Chapter 2

Quantum Mechanical Path Integrals

In this chapter the standard version of nonrelativistic quantum mechanics will be reformulated in terms of a path integral. The path integral will be derived as a limiting expression from the fundamental structure of nonrelativistic quantum mechanics, and will be valid for a wide variety of systems. In this sense the path integral is a representation of quantum mechanical amplitudes equivalent to the usual wave mechanical or matrix formulations of these same amplitudes. This is extremely useful since there is no ambiguity in the path integral's definition. For this reason the form of the path integral derived in this case serves as a motivating form for a generalization of the path integral to all quantum processes.

In Sec. 2.1 the relevant aspects of basic quantum mechanics are reviewed. In Sec. 2.2 these are used to find the path integral form for a quantum mechanical amplitude. In Sec. 2.3 the idea of the path integral as a "sum over histories" is presented as a conceptual generalization of the results of Sec. 2.2. Some of the formidable mathematical difficulties associated with this generalization are sketched.

2.1 Quantum Mechanics

The Hamiltonian formulation of classical mechanics, discussed in Sec. 1.3, serves as the starting point for the operator form of quantum mechanics [1, 2, 3]. In the Hamiltonian formalism the generalized coordinates, q_j, and their canonically conjugate momenta, p_j, are the fundamental mechanical

"observables" of a particle or system. In quantum mechanics these become operators defined on an abstract Hilbert space $\mathcal{H}$ that represents all possible quantum mechanical configurations in which the system may be observed. These operators, denoted Q_j and P_j, are assumed to obey the commutation relation

$$[Q_j, P_k] \equiv Q_j P_k - P_k Q_j = i\hbar\delta_{jk} , \tag{2.1}$$

where $\hbar$ is Planck's constant. The elements of the Hilbert space $\mathcal{H}$ are called *states* and are written $|\psi\rangle$. The operators Q and P are assumed to have a complete set of eigenstates $|q\rangle$ and $|p\rangle$ such that

$$Q_j|q\rangle = q_j|q\rangle , \; P_j|p\rangle = p_j|p\rangle , \tag{2.2}$$

so that q_j and p_j are the eigenvalues of the respective operators.

The Hilbert space $\mathcal{H}$ is equipped with an inner product. If $|\psi\rangle$ and $|\phi\rangle$ are any two states in $\mathcal{H}$, then their inner product is denoted $\langle\psi|\phi\rangle$, and obeys

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* , \tag{2.3}$$

so that its form is analogous to the inner product for the functions of Sec. 1.3 or the vectors of Sec. 1.4. The inner products of the $|p\rangle$ and $|q\rangle$ states are assumed to obey

$$\langle q|q'\rangle = \delta^n(q-q') , \; \langle p|p'\rangle = \delta^n(p-p') , \tag{2.4}$$

so that these states are orthonormal in the continuum sense. The Dirac delta appearing in (2.4) is understood to have the test function space L^2, the space of all square integrable functions. It is also assumed that these states are complete, so that the states $|p\rangle$ and $|q\rangle$ both span the Hilbert space $\mathcal{H}$. In the continuum normalization of (2.4) this means that

$$\int d^n p\,|p\rangle\langle p| = 1 , \; \int d^n q\,|q\rangle\langle q| = 1 , \tag{2.5}$$

where the limits on the integrals of (2.5) must run over the entirety of the phase space available to the system. Coupling the algebra of (2.1) with the inner product (2.4) gives the coordinate representation of the momentum operator

$$\langle q|P_j|q'\rangle = -i\hbar\frac{\partial}{\partial q_j}\delta^n(q-q') . \tag{2.6}$$

This, in turn, gives the inner product

$$\langle q|p\rangle = \frac{1}{(2\pi\hbar)^{n/2}}\exp\left(\frac{i}{\hbar}p\cdot q\right) . \tag{2.7}$$

The factors present in (2.7) are necessary in order that

$$\langle q \,|\, q' \rangle = \int_{-\infty}^{\infty} d^n p \, \langle q \,|\, p \rangle \langle p \,|\, q' \rangle$$
$$= \int_{-\infty}^{\infty} \frac{d^n p}{(2\pi\hbar)^n} \, e^{ip\cdot(q-q')/\hbar} = \delta^n(q - q') \, . \tag{2.8}$$

The formal similarity of (2.1) to (1.50) indicates that the classical mechanical Poisson brackets of two observables, $A(p,q)$ and $B(p,q)$, must be replaced in quantum mechanics by commutators in the manner

$$\{A(p,q), B(p,q)\}_{p,q} \rightarrow \frac{1}{i\hbar}[A(P,Q), B(P,Q)] \, . \tag{2.9}$$

If O is a quantum mechanical observable, i.e., some function of Q, P, and possibly t, then (1.49) and the formal identity (2.9) gives

$$i\hbar \frac{dO}{dt} = i\hbar \frac{\partial O}{\partial t} + [O, H] \, , \tag{2.10}$$

where $H = H(P,Q,t)$ is the Hamiltonian of the system under analysis. Thus, the time development of a quantum mechanical observable is driven by the Hamiltonian of the system, just as it is in classical mechanics.

The physical system is represented by a state $|\, \psi \rangle$ in the Hilbert space $\mathcal{H}$, and the state is assumed to be of unit length, so that $\langle \psi \,|\, \psi \rangle = 1$. It follows from (2.10) that the time development of the state $|\, \psi \rangle$ is given by the Schrödinger equation

$$H |\, \psi, t \rangle_s = i\hbar \frac{\partial}{\partial t} |\, \psi, t \rangle_s \, . \tag{2.11}$$

The standard differential version of the Schrödinger equation used in wave mechanics may be obtained from (2.11) by forming the inner product with the position eigenstate $|\, q \rangle$, and identifying the wave-function $\psi(q,t) = \langle q \,|\, \psi, t \rangle_s$. This results in the differential equation

$$H(-i\hbar \frac{\partial}{\partial q}, q) \, \psi(q,t) = i\hbar \frac{\partial}{\partial t} \psi(q,t) \, . \tag{2.12}$$

When the system is in the state $|\, \psi \rangle$, the expectation value of a measurement of the observable $O(P,Q)$ is given by

$$\langle O \rangle = \langle \psi \,|\, O(P,Q) \,|\, \psi \rangle = \int dq \, \psi^*(q,t) \, O(-i\hbar \frac{\partial}{\partial q}, q) \, \psi(q,t) \, , \tag{2.13}$$

leading to the interpretation of $|\psi(q)|^2$ as a probability density. The normalization of the state,

$$\langle \psi \,|\, \psi \rangle = \int dq \, |\psi(q,t)|^2 = 1 \,, \tag{2.14}$$

is simply a reflection of the fact that the total probability of observing the particle must be unity.

In the Schrödinger picture of quantum mechanics the states, $|\,\psi\rangle_S$, are manifestly time dependent, while the observables are not, so that, if H has no explicit time dependence, the state at time t evolves from the state at $t = 0$ according to

$$|\,\psi, t\rangle_S = \exp\left(-\frac{i}{\hbar} H t\right) |\,\psi\rangle_S \,. \tag{2.15}$$

If H is time dependent, then (2.15) must be replaced with the time-ordered integral of H. This is denoted by

$$|\,\psi, t\rangle_S = T\left\{\exp\left[-\frac{i}{\hbar}\int_0^t d\tau \, H(\tau)\right]\right\} |\,\psi\rangle_S \,. \tag{2.16}$$

Time ordering means expanding the exponential in (2.16) so that the operators are ordered sequentially according to their time argument, with the latest at the left and earliest at the right. This is most easily expressed by introducing the step function $\theta(\tau)$, which is defined as

$$\theta(\tau) = \begin{cases} 1 & \text{if } \tau > 0, \\ \\ 0 & \text{if } \tau < 0. \end{cases} \tag{2.17}$$

Exercise 2.1: Show that $\theta(\tau)$ has the integral representation

$$\theta(\tau) = \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{i\omega\tau}}{\omega - i\epsilon} \,, \tag{2.18}$$

and that

$$\frac{\partial}{\partial t}\theta(t) = \delta(t) \,. \tag{2.19}$$

Using the step function, the time-ordered product of two time-dependent operators can be written

$$T\{A(t_1)B(t_2)\} = \theta(t_1 - t_2)A(t_1)B(t_2) + \theta(t_2 - t_1)B(t_2)A(t_1) \,. \tag{2.20}$$

The generalization of (2.20) to the time-ordered product of many operators is obvious.

In the Heisenberg picture of quantum mechanics the observables, O_H, are time dependent, and from (2.10), they satisfy

$$i\hbar\frac{d}{dt}O_H = i\hbar\frac{\partial}{\partial t}O_H + [O_H, H] \,. \tag{2.21}$$

The equality of the matrix elements in the respective pictures gives

$${}_H\langle\, \psi \,|O_H(t)|\, \phi \,\rangle_H = {}_S\langle\, \psi, t \,|O_S|\, \phi, t \,\rangle_S \,, \tag{2.22}$$

so that differentiation of (2.22) gives

$$i\hbar\frac{\partial O_H}{\partial t} = [O_H, H] \,. \tag{2.23}$$

If H has no explicit time dependence, then the Heisenberg picture operators of (2.23) at time t can written in terms of the operators at $t = 0$ in the form

$$O_H(t) = e^{iHt/\hbar}O_H e^{-iHt/\hbar} \,. \tag{2.24}$$

If H is explicitly time dependent, then it is necessary to use time ordering, as in (2.16). The Heisenberg picture states, $|\,\psi\,\rangle_H$, are time independent. It is clear that the Schrödinger picture and Heisenberg picture can be chosen to coincide at some specific time. In what follows it will be assumed that this time is $t = 0$, and any state with no explicit time dependence displayed can be considered to be either a Heisenberg picture state or a Schrödinger picture state at $t = 0$.

In the path integral formulation of quantum mechanics the object of utmost interest is the transition amplitude. If the system is in the Schrödinger picture state $|\,\phi, t_a\,\rangle$ at the time t_a, then the transition amplitude to the state $|\,\psi, t_b\,\rangle$ at the time t_b is defined as

$$Z(\psi, \phi) = \langle\, \psi, t_b \,|\, \phi, t_a \,\rangle \,. \tag{2.25}$$

The transition amplitude then gives the probability of the system transiting between the respective states as $P = |Z|^2$, so that Z describes a *quantum process*. In the next section the transition amplitude is given a path integral representation.

2.2 The Path Integral Derived

In this section the transition amplitude will be given a path integral representation by applying the results of the previous section. The pivotal

idea, first noted by Dirac [4], is that the infinitesimal quantum mechanical transition amplitude is governed by the value of the classical action. Using fairly intuitive arguments, this idea was developed by Feynman [5, 6] into the path integral representation of the finite transition amplitude, and later presented in detail in the book by Feynman and Hibbs [7]. The path integral derived in this section will be identical in form to that first developed by Feynman. However, a derivation based on the canonical structure of quantum mechanics has the advantage of demonstrating that the path integral must yield results identical to those obtained by the standard methods of wave mechanics or matrix manipulation. For that reason it is an immensely valuable heuristic device for testing generalizations of the path integral form to systems where a rigorous derivation is impossible.

It is therefore very important to list the assumptions that go into this derivation, so that they may be kept in mind during any generalization. First, it will be assumed that the limits on the statement of completeness (2.5) are $\pm\infty$. Second, it will be assumed that the Hamiltonian H has no explicit time dependence, although this is not necessary. Third, and this is for simplicity of notation, the system will be considered to be that of a one-dimensional single particle moving in a potential.

The first step in the derivation of the path integral [3, 8, 9] is to construct the "instantaneous" eigenstates, $|q,t\rangle$ and $|p,t\rangle$, of the Heisenberg picture operators $Q(t)$ and $P(t)$. These are defined by

$$|q,t\rangle = e^{iHt/\hbar}|q\rangle\,, \quad |p,t\rangle = e^{iHt/\hbar}|p\rangle\,. \tag{2.26}$$

It is to be noted that these states are *not* Schrödinger picture states. However, these states are complete, since it follows from (2.5) that

$$\begin{aligned}&\int_{-\infty}^{\infty} dq\,|q,t\rangle\langle q,t| \\ &= \exp(iHt/\hbar)\left(\int_{-\infty}^{\infty} dq\,|q\rangle\langle q|\right)\exp(-iHt/\hbar) = 1\,.\end{aligned} \tag{2.27}$$

The state $|q,t\rangle$ is an eigenstate of the Heisenberg picture operator $Q(t)$ in the sense that

$$Q(t)\,|q,t\rangle = q\,|q,t\rangle\,. \tag{2.28}$$

These states also have the valuable property that, for $|\psi,t\rangle$ a Schrödinger picture state,

$$\langle q,-t\,|\,\psi,t\rangle = \langle q\,|\,\psi\rangle = \psi(q)\,. \tag{2.29}$$

A similar pair of statements holds for the instantaneous momentum eigenstates.

These states can be used to derive the path integral form for the transition element between Schrödinger picture states. The object of interest, Z, is defined as the inner product of the instantaneous eigenstates at different times, so that

$$Z(q_a, t_a, q_b, t_b) = \langle\, q_b, t_b \,|\, q_a, t_a \,\rangle\,, \tag{2.30}$$

where it is assumed that $t_b > t_a$. Knowledge of the form for Z allows the calculation of the more general form (2.25), since it follows that the transition element between Schrödinger picture states is given by

$$\begin{aligned}
&\langle\, \psi, -t_b \,|\, \phi, -t_a \,\rangle \\
&= \int_{-\infty}^{\infty} dq_a\, dq_b\, \langle\, \psi, -t_b \,|\, q_b, t_b \,\rangle \langle\, q_b, t_b \,|\, q_a, t_a \,\rangle \langle\, q_a, t_a \,|\, \phi, -t_a \,\rangle \\
&= \int_{-\infty}^{\infty} dq_a\, dq_b\, \psi^*(q_b) \phi(q_a) Z(q_a, t_a, q_b, t_b)\,,
\end{aligned} \tag{2.31}$$

where properties (2.27) and (2.29) have been used. Once the initial and final states of the system are specified by the normalized forms for $\psi(q)$ and $\phi(q)$, the system propagates in time from ψ to ϕ through the function Z. For this reason the transition element (2.30) is sometimes referred to as the *propagator*, since it contains all the information regarding the time development of the system.

The time interval $t_b - t_a$ is first partitioned into N infinitesimal steps of duration $\epsilon = (t_b - t_a)/N$, where the limit $N \to \infty$ is understood in everything that follows. Next, $N-1$ complete sets of intermediate instantaneous $|\, q \,\rangle$ eigenstates are inserted into the transition element sequentially at each of the respective times $t_n = t_a + n\epsilon$. This gives

$$\begin{aligned}
Z(q_a, t_a, q_b, t_b) \;=\; &\int_{-\infty}^{\infty} dq_1 \cdots dq_{N-1}\, \langle\, q_b, t_b \,|\, q_{N-1}, t_{N-1} \,\rangle \\
&\times \langle\, q_{N-1}, t_{N-1} \,|\, \cdots \,|\, q_1, t_1 \,\rangle \langle\, q_1, t_1 \,|\, q_a, t_a \,\rangle\,,
\end{aligned} \tag{2.32}$$

so that the whole transition element has been reduced to the product of N transition elements, which are infinitesimal in the sense that their time difference approaches zero. Each one of the infinitesimal transition elements may now be analyzed. Since the time difference is ϵ between the two states, it follows from the definition (2.26) that the jth element is given by

$$\langle\, q_{j+1}, t_{j+1} \,|\, q_j, t_j \,\rangle = \langle\, q_{j+1} \,|\, e^{-i\epsilon H(P,Q)/\hbar} \,|\, q_j \,\rangle\,. \tag{2.33}$$

In order to proceed further it is necessary to select a convention that will be used consistently to reduce all the infinitesimal elements. To evaluate the matrix element of the exponentiated Hamiltonian, the exponential must

be expanded in a power series. After the expansion all the P operators will be moved to the left and all the Q operators will be moved to the right. For want of a better name this will be referred to as *coordinate ordering*. The final result of coordinate ordering a product of P's and Q's will be that all the P operators lie on the left side of the expression and all the Q operators will lie on the right side of the expression. The coordinate ordering operation will be denoted by $C\{\cdots\}$, so that, for example,

$$C\{PQP^2\} = P^3Q\,. \tag{2.34}$$

Obviously, the opposite convention can be selected, and it is natural to consider the possibility that the existence of different ordering schemes might induce some ambiguity in the resulting path integral [10]. That the same form results is given as Exercise 2.4. The advantage of coordinate ordering is that an arbitrary function of Q and P, denoted $f(Q,P)$, has the matrix element

$$\langle p\,|\,C\{f(Q,P)\}\,|\,q\rangle = f(q,p)\,\langle p\,|\,q\rangle\,, \tag{2.35}$$

so that a coordinate-ordered function of the operators may be reduced to a c-number (classical number) function by taking its matrix element. Result (2.35) can be demonstrated by using a power series representation of the c-number function f and by noting that coordinate ordering suppresses the presence of any commutators between Q and P.

The next step in evaluating (2.33) is to observe that

$$e^{-i\epsilon H(P,Q)/\hbar} = C\left\{e^{-i\epsilon H(P,Q)/\hbar}\right\} + O(\epsilon^2)\,. \tag{2.36}$$

The proof of this statement for a general Hamiltonian is given as Exercise 2.2. However, a demonstration for the particularly simple but physically meaningless form $H = aP + bQ$ is instructive because of its use of the Baker–Campbell–Hausdorff theorem. The operator version of this theorem is identical to the form proved in Sec. 1.4 for matrices. Using this theorem shows that

$$e^{-i\epsilon(aP+bQ)/\hbar} = e^{-i\epsilon aP/\hbar}e^{-i\epsilon bQ/\hbar}e^{i\epsilon^2 ab/2\hbar}\,, \tag{2.37}$$

so that the effects of the commutator (2.1) are $O(\epsilon^2)$ and are therefore irrelevant in the $\epsilon \to 0$ limit. Since the commutator represents quantum effects, or *quantum corrections*, this verifies the intuitive notion that, for infinitesimal time periods, the time development of the system is overwhelmingly dominated by classical dynamics. The generalization of this result, showing that the $O(\epsilon^2)$ term in (2.36) is ignorable, can be accomplished by using

the Trotter product formula [11, 12]. If A and B are any two bounded operators, the Trotter product formula gives

$$\exp[t(A+B)] = \lim_{n\to\infty}\left[\exp\left(\frac{t}{n}A\right)\exp\left(\frac{t}{n}B\right)\right]^n . \tag{2.38}$$

Exercise 2.2: Prove (2.38) and adapt the theorem to demonstrate that, in the $\epsilon \to 0$ limit, the commutators generated by a Hamiltonian of the form $H = P^2/2m + V(Q)$ are irrelevant to the evaluation of (2.33).

These results show that the infinitesimal transition element (2.33) becomes, for $\epsilon \approx 0$,

$$\begin{aligned}
&\langle\, q_{j+1} \,|e^{-i\epsilon H(P,Q)/\hbar}|\, q_j \,\rangle \\
&= \int_{-\infty}^{\infty} dp_j \,\langle\, q_{j+1} \,|\, p_j \,\rangle\langle\, p_j \,|\, e^{-i\epsilon H(P,Q)/\hbar} \,|\, q_j \,\rangle \\
&\approx \int_{-\infty}^{\infty} dp_j \, e^{-i\epsilon H(p_j,q_j)/\hbar}\langle\, q_{j+1} \,|\, p_j \,\rangle\langle\, p_j \,|\, q_j \,\rangle \,.
\end{aligned} \tag{2.39}$$

This infinitesimal element can be simplified further by using (2.7) to give

$$\langle\, q_{j+1} \,|\, p_j \,\rangle\langle\, p_j \,|\, q_j \,\rangle = \frac{1}{2\pi\hbar} e^{ip_j(q_{j+1}-q_j)/\hbar} \,. \tag{2.40}$$

Using the fact that q_j is the coordinate value associated with the state at time t_j allows the *formal* identification

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}(q_{j+1}-q_j) = \frac{dq_j}{dt} \equiv \dot{q}_j \,. \tag{2.41}$$

Using this identification, the infinitesimal matrix element can be written

$$\begin{aligned}
\langle\, q_{j+1}, t_{j+1} \,|\, q_j, t_j \,\rangle \;&\approx\; \int_{-\infty}^{\infty} \frac{dp_j}{2\pi\hbar} \exp\left\{-\frac{i}{\hbar}\epsilon\left[p_j\dot{q}_j - H(p_j,q_j)\right]\right\} \\
&=\; \int_{-\infty}^{\infty} \frac{dp_j}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\epsilon\,\mathcal{L}(p_j,q_j)\right] \,,
\end{aligned} \tag{2.42}$$

where

$$\mathcal{L}(p_j,q_j) = p_j\dot{q}_j - H(p_j,q_j) \,. \tag{2.43}$$

First discussed in Sec. 1.3, $\mathcal{L}(p_j,q_j)$ is the Lagrangian density in Hamilton's formulation of the classical mechanical system.

The finite transition element Z can finally be written as the product of the N infinitesimal elements, giving

$$\langle q_b, t_b \,|\, q_a, t_a \rangle$$
$$= \int_{-\infty}^{\infty} \frac{dp_0}{2\pi\hbar} \cdots \frac{dp_{N-1}}{2\pi\hbar}\, dq_1 \cdots dq_{N-1} \exp\left[\frac{i}{\hbar} \sum_{j=0}^{N-1} \epsilon\, \mathcal{L}(p_j, q_j)\right] , \quad (2.44)$$

where the identifications $q_0 = q_a$ and $q_N = q_b$ are implicit in (2.44). The argument of the exponential in (2.44) has the form of a Riemann sum, enabling the identification

$$\lim_{\epsilon \to 0} \sum_{j=0}^{N-1} \epsilon\, \mathcal{L}(p_j, q_j) = \int_{t_a}^{t_b} dt\, \mathcal{L}(p, q) = S\,[p(t), q(t), t_a, t_b] \ , \quad (2.45)$$

Thus, the classical action has appeared in the quantum mechanical transition element. The *path integral measure* appearing in (2.44) is written formally as

$$\lim_{N \to \infty} \frac{dp_0}{2\pi\hbar} \cdots \frac{dp_{N-1}}{2\pi\hbar}\, dq_1 \cdots dq_{N-1} \equiv \mathcal{D}p\,\mathcal{D}q \ . \quad (2.46)$$

Form (2.46), when combined with the exponential of the action, technically does not meet the mathematical criteria required for a probability measure [13]; nevertheless, it will be referred to as the path integral measure throughout what follows. This problem is discussed further in Sec. 2.3.

The final form of the transition element is then given by

$$\langle q_b, t_b \,|\, q_a, t_a \rangle = \int_{q_a}^{q_b} \mathcal{D}p\,\mathcal{D}q \, \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} dt\, \mathcal{L}(p, q)\right\} \ , \quad (2.47)$$

where the limits on the q integrals are present to remind the user that q_0 and q_N are identified as q_a and q_b. Expression (2.47) is the fundamental form for the path integral version of the propagator. The measure appearing in (2.47) ranges over the entire *phase space* available to the particle as it propagates from q_a to q_b.

Exercise 2.3: Consider a Hamiltonian H that is explicitly time dependent in the sense that time-dependent c-number functions (*not* velocity-dependent potentials) may appear in the Lagrangian density. Use (2.16) to show that the resulting path integral representation of the transition element is unchanged in form.

Exercise 2.3 gives the important result that Lagrangian densities describing systems with time-dependent parameters can immediately be given a path integral representation with no difficulty.

Exercise 2.4: Consider a definition of coordinate ordering where the P operator is moved to the right and the Q operator is moved to the left. Derive the form of the path integral for this definition.

Exercise 2.5: Extend the path integral formalism to a system with n degrees of freedom.

Some applications of the path integral found in the literature do not have $\mathcal{D}p$ appearing in the measure. This is not necessarily incorrect since it is possible to integrate all the p_j appearing in (2.42) for a large class of Lagrangians. An example of this occurs when the Lagrangian density of the system has the form

$$\mathcal{L}(p,q) = p\dot{q} - \frac{p^2}{2m} - V(q)\,, \tag{2.48}$$

Since this gives rise to an integral Gaussian in p, it is possible to evaluate exactly the p integration in all the infinitesimal transition elements (2.42). It follows from (1.107) that

$$\begin{aligned}
&\int_{-\infty}^{\infty} \frac{dp_j}{2\pi\hbar} \exp\frac{i}{\hbar}\left[p_j(q_{j+1}-q_j) - \epsilon\frac{p_j^2}{2m} - \epsilon V(q_j)\right] \\
&= \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \exp\frac{i}{\hbar}\epsilon\left[\frac{1}{2}m\left(\frac{q_{j+1}-q_j}{\epsilon}\right)^2 - V(q_j)\right] \\
&= \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \exp\left[\frac{i}{\hbar}\epsilon\,\mathcal{L}(\dot{q},q)\right]\,,
\end{aligned} \tag{2.49}$$

where the identification (2.41) has again been made. In this case the path integral has become

$$\langle\, q_b, t_b \,|\, q_a, t_a \,\rangle = \int_{q_a}^{q_b} \overline{\mathcal{D}}q \, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \mathcal{L}(\dot{q},q)\right\}\,, \tag{2.50}$$

where

$$\mathcal{L}(\dot{q},q) = \tfrac{1}{2}m\dot{q}^2 - V(q)\,. \tag{2.51}$$

The factors resulting from the dp integrations have been absorbed into the measure, giving the definition

$$\overline{\mathcal{D}}q \equiv \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} dq_1\cdots dq_{N-1}\,. \tag{2.52}$$

The form (1.38) of the classical mechanical action has emerged in this case. It is form (2.50) which will be used to generalize the path integral in the next section, although (2.47) is a more general and useful form than (2.50).

The path integral form (2.50) has been derived assuming that the potential $V(q)$ appearing in the Lagrangian density is not velocity dependent. Some physical systems are characterized by a velocity-dependent potential. It is still possible to derive a path integral for the propagator; however, there may be ambiguities in the final form. The demonstration of this is left as the following exercise.

Exercise 2.6: Consider a one-dimensional system with a point mass moving in the velocity-dependent potential

$$V(\dot{q},q) = \tfrac{1}{2}\alpha\dot{q}^2q^2\,.$$

Derive the form of the path integral equivalent to (2.50) and discuss any ambiguities that are present in the coordinate ordering problem for this potential.

2.3 The Sum over Histories

In the previous section the path integral expression for the transition amplitude was derived from the standard operator formulation of quantum mechanics. Although the measure in the second form (2.50) of the path integral is singular in the $\epsilon \to 0$ limit, the path integral, as defined in the previous section, must yield results that are identical to any other valid approach to the same problem. That this is true will be seen in detail in the next chapter. However, for the moment the explicit evaluation of the path integral will be deferred and attention will be focussed on generalizing the concepts contained in, and indicated by, the form of the path integral in hand. It will be argued that such a generalization is not rigorously defensible at this time, and that it is well to remember this when applying path integrals to new problems. In generalizing the concepts of the path

integral it is also necessary to remember the assumptions that went into the derivation of the previous section.

It is the outstanding feature of the path integral that the classical action of the system has appeared in a quantum mechanical expression, and it is this feature that is considered central to any extension of the path integral formalism. It is the path integral of (2.50), obtained by integrating the momenta p_j, that will serve as the form for motivating the conceptual generalization. In the first step, the integrations over the q_j will be replaced by a Riemann sum of the form

$$\int_{-\infty}^{\infty} dq_j \rightarrow \sum_{n_j=-\infty}^{\infty} \epsilon_q \,, \tag{2.53}$$

where ϵ_q is understood to be the infinitesimal measure element on all the q_j integrations. The path integral (2.50) then becomes

$$\begin{aligned} \langle q_b, t_b \,|\, q_a, t_a \rangle \;\rightarrow\; & \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \sum_{n_1=-\infty}^{\infty} \epsilon_q \cdots \sum_{n_{N-1}=-\infty}^{\infty} \epsilon_q \\ & \times \exp\left[\frac{i}{\hbar}\sum_{j=0}^{N-1} \epsilon\, \mathcal{L}\left([n_{j+1}-n_j]\frac{\epsilon_q}{\epsilon}, n_j\epsilon_q\right)\right] , \end{aligned} \tag{2.54}$$

where n_0 and n_{N-1} are defined by $q_a = n_0\epsilon_q$ and $q_b = n_N\epsilon_q$.

This form of the path integral then represents the sum over all possible sets of values for the $N-1$ integer variables $\{n_j\}$. Each set of values is weighted by the exponential of the value of the action for that set of values. Specifying a set of $\{n_j\}$ is equivalent to specifying a set of $\{q_j\}$, and these values represent the intermediate values of the particle's position as it moves from q_a to q_b. In effect, specifying a set of values $\{n_j\}$ defines a *discrete path* from q_a to q_b, i.e., a set of $N-1$ intermediate positions for the particle. In the $\epsilon_q \rightarrow 0$ limit any piecewise continuous path from q_a to q_b can be represented in this manner. Thus, in the limit, the path integral can be viewed as a sum over all piecewise continuous paths from q_a to q_b in the time interval $t_b - t_a$, with each path receiving a weighting factor given by the exponential of the *classical* action along that path. In this way every piecewise continuous path represents a possible "history" of the particle's motion, and the path integral representation of the transition element is a weighted sum over all possible histories.

It is this observation that is the starting point for the generalization of the path integral, derived in the last section, to systems whose quantization by other techniques may not be well understood. In this approach to

describing a quantum process, one begins by writing the classical action S for the system under consideration. This specifies the dynamical variables of the system, e.g., $q(t)$ in the case of quantum mechanics. The transition amplitude Z of the *quantized* system is then assumed to be given by

$$Z = \sum_{\text{paths}} e^{iS/\hbar} , \tag{2.55}$$

where the paths must be chosen to go from some initial configuration of the dynamical variables to some final configuration. In (2.55) the formal derivatives of (2.41) are taken to be the exact statements, and in that sense (2.55) is a *continuum* version of the path integral derived in the previous section. The advantage of such a picture for quantum processes is the intuitive power that it brings. In the path integral formulation the classical paths of Newton have reappeared in the quantized system, allowing a graphical interpretation of quantum processes. However, the deceptive simplicity of statement (2.55) cloaks many subtle, and as yet unresolved, mathematical difficulties, and at least a cursory discussion of some of these must be made.

First, there are numerous classical systems for which no sensible quantum theory exists. Cases of this are very easy to find, even in simple one-dimensional quantum mechanical systems. A simple example is the potential $V = \alpha q^2 - \beta q^4$. If β is a positive constant the potential is unbounded from below. Even though it is possible, at least formally, to write down classical solutions to the equation of motion, the quantum theory cannot be stable since there is no normalizable ground state. Another problem associated with converting a classical mechanical system to a quantum mechanical path integral is that it is not obvious, at first glance, how to implement classical constraints on motion in a quantum mechanically consistent manner. At an even more subtle level, it will be seen that some field theories cannot be consistently quantized because of quantum mechanical anomalies in their conservation laws. The path integral approach cannot possibly improve such situations, and it may even obscure some of the problems if it is indiscriminately applied.

Second, the motivating form (2.54) indicates that the only difference in weighting each path receives is the exponential of the value of the action associated with the path, and that the prefactors, i.e., the ϵ factors in (2.54), are the same for all paths. That this is true for all quantum systems, or rather might be an artifact of the assumptions made in deriving the form (2.50), is not *a priori* obvious. For example, the assumption was made that the limits on the intermediate q_j integrations were $\pm\infty$. If, instead, the system under consideration is a particle in a one-dimensional box of

width L, then clearly the integrations over the q_j should have the range 0 to L, and that in itself will give a different result for (2.47). Obtaining a form similar to (2.50) raises additional difficulties. Later in this section a similar system, a point mass on a circle, will be analyzed, and these points will become manifestly clear. There it will not be apparent that the path integral derived from the quantum mechanical solution to the problem has any reference to the classical action for the system.

Third, to say that there are "many" paths from q_a to q_b would be something of an understatement. However, there are many pathological paths that cannot contribute. For example, if t_a is a rational number and t_b is an irrational number, then a possible path would be given by the Dirichlet function,

$$q(t) = \begin{cases} q_a & \text{if } t \text{ is rational,} \\ \\ q_b & \text{if } t \text{ is irrational.} \end{cases} \tag{2.56}$$

Such a path is not piecewise continuous and by that criterion should be excluded from the sum. In addition, the set of all piecewise continuous paths contains both discontinous and nondifferentiable paths, and these are, in some sense, "far away" from the typically smooth and completely continuous classical trajectories that extremize the action. Intuitively, paths far from the classical trajectories would be expected to contribute little to the path integral, since a gross deviation from classical behavior violates the idea that quantum corrections to most physical processes are small. Of course, quantum mechanics counters this intuition with the presence of a discrete set of bound states. This is far from the classical behavior of the system, which allows a continuum of bound states to occur in attractive potentials. In the path integral it is unclear how the bound state structure is manifested in a sum over histories, since a discrete set of bound states corresponds classically to a discrete set of bounded trajectories.

That paths associated with large values for the action do not contribute significantly to the path integral can be inferred from the Riemann–Lebesgue lemma [14]. This states that, if $f(\alpha)$ is an integrable function,

$$\lim_{t\to\infty} \int d\alpha\, f(\alpha) \sin(\alpha t) = 0\,. \tag{2.57}$$

The Riemann–Lebesgue lemma can be proved by treating $\lim_{t\to\infty} \sin(\alpha t)$ as a distribution. It then follows that

$$\lim_{t\to\infty} \sin(\alpha t) = \int_0^\infty dt\, \frac{d}{dt} \sin(\alpha t) = \tfrac{1}{2}\alpha \int_{-\infty}^{\infty} dt\, e^{i\alpha t} = \pi\alpha\, \delta(\alpha)\,, \tag{2.58}$$

which agrees with result (2.57).

Exercise 2.7: Show that $\lim_{t\to\infty} \cos(\alpha t) = 0$.

These results show that, as a distribution,

$$\lim_{t\to\infty} e^{i\alpha t} = \pi i \alpha\, \delta(\alpha)\,, \tag{2.59}$$

which vanishes when integrated against a well-behaved function. In this sense, paths with infinite values for the action will not contribute to the path integral.

These remarks serve to draw attention to the major difficulty in generalizing the path integral to a sum over histories, and that is the question of precisely how this sum is to be performed or defined in a sensible way. The idea of summing or integrating over paths can be made mathematically rigorous only by the formal definition of a *path measure* on the space of all paths [15, 16]. This measure must be defined consistently with the weighting factor of the exponentiated action, since that is the functional being integrated. To motivate this with a familiar example, it is recalled that the dt appearing in the Riemann sum of the exponential is an example of a type of measure called the Jordan measure and has the form $t_{j+1} - t_j$. This is by no means the most general form of measure, even for the real line. To demonstrate the relation between the function being integrated and the measure used to integrate it, one need only point out that the function $q(t)$ defined by (2.56) is not an integrable function using Jordan measure. If such a pathological function is to be rendered integrable, then a more general measure, referred to as the *Lebesgue measure*, must be defined. The discussion of formal measure theory and, in particular, the problem of defining a measure over the space of paths is very difficult and requires a level of mathematics well beyond the scope of this book [17]. However, some aspects of summing over paths can be made clearer with a modicum of effort.

One of the chief difficulties in constructing a rigorous measure for the continuum version of the path integral is the presence of the i in its definition. The oscillatory nature of the exponential creates difficulties in including "unruly" paths, i.e., nondifferentiable and discontinuous paths, since the exponentiated action tends toward a distribution. A simple exclusion of the unruly paths would be incorrect. This is so because, while the differentiable and continuous paths are everywhere *dense* in the set of all paths, it can be shown that, taken alone, they are inadequate to give a correct evaluation of the path integral. In point of fact, a careful analysis

of the situation shows that these paths form a set of measure zero [18]. The situation is much like that of the real number line, where the set of all rational numbers can be shown to be a set of measure zero, even though they are everywhere dense in the real line.

Unfortunately, because the exponentiated action tends toward a distribution, the path integral defined by (2.55) prevents the definition of a well-behaved measure, and therefore an alternate scheme must be found if a mathematical definition is to be made. It is the oscillatory nature of the path integral that gives rise to the distributions. If the oscillations were suppressed, then it might be possible to define a sensible measure for paths. It is with this hope that much of the rigorous work done on path integrals defines them for Euclidean time. This means that the integrand of the action undergoes the so-called Wick rotation, which amounts to replacing t with $-i\tau$. In effect, the path integral is analytically continued to imaginary time, evaluated, and analytically continued back by the inverse Wick rotation, $\tau \rightarrow it$, to yield the final result. The necessity of this analytic continuation arises from the need to evaluate the generalization of the oscillatory Gaussian integrals first encountered in Sec. 1.5. There, the integration was defined by an analytic continuation identical to the Wick rotation. Under the Wick rotation the form (2.50) for the path integral becomes

$$Z = \int_{q_a}^{q_b} \overline{\mathcal{D}}q \, e^{-S_E/\hbar} \, , \tag{2.60}$$

where, for the simple case (2.48), the *Euclidean action* S_E is given by

$$S_E = \int_{t_a}^{t_b} d\tau \left\{ \frac{1}{2} m \left(\frac{dq}{d\tau} \right)^2 + V(q) \right\} . \tag{2.61}$$

The factors in the measure of the path integral become real under the Wick rotation, so that

$$\overline{\mathcal{D}}q = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar\epsilon_\tau} \right)^{N/2} dq_1 \cdots dq_{N-1} \, , \tag{2.62}$$

where ϵ_τ is effectively $d\tau$. The Euclidean action (2.61) is identical in form to the integral of the Hamiltonian, written in terms of $\dot{q}$ instead of p. It will be shown in Chapter 4 that this is no coincidence. However, for now it is necessary only to notice that, unless the potential is unbounded from below, large deviations from the classical trajectory, as well as unruly paths, are exponentially suppressed. The Wick rotation makes a mathematically meaningful measure possible.

It is worth noting that, under a Wick rotation, the differential form of the Schrödinger equation, for $V = 0$, becomes

$$\frac{\hbar^2}{2m}\nabla^2\psi = \hbar\frac{d}{d\tau}\psi\,, \tag{2.63}$$

which is the diffusion equation that governs Brownian motion. Wiener [19] was the first to construct a path integral representation for Brownian motion and to show that a well-behaved measure could be defined. It has been argued, using sophisticated techniques, that the path integral has a well-defined measure in the Euclidean region, and this argument will be taken over in the remainder of this book. The interested reader is recommended to the books by Rivers [13] and by Glimm and Jaffe [20].

At best, these remarks may convey the difficulty in making the continuum path integral of (2.55) a well-defined mathematical object. In practice it is common to approximate the sum over paths by using the subset of piecewise continuous paths that are differentiable and continuous and that yield a finite action. In particular the classical trajectory is believed to represent the maximum weight path. It is hoped, but unsubstantiated in most cases, that this approximation gives the most important properties of the quantum transition amplitude. In Chapter 3 the role of the classical trajectory in the quantum transition amplitude will be discussed for several extremely simple cases.

This section will close with the derivation of the path integral representation for the transition amplitude in a simple one-dimensional quantum system with properties significantly different than those originally assumed. The system is that of a point mass constrained to move on a circle of radius R. The classical action for this system, in terms of the angular variable θ, is given by

$$\mathcal{L}(\dot\theta,\theta) = \tfrac{1}{2}mR^2\dot\theta^2 - V(\theta)\,. \tag{2.64}$$

The potential V is assumed to be periodic, so that $V(\theta + 2\pi n) = V(\theta)$, where n is an arbitrary integer. The Hamiltonian has the standard form

$$H(p_\theta,\theta) = \frac{1}{2m}{p_\theta}^2 + V(\theta)\,. \tag{2.65}$$

The position eigenstates of the system are $|\,\theta\,\rangle$, and these are complete in the sense that

$$\int_0^{2\pi} d\theta\,|\,\theta\,\rangle\langle\,\theta\,| = 1\,. \tag{2.66}$$

The configuration space representation of the momentum operator is

$$\langle\,\theta\,|\,P\,|\,\theta'\,\rangle = -i\frac{\hbar}{R}\frac{\partial}{\partial\theta}\delta(\theta-\theta')\,. \tag{2.67}$$

Because the system is on a circle, the eigenfunctions of all observables must be periodic. It is straightforward to show that the eigenstates of the observable p_θ are no longer continuous, but are indexed by an integer n, and are therefore denoted $|\, p_n \,\rangle$. It follows from (2.67) that the normalized momentum eigenfunctions for the system are given by

$$\langle\, \theta \,|\, p_n \,\rangle = \frac{1}{\sqrt{2\pi}} e^{in\theta} \,. \tag{2.68}$$

These eigenfunctions are orthonormal

$$\langle\, p_n \,|\, p_m \,\rangle = \int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{i(m-n)\theta} = \delta_{mn} \,, \tag{2.69}$$

and complete in the sense that

$$\sum_{n=-\infty}^{\infty} \langle\, \theta \,|\, p_n \,\rangle\langle\, p_n \,|\, \theta' \,\rangle = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{in(\theta-\theta')} = \delta(\theta - \theta') \,, \tag{2.70}$$

where the Dirac delta is clearly periodic. These results can be used to derive the path integral form for the transition element $\langle\, \theta_b, t_b \,|\, \theta_a, t_a \,\rangle$.

Exercise 2.8: Use the previous results to show that the path integral representation of the transition amplitude is given by

$$\begin{aligned} &\langle\, \theta_b, t_b \,|\, \theta_a, t_a \,\rangle = \\ &\lim_{N\to\infty} \int_{\theta_a}^{\theta_b} d\theta_1 \cdots d\theta_{N-1}\, \frac{1}{(2\pi)^N} \sum_{n_0=-\infty}^{\infty} \cdots \sum_{n_{N-1}=-\infty}^{\infty} \\ &\times \exp\left\{ \frac{i}{\hbar} \sum_{j=0}^{N-1} \left[n_j \hbar(\theta_{j+1} - \theta_j) - \epsilon \frac{n_j^2 \hbar^2}{2mR^2} - \epsilon V(\theta_j) \right] \right\} \,, \end{aligned} \tag{2.71}$$

where the integrations over the θ_j are from 0 to 2π.

There are formal similarities between (2.71) and the general form (2.47) if the classical momentum is identified as $p = n\hbar/R$. However, this forces the classical momentum to be discrete, and such a constraint is never present in classical mechanics. Furthermore, it is not clear at this stage that a form similar to (2.50) can be obtained or, if it can be, what the limits on the θ integrations should be. Thus, passing over to a path integral of the form (2.55) for this system seems, at this point, a questionable step. This problem will be resolved in the next chapter when (2.71) is analyzed to reveal its underlying structure.

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