left(\frac{iHt_0}{\hbar}\right)|\mathbf{x}'\rangle \\ &= \langle \mathbf{x}'', t|\mathbf{x}', t_0\rangle, \qquad (2.5.26)\end{aligned}$$

where $|\mathbf{x}', t_0\rangle$ and $\langle \mathbf{x}'', t|$ are to be understood as an eigenket and an eigenbra of the position operator in the Heisenberg picture. In Section 2.1 we showed that $\langle b', t|a'\rangle$, in the Heisenberg-picture notation, is the probability amplitude for a system originally prepared to be an eigenstate of A with eigenvalue a' at some initial time $t_0 = 0$ to be found at a later time t in an eigenstate of B with eigenvalue b', and we called it the transition amplitude for going from state $|a'\rangle$ to state $|b'\rangle$. Because there is nothing special about the choice of t_0—only the time difference $t - t_0$ is relevant—we can identify $\langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$ as the probability amplitude for the particle prepared at t_0 with position eigenvalue $\mathbf{x}'$ to be found at a later time t at $\mathbf{x}''$. Roughly speaking, $\langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$ is the amplitude for the particle to go from a space-time point $(\mathbf{x}', t_0)$ to another space-time point $(\mathbf{x}'', t)$, so the term *transition amplitude* for this expression is quite appropriate. This interpretation is, of course, in complete accord with the interpretation we gave earlier for $K(\mathbf{x}'', t; \mathbf{x}', t_0)$.

Yet another way to interpret $\langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$ is as follows. As we emphasized earlier, $|\mathbf{x}', t_0\rangle$ is the position eigenket at t_0 with the eigenvalue $\mathbf{x}'$ in the Heisenberg picture. Because at any given time the Heisenberg-picture eigenkets of an observable can be chosen as base kets, we can regard $\langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$ as the transformation function that connects the two sets of base kets at *different* times. So in the Heisenberg picture, time evolution can be viewed as a *unitary transformation*, in the sense of changing bases, that connects one set of base kets formed by $\{|\mathbf{x}', t_0\rangle\}$ to another formed by $\{|\mathbf{x}'', t\rangle\}$. This is reminiscent of classical physics, in which the time development of a classical dynamic variable such as $\mathbf{x}(t)$ is viewed as a canonical (or contact) transformation generated by the classical Hamiltonian (Goldstein 1980, 407–8).

It turns out to be convenient to use a notation that treats the space and time coordinates more symmetrically. To this end we write $\langle \mathbf{x}'', t'' | \mathbf{x}', t' \rangle$ in place of $\langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$. Because at any given time the position kets in the Heisenberg picture form a complete set, it is legitimate to insert the identity operator written as

$$\int d^3x'' |\mathbf{x}'', t''\rangle \langle \mathbf{x}'', t''| = 1 \tag{2.5.27}$$

at any place we desire. For example, consider the time evolution from t' to t'''; by dividing the time interval (t', t''') into two parts, (t', t'') and (t'', t'''), we have

$$\langle \mathbf{x}''', t''' | \mathbf{x}', t' \rangle = \int d^3x'' \langle \mathbf{x}''', t''' | \mathbf{x}'', t'' \rangle \langle \mathbf{x}'', t'' | \mathbf{x}', t' \rangle, \qquad (t''' > t'' > t'). \tag{2.5.28}$$

We call this the **composition property** of the transition amplitude.* Clearly, we can divide the time interval into as many smaller subintervals as we wish. We have

$$\langle \mathbf{x}'''', t'''' | \mathbf{x}', t' \rangle = \int d^3x''' \int d^3x'' \langle \mathbf{x}'''', t'''' | \mathbf{x}''', t''' \rangle \langle \mathbf{x}''', t''' | \mathbf{x}'', t'' \rangle \times \langle \mathbf{x}'', t'' | \mathbf{x}', t' \rangle, \quad (t'''' > t''' > t'' > t'), \tag{2.5.29}$$

*The analogue of (2.5.28) in probability theory is known as the Chapman-Kolmogoroff equation, and in diffusion theory, the Smoluchowsky equation.

and so on. If we somehow guess the form of $\langle \mathbf{x}'', t''|\mathbf{x}', t'\rangle$ for an *infinitesimal* time interval (between t' and $t'' = t' + dt$), we should be able to obtain the amplitude $\langle \mathbf{x}'', t''|\mathbf{x}', t'\rangle$ for a finite time interval by compounding the appropriate transition amplitudes for infinitesimal time intervals in a manner analogous to (2.5.29). This kind of reasoning leads to an *independent formulation* of quantum mechanics due to R. P. Feynman, published in 1948, to which we now turn our attention.

Path Integrals as the Sum Over Paths

Without loss of generality we restrict ourselves to one-dimensional problems. Also, we avoid awkward expressions like

$$\underbrace{x'''' \quad \cdots \quad x'''}_{N \text{ times}}$$

by using notation such as x_N. With this notation we consider the transition amplitude for a particle going from the initial space-time point (x_1, t_1) to the final space-time point (x_N, t_N). The entire time interval between t_1 and t_N is divided into $N-1$ equal parts:

$$t_j - t_{j-1} = \Delta t = \frac{(t_N - t_1)}{(N-1)}. \tag{2.5.30}$$

Exploiting the composition property, we obtain

$$\begin{aligned}\langle x_N, t_N|x_1, t_1\rangle = \int dx_{N-1}\int dx_{N-2}\cdots\int dx_2 \langle x_N, t_N|x_{N-1}, t_{N-1}\rangle \\ \times\langle x_{N-1}, t_{N-1}|x_{N-2}, t_{N-2}\rangle\cdots\langle x_2, t_2|x_1, t_1\rangle.\end{aligned} \tag{2.5.31}$$

To visualize this pictorially, we consider a space-time plane, as shown in Figure 2.2. The initial and final space-time points are fixed to be (x_1, t_1) and (x_N, t_N), respectively. For each time segment, say between t_{n-1} and t_n, we are instructed to consider the transition amplitude to go from (x_{n-1}, t_{n-1}) to (x_n, t_n); we then integrate over $x_2, x_3, \ldots, x_{N-1}$. This means that we must *sum over all possible paths* in the space-time plane with the end points fixed.

Before proceeding further, it is profitable to review here how paths appear in classical mechanics. Suppose we have a particle subjected to a force field derivable from a potential $V(x)$. The *classical* Lagrangian is written as

$$L_{\text{classical}}(x, \dot{x}) = \frac{m\dot{x}^2}{2} - V(x). \tag{2.5.32}$$

Given this Lagrangian with the end points (x_1, t_1) and (x_N, t_N) specified, we do *not* consider just any path joining (x_1, t_1) and (x_N, t_N) in classical mechanics. On the contrary, there exists a *unique path* that corresponds to

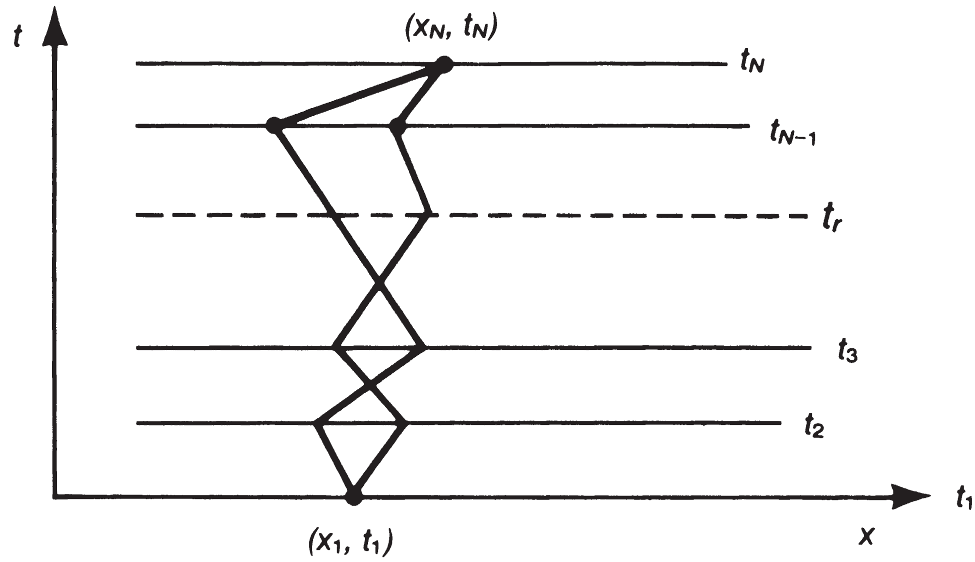

FIGURE 2.2. Paths in xt-plane.

the actual motion of the classical particle. For example, given

$$V(x) = mgx, \qquad (x_1, t_1) = (h, 0), \qquad (x_N, t_N) = \left(0, \sqrt{\frac{2h}{g}}\right), \tag{2.5.33}$$

where h may stand for the height of the Leaning Tower of Pisa, the classical path in the xt-plane can *only* be

$$x = h - \frac{gt^2}{2}. \tag{2.5.34}$$

More generally, according to Hamilton's principle, the unique path is that which minimizes the action, defined as the time integral of the classical Lagrangian:

$$\delta \int_{t_1}^{t_2} dt\, L_{\text{classical}}(x, \dot{x}) = 0, \tag{2.5.35}$$

from which Lagrange's equation of motion can be obtained.

Feynman's Formulation

The basic difference between classical mechanics and quantum mechanics should now be apparent. In classical mechanics a definite path in the xt-plane is associated with the particle's motion; in contrast, in quantum mechanics all possible paths must play roles including those which do not bear any resemblance to the classical path. Yet we must somehow be able to reproduce classical mechanics in a smooth manner in the limit $\hbar \to 0$. How are we to accomplish this?

As a young graduate student at Princeton University, R. P. Feynman tried to attack this problem. In looking for a possible clue, he was said to be intrigued by a mysterious remark in Dirac's book which, in our notation, amounts to the following statement:

$$\exp\left[i\int_{t_1}^{t_2} \frac{dt\, L_{\text{classical}}(x,\dot{x})}{\hbar} \right] \quad \text{corresponds to} \quad \langle x_2, t_2 | x_1, t_1 \rangle.$$

Feynman attempted to make sense out of this remark. Is "corresponds to" the same thing as "is equal to" or "is proportional to"? In so doing he was led to formulate a space-time approach to quantum mechanics based on *path integrals*.

In Feynman's formulation the classical action plays a very important role. For compactness, we introduce a new notation:

$$S(n, n-1) \equiv \int_{t_{n-1}}^{t_n} dt\, L_{\text{classical}}(x, \dot{x}). \tag{2.5.36}$$

Because $L_{\text{classical}}$ is a function of x and $\dot{x}$, $S(n, n-1)$ is defined only after a definite path is specified along which the integration is to be carried out. So even though the path dependence is not explicit in this notation, it is understood that we are considering a particular path in evaluating the integral. Imagine now that we are following some prescribed path. We concentrate our attention on a small segment along that path, say between (x_{n-1}, t_{n-1}) and (x_n, t_n). According to Dirac, we are instructed to associate $\exp[iS(n, n-1)/\hbar]$ with that segment. Going along the definite path we are set to follow, we successively multiply expressions of this type to obtain

$$\prod_{n=2}^{N} \exp\left[\frac{iS(n,n-1)}{\hbar}\right] = \exp\left[\left(\frac{i}{\hbar}\right)\sum_{n=2}^{N} S(n,n-1)\right] = \exp\left[\frac{iS(N,1)}{\hbar}\right]. \tag{2.5.37}$$

This does not yet give $\langle x_N, t_N | x_1, t_1 \rangle$; rather, this equation is the contribution to $\langle x_N, t_N | x_1, t_1 \rangle$ arising from the particular path we have considered. We must still integrate over $x_2, x_3, \ldots, x_{N-1}$. At the same time, exploiting the composition property, we let the time interval between t_{n-1} and t_n be infinitesimally small. Thus our candidate expression for $\langle x_N, t_N | x_1, t_1 \rangle$ may be written, in some loose sense, as

$$\langle x_N, t_N | x_1, t_1 \rangle \sim \sum_{\text{all paths}} \exp\left[\frac{iS(N,1)}{\hbar}\right], \tag{2.5.38}$$

where the sum is to be taken over an innumerably infinite set of paths!

Before presenting a more precise formulation, let us see whether considerations along this line make sense in the classical limit. As $\hbar \to 0$, the exponential in (2.5.38) oscillates very violently, so there is a tendency for cancellation among various contributions from neighboring paths. This is because $\exp[iS/\hbar]$ for some definite path and $\exp[iS/\hbar]$ for a slightly different path have very different phases because of the smallness of $\hbar$. So most paths do *not* contribute when $\hbar$ is regarded as a small quantity. However, there is an important exception.

Suppose that we consider a path that satisfies

$$\delta S(N,1)=0, \tag{2.5.39}$$

where the change in S is due to a slight deformation of the path with the end points fixed. This is precisely the classical path by virtue of Hamilton's principle. We denote the S that satisfies (2.5.39) by $S_{\min}$. We now attempt to deform the path a little bit from the classical path. The resulting S is still equal to $S_{\min}$ to first order in deformation. This means that the phase of $\exp[iS/\hbar]$ does not vary very much as we deviate slightly from the classical path even if $\hbar$ is small. As a result, as long as we stay near the classical path, constructive interference between neighboring paths is possible. In the $\hbar \to 0$ limit, the major contributions must then arise from a very narrow strip (or a tube in higher dimensions) containing the classical path, as shown in Figure 2.3. Our (or Feynman's) guess based on Dirac's mysterious remark makes good sense because the classical path gets singled out in the $\hbar \to 0$ limit.

To formulate Feynman's conjecture more precisely, let us go back to $\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle$, where the time difference $t_n - t_{n-1}$ is assumed to be infinitesimally small. We write

$$\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle = \left[\frac{1}{w(\Delta t)}\right]\exp\left[\frac{iS(n,n-1)}{\hbar}\right], \tag{2.5.40}$$

where we evaluate $S(n, n-1)$ in a moment in the $\Delta t \to 0$ limit. Notice that we have inserted a weight factor, $1/w(\Delta t)$, which is assumed to depend only on the time interval $t_n - t_{n-1}$ and not on $V(x)$. That such a factor is needed is clear from dimensional considerations; according to the way we

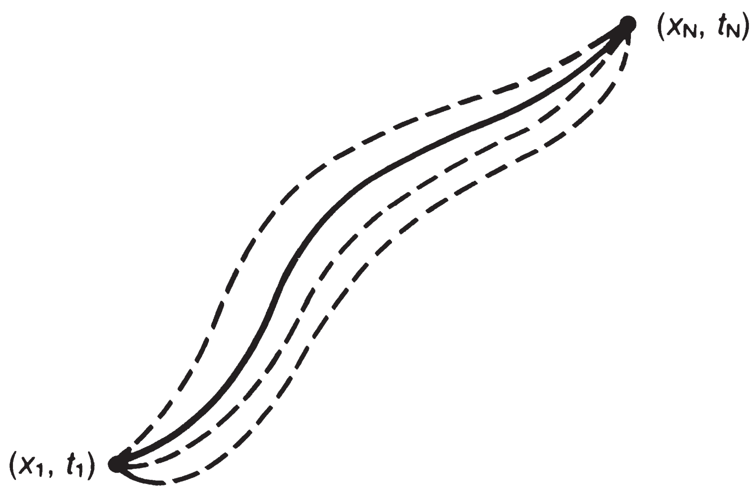

FIGURE 2.3. Paths important in the $\hbar \to 0$ limit.

normalized our position eigenkets, $\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle$ must have the dimension of 1/length.

We now look at the exponential in (2.5.40). Our task is to evaluate the $\Delta t \to 0$ limit of $S(n, n-1)$. Because the time interval is so small, it is legitimate to make a straight-line approximation to the path joining (x_{n-1}, t_{n-1}) and (x_n, t_n) as follows:

$$\begin{aligned} S(n,n-1) &= \int_{t_{n-1}}^{t_n} dt\left[\frac{m\dot{x}^2}{2} - V(x)\right] \\ &= \Delta t\left\{\left(\frac{m}{2}\right)\left[\frac{(x_n - x_{n-1})}{\Delta t}\right]^2 - V\left(\frac{(x_n + x_{n-1})}{2}\right)\right\}. \end{aligned} \tag{2.5.41}$$

As an example, we consider specifically the free-particle case, $V = 0$. Equation (2.5.40) now becomes

$$\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle = \left[\frac{1}{w(\Delta t)}\right]\exp\left[\frac{im(x_n - x_{n-1})^2}{2\hbar\,\Delta t}\right]. \tag{2.5.42}$$

We see that the exponent appearing here is completely identical to the one in the expression for the free-particle propagator (2.5.16). The reader may work out a similar comparison for the simple harmonic oscillator.

We remarked earlier that the weight factor $1/w(\Delta t)$ appearing in (2.5.40) is assumed to be independent of $V(x)$, so we may as well evaluate it for the free particle. Noting the orthonormality, in the sense of δ-function, of Heisenberg-picture position eigenkets at equal times,

$$\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle|_{t_n = t_{n-1}} = \delta(x_n - x_{n-1}), \tag{2.5.43}$$

we obtain

$$\frac{1}{w(\Delta t)} = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}, \tag{2.5.44}$$

where we have used

$$\int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar\,\Delta t}\right) = \sqrt{\frac{2\pi i\hbar\,\Delta t}{m}} \tag{2.5.45a}$$

and

$$\lim_{\Delta t\to 0}\sqrt{\frac{m}{2\pi i\hbar\,\Delta t}}\exp\left(\frac{im\xi^2}{2\hbar\,\Delta t}\right) = \delta(\xi). \tag{2.5.45b}$$

This weight factor is, of course, anticipated from the expression for the free-particle propagator (2.5.16).

To summarize, as $\Delta t \to 0$, we are led to

$$\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle = \sqrt{\frac{m}{2\pi i\hbar\,\Delta t}}\exp\left[\frac{iS(n,n-1)}{\hbar}\right]. \tag{2.5.46}$$

The final expression for the transition amplitude with $t_N - t_1$ finite is

$$\langle x_N, t_N | x_1, t_1 \rangle = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \, \Delta t} \right)^{(N-1)/2} \times \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \prod_{n=2}^{N} \exp\left[\frac{iS(n, n-1)}{\hbar} \right], \tag{2.5.47}$$

where the $N \to \infty$ limit is taken with x_N and t_N fixed. It is customary here to define a new kind of multidimensional (in fact, infinite-dimensional) integral operator

$$\int_{x_1}^{x_N} \mathscr{D}[x(t)] \equiv \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \, \Delta t} \right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \tag{2.5.48}$$

and write (2.5.47) as

$$\langle x_N, t_N | x_1, t_1 \rangle = \int_{x_1}^{x_N} \mathscr{D}[x(t)] \exp\left[i \int_{t_1}^{t_N} dt \frac{L_{\text{classical}}(x, \dot{x})}{\hbar} \right]. \tag{2.5.49}$$

This expression is known as **Feynman's path integral**. Its meaning as the sum over all possible paths should be apparent from (2.5.47).

Our steps leading to (2.5.49) are not meant to be a derivation. Rather, we (or Feynman) have attempted a new formulation of quantum mechanics based on the concept of paths, motivated by Dirac's mysterious remark. The only ideas we borrowed from the conventional form of quantum mechanics are (1) the superposition principle (used in summing the contributions from various alternate paths), (2) the composition property of the transition amplitude, and (3) classical correspondence in the $\hbar \to 0$ limit.

Even though we obtained the same result as the conventional theory for the free-particle case, it is now obvious, from what we have done so far, that Feynman's formulation is completely equivalent to Schrödinger's wave mechanics. We conclude this section by proving that Feynman's expression for $\langle x_N, t_N | x_1, t_1 \rangle$ indeed satisfies Schrödinger's time-dependent wave equation in the variables x_N, t_N, just as the propagator defined by (2.5.8).

We start with

$$\begin{aligned} \langle x_N, t_N | x_1, t_1 \rangle &= \int dx_{N-1} \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle \langle x_{N-1}, t_{N-1} | x_1, t_1 \rangle \\ &= \int_{-\infty}^{\infty} dx_{N-1} \sqrt{\frac{m}{2\pi i \hbar \, \Delta t}} \exp\left[\left(\frac{im}{2\hbar} \right) \frac{(x_N - x_{N-1})^2}{\Delta t} - \frac{iV \Delta t}{\hbar} \right] \\ &\quad \times \langle x_{N-1}, t_{N-1} | x_1, t_1 \rangle, \end{aligned} \tag{2.5.50}$$

where we have assumed $t_N - t_{N-1}$ to be infinitesimal. Introducing

$$\xi = x_N - x_{N-1} \tag{2.5.51}$$

and letting $x_N \to x$ and $t_N \to t + \Delta t$, we obtain

$$\langle x, t+\Delta t | x_1, t_1\rangle = \sqrt{\frac{m}{2\pi i\hbar\,\Delta t}} \int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar\,\Delta t} - \frac{iV\Delta t}{\hbar}\right)\langle x-\xi, t|x_1, t_1\rangle. \tag{2.5.52}$$

As is evident from (2.5.45b), in the limit $\Delta t \to 0$, the major contribution to this integral comes from the $\xi \simeq 0$ region. It is therefore legitimate to expand $\langle x-\xi, t|x_1, t_1\rangle$ in powers of ξ. We also expand $\langle x, t+\Delta t|x_1, t_1\rangle$ and $\exp(-iV\Delta t/\hbar)$ in powers of Δt, so

$$\begin{aligned}\langle x, t|x_1, t_1\rangle &+ \Delta t \frac{\partial}{\partial t}\langle x, t|x_1, t_1\rangle \\ &= \sqrt{\frac{m}{2\pi i\hbar\,\Delta t}} \int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar\,\Delta t}\right)\left(1 - \frac{iV\Delta t}{\hbar} + \cdots\right) \\ &\quad \times \left[\langle x, t|x_1, t_1\rangle + \left(\frac{\xi^2}{2}\right)\frac{\partial^2}{\partial x^2}\langle x, t|x_1, t_1\rangle + \cdots\right],\end{aligned} \tag{2.5.53}$$

where we have dropped a term linear in ξ because it vanishes when integrated with respect to ξ. The $\langle x, t|x_1, t_1\rangle$ term on the left-hand side just matches the leading term on the right-hand side because of (2.5.45a). Collecting terms first order in Δt, we obtain

$$\begin{aligned}\Delta t \frac{\partial}{\partial t}\langle x, t|x_1, t_1\rangle &= \left(\sqrt{\frac{m}{2\pi i\hbar\,\Delta t}}\right)(\sqrt{2\pi})\left(\frac{i\hbar\,\Delta t}{m}\right)^{3/2}\frac{1}{2}\frac{\partial^2}{\partial x^2}\langle x, t|x_1, t_1\rangle \\ &\quad - \left(\frac{i}{\hbar}\right)\Delta t\, V\langle x, t|x_1, t_1\rangle,\end{aligned} \tag{2.5.54}$$

where we have used

$$\int_{-\infty}^{\infty} d\xi\, \xi^2 \exp\left(\frac{im\xi^2}{2\hbar\,\Delta t}\right) = \sqrt{2\pi}\left(\frac{i\hbar\,\Delta t}{m}\right)^{3/2}, \tag{2.5.55}$$

obtained by differentiating (2.5.45a) with respect to Δt. In this manner we see that $\langle x, t|x_1, t_1\rangle$ satisfies Schrödinger's time-dependent wave equation:

$$i\hbar \frac{\partial}{\partial t}\langle x, t|x_1, t_1\rangle = -\left(\frac{\hbar^2}{2m}\right)\frac{\partial^2}{\partial x^2}\langle x, t|x_1, t_1\rangle + V\langle x, t|x_1, t_1\rangle. \tag{2.5.56}$$

Thus we can conclude that $\langle x, t|x_1, t_1\rangle$ constructed according to Feynman's prescription is the same as the propagator in Schrödinger's wave mechanics.

Feynman's space-time approach based on path integrals is not too convenient for attacking practical problems in nonrelativistic quantum mechanics. Even for the simple harmonic oscillator it is rather cumbersome to evaluate explicitly the relevant path integral.* However, his approach is extremely gratifying from a conceptual point of view. By imposing a certain set of sensible requirements on a physical theory, we are inevitably led to a formalism equivalent to the usual formulation of quantum mechanics. It makes us wonder whether it is at all possible to construct a sensible alternative theory that is equally successful in accounting for microscopic phenomena.

Methods based on path integrals have been found to be very powerful in other branches of modern physics, such as quantum field theory and statistical mechanics. In this book the path-integral method will appear again when we discuss the Aharonov-Bohm effect.†

2.6. POTENTIALS AND GAUGE TRANSFORMATIONS

Constant Potentials

In classical mechanics it is well known that the zero point of the potential energy is of no physical significance. The time development of dynamic variables such as $\mathbf{x}(t)$ and $\mathbf{L}(t)$ is independent of whether we use $V(\mathbf{x})$ or $V(\mathbf{x})+V_0$ with V_0 constant both in space and time. The force that appears in Newton's second law depends only on the gradient of the potential; an additive constant is clearly irrelevant. What is the analogous situation in quantum mechanics?

We look at the time evolution of a Schrödinger-picture state ket subject to some potential. Let $|\alpha, t_0; t\rangle$ be a state ket in the presence of $V(\mathbf{x})$, and $\widetilde{|\alpha, t_0; t\rangle}$, the corresponding state ket appropriate for

$$\tilde{V}(\mathbf{x}) = V(\mathbf{x}) + V_0. \tag{2.6.1}$$

To be precise let us agree that the initial conditions are such that both kets coincide with $|\alpha\rangle$ at $t = t_0$. If they represent the same physical situation, this can always be done by a suitable choice of the phase. Recalling that the state ket at t can be obtained by applying the time-evolution operator

*The reader is challenged to solve the simple harmonic oscillator problem using the Feynman path integral method in Problem 2-31.

†The reader who is interested in the fundamentals and applications of path integrals may consult Feynman and Hibbs 1965.