

# Modern Quantum Mechanics Revised Edition

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and so on. If we somehow guess the form of  $\langle x'', t'' | x', t' \rangle$  for an *infinitesimal* time interval (between  $t'$  and  $t'' = t' + dt$ ), we should be able to obtain the amplitude  $\langle x'', t'' | x', t' \rangle$  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

$$x'''' \cdots x'''' \\ N \text{ times}$$

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:

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

Exploiting the composition property, we obtain

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

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  $x_2, x_3, \dots, x_{N-1}$ . 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

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

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

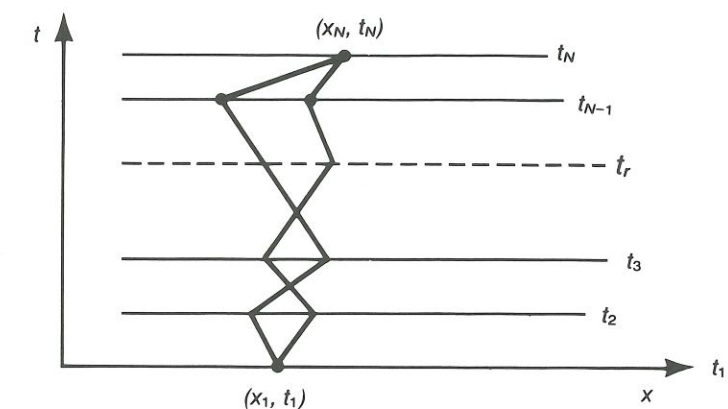


FIGURE 2.2. Paths in  $xt$ -plane.

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

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

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

$$x = h - \frac{gt^2}{2}. \quad (2.5.34)$$

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:

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

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  $\hbar \rightarrow 0$ . 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:

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

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:

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

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

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

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  $x_2, x_3, \dots, x_{N-1}$ . 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

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

where the sum is to be taken over an innumerable 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  $\hbar \rightarrow 0$ , 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

$$\delta S(N, 1) = 0, \quad (2.5.39)$$

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  $S_{\text{min}}$ . We now attempt to deform the path a little bit from the classical path. The resulting  $S$  is still equal to  $S_{\text{min}}$  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  $\hbar \rightarrow 0$  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  $\hbar \rightarrow 0$  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

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

where we evaluate  $S(n, n-1)$  in a moment in the  $\Delta t \rightarrow 0$  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

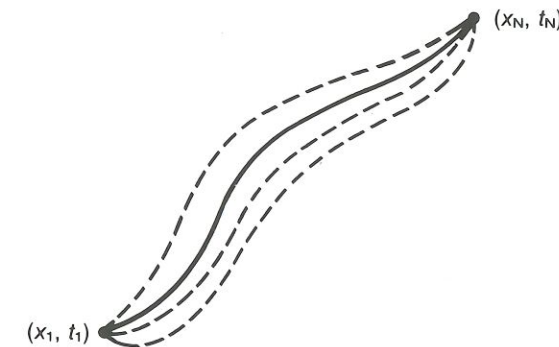


FIGURE 2.3. Paths important in the  $\hbar \rightarrow 0$  limit.

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  $\Delta t \rightarrow 0$  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:

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

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

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

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  $\delta$ -function, of Heisenberg-picture position eigenkets at equal times,

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

we obtain

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

where we have used

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

and

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

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

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

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

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

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

where the  $N \rightarrow \infty$  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

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

and write (2.5.47) as

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

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  $\hbar \rightarrow 0$  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

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

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

$$\xi = x_N - x_{N-1} \quad (2.5.51)$$

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

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

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

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

where we have dropped a term linear in  $\xi$  because it vanishes when integrated with respect to  $\xi$ . 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  $\Delta t$ , we obtain

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

where we have used

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

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

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

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  $|\alpha, t_0; t\rangle$ , the corresponding state ket appropriate for

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

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.