Path Integrals

Path integrals were invented by Feynman (while a graduate student!) as an alternative formulation of quantum mechanics. Our goal in this chapter is to show that quantum mechanics and quantum field theory can be completely reformulated in terms of path integrals. The path integral formulation is particularly useful for quantum field theory.

1 From Quantum Mechanics to Path Integrals

Before discussing field theory, we derive the path integral for the quantum mechanics of a single particle with position q and conjugate momentum p. The corresponding quantum operators are denoted by \hat{p} and \hat{q} , and satisfy

$$[\hat{q}, \hat{p}] = i,$$

$$[\hat{q}, \hat{q}] = [\hat{p}, \hat{p}] = 0.$$
(1.1)

(We use units where $\hbar = 1$.) In this chapter, we will always use hats to distinguish quantum operators from classical quantities in order to emphasize the distinction. We use the standard 'bra-ket' notation of Dirac for quantum states, so we write equations such as

$$\hat{q}|q\rangle = q|q\rangle,\tag{1.2}$$

which says that $|q\rangle$ is the eigenstate of the operator \hat{q} with eigenvalue q.

In quantum mechanics, the state of the system at the time t is specified by a ket vector $|\psi(t)\rangle$. The state ket evolves in time according to the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle.$$
 (1.3)

Suppose that at some initial time $t = t_i$ the system is prepared in the state $|\psi_0\rangle$. As long as the Hamiltonian has no explicit dependence on time, we can write a formal solution to the Schrödinger equation:

$$|\psi(t)\rangle = e^{-i\hat{H}\cdot(t-t_i)}|\psi_0\rangle, \qquad (1.4)$$

where the exponential of an operator is defined by its power series:

$$e^{\hat{\Omega}} \stackrel{\text{\tiny def}}{=} \sum_{n=0}^{\infty} \frac{1}{n!} \hat{\Omega}^n.$$
(1.5)

Eq. (1.4) can be checked by differentiating both sides with respect to t and verifying that $|\psi(t)\rangle$ as defined by Eq. (1.4) satisfies the Schrödinger equation, and also the correct boundary condition

$$\lim_{t \to t_i} |\psi(t)\rangle = |\psi_0\rangle. \tag{1.6}$$

We call the solution Eq. (1.4) 'formal' only because is no easier to evaluate the exponential of the Hamiltonian than it is to solve the Schrödinger equation. The real use of Eq. (1.4) is for proving general results.

The quantity

$$\hat{U}(t,t_i) \stackrel{\text{def}}{=} e^{-i\hat{H} \cdot (t-t_i)} \tag{1.7}$$

that appears in Eq. (1.4) is called the **time evolution operator**. If we know this operator, it is clear that we know everything there is to know about the way the system evolves in time. It is also sufficient to find the matrix element of \hat{U} between arbitrary position eigenstates

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle.$$
 (1.8)

This quantity is sometimes called the **time evolution kernel**. (Note that the final state appears on the left. We will always write our expressions so that 'later times are on the left.')

We begin our derivation of the path integral by dividing the time interval from t_i to t_f into N equal intervals of length

$$\Delta t = \frac{t_f - t_i}{N}.\tag{1.9}$$

(We will eventually take the limit $N \to \infty$, $\Delta t \to 0$.) We write the time evolution operator as

$$e^{-i\hat{H}\cdot(t-t_i)} = \underbrace{e^{-i\hat{H}\Delta t}e^{-i\hat{H}\Delta t}\cdots e^{-i\hat{H}\Delta t}}_{N \text{ factors}}.$$
(1.10)

We then insert a complete set of states between each of the factors above using the completeness relation

$$1 = \int dq \, |q\rangle\langle q|. \tag{1.11}$$

In this way, we obtain

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = \int dq_{N-1} \cdots \int dq_1$$

$$\times \langle q_f | e^{-i\hat{H}\Delta t} | q_{N-1} \rangle \langle q_{N-1} | e^{-i\hat{H}\Delta t} | q_{N-2} \rangle \cdots \langle q_1 | e^{-i\hat{H}\Delta t} | q_i \rangle.$$

$$(1.12)$$

The integration variables q_1, \ldots, q_N can be viewed as the positions at time intervals Δt along a path from q_i to q_f . In this sense, Eq. (1.12) already has the form of an integral over paths. We will eventually take the limit where $N \to \infty$ (and $\Delta t \to 0$), so we really are summing over all paths in some sense.

We define

$$T_{q',q} \stackrel{\text{def}}{=} \langle q' | e^{-i\hat{H}\Delta t} | q \rangle, \qquad (1.13)$$

so that we can write

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = \int dq_{N-1} \cdots \int dq_1 T_{q_f, q_{N-1}} T_{q_{N-1}, q_{N-2}} \cdots T_{q_1, q_i}.$$
 (1.14)

If we regard $T_{q',q}$ as a 'matrix' with 'indices' q' and q, this gives the time evolution kernel as a product of matrices. (The 'indices' are integrated over rather than summed because they are continuous.) T is called the **transfer matrix** of the system.

To proceed further, we assume that the Hamiltonian has the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}).$$
(1.15)

This describes a particle moving in a potential V(q). We evaluate the transfer matrix with the help of the matrix identity

$$e^{A+B} = e^{A}e^{B}\left(1 - \frac{1}{2}[A, B] + \cdots\right)$$
(1.16)

This generalizes the multiplicative property of the exponential that holds for commuting numbers with correction terms that depend on commutators of the matrices. Using this identity we have

$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t\hat{p}^2/(2m)}e^{-i\Delta tV(\hat{q})} \left(1 + \text{commutator terms}\right).$$
(1.17)

The commutator terms are $\mathcal{O}(\Delta t^2)$, and can therefore be neglected in the limit $\Delta t \rightarrow 0$. We can then evaluate the transfer matrix by inserting a complete set of momentum eigenstates

$$T_{q',q} = \int dp \langle q' | e^{-i\Delta t \hat{p}^2/(2m)} | p \rangle \langle p | e^{-i\Delta t V(\hat{q})} | q \rangle$$
$$= \int \frac{dp}{2\pi} e^{-ip(q'-q)} e^{-iH(p,q)\Delta t}.$$
(1.18)

Here we have used

$$\langle p|q\rangle = \frac{1}{(2\pi)^{1/2}}e^{-ipq},$$
 (1.19)

and the identities

$$f(\hat{q})|q\rangle = f(q)|q\rangle, \qquad \langle p|f(\hat{p}) = \langle p|f(p), \qquad (1.20)$$

which hold for an arbitrary function f. Notice what has happened in Eq. (1.18): we have used the completeness relation to replace the operators \hat{p} and \hat{q} with integrals over classical quantities p and q.

Substituting Eq. (1.18) into Eq. (1.14), we obtain

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = \int dq_{N-1} \frac{dp_{N-1}}{2\pi} \cdots \int dq_1 \frac{dp_1}{2\pi} \int \frac{dp_0}{2\pi} \\ \times \exp\left\{ i \sum_{n=0}^{N-1} \Delta t \left[p_n \frac{q_{n+1} - q_n}{\Delta t} - H(p_n, q_n) \right] \right\}.$$

$$(1.21)$$

In the continuum limit $N \to \infty$, $\Delta t \to 0$, we can identify

$$\frac{q_{n+1} - q_n}{\Delta t} \to \dot{q}(t), \quad \sum_{n=0}^{N-1} \Delta t f(t_n) \to \int_{t_i}^{t_f} dt f(t).$$
(1.22)

We can then write Eq. (1.21) in the compact form

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = \int_{q_i}^{q(t_f) = q_f} d[p] d[q] e^{iS_{\mathrm{H}}[p,q]},$$

$$(1.23)$$

where

$$S_{\rm H}[p,q] = \int_{t_i}^{t_f} dt \Big[p(t)\dot{q}(t) - H(p(t),q(t)) \Big],$$
(1.24)

and we have used the abbreviations

$$d[p] \stackrel{\text{def}}{=} \prod_{n=0}^{N-1} \frac{dp_n}{2\pi}, \qquad d[q] \stackrel{\text{def}}{=} \prod_{n=1}^{N-1} dq_n.$$
 (1.25)

Eq. (1.23) is called a **path integral** (or **functional integral**) because the integral is over all 'phase-space paths' (p(t), q(t)). The path q(t) must satisfy the boundary conditions $q(t_i) = q_i$, $q(t_f) = q_f$, while the path p(t) is completely unconstrained and is not related to q(t) (or $\dot{q}(t)$) in any way. We emphasize that p(t) and q(t) are defined by integrating over the values of p(t) and q(t) independently at each value of t, so the paths that contribute to the functional integral are in general highly discontinuous. It is often useful to have an intuitive picture of the path integral as stating that a quantum particle samples 'all possible paths,' but it is important to remember that the integral is not restricted to 'physical' paths in any sense.

The quantity S[p,q] defined in Eq. (1.24) is called the **Hamiltonian action** of the system.¹ Note that S[p,q] is a number that depends on the full phase space path from t_i to t_f . S[p,q] is therefore a 'function of a function,' or a **functional**. We will write the arguments of functionals in square brackets to emphasize this point.

The Hamiltonian form of the path integral is not used much in practice. We can obtain a simpler form of the path integral by carrying out the integral over the momenta. To do this, we go back to the transfer matrix for finite Δt . We must therefore compute

$$T_{q',q} = \int \frac{dp}{2\pi} \exp\left\{i(q'-q)p - i\Delta t \left[\frac{p^2}{2m} + V(q)\right]\right\}.$$
 (1.26)

This integral is not well-defined because the integrand does not fall off as $p \to \pm \infty$. (The same problem occurs in the q integral.) However, the integral can be defined by analytic continuation.

One way to make the expressions above well-defined is to evaluate the timeevolution kernel for imaginary values of the initial and final times. That is, we consider the quantity

$$\langle q_f | \hat{U}(-i\tau_f, -i\tau_0) | q_i \rangle = \langle q_f | e^{-\hat{H} \cdot (\tau_f - \tau_0)} | q_i \rangle.$$
(1.27)

Repeating the steps above, we find a transfer matrix

$$T_{q',q} = \int \frac{dp}{2\pi} \exp\left\{i(q'-q)p - \Delta\tau \left[\frac{p^2}{2m} + V(q)\right]\right\}.$$
 (1.28)

This integrand is exponentially damped for large p, so the integral converges. For reasons that will become clear later, this is called the **Euclidean time** approach. In this approach, we must analytically continue back to real time at the end of the calculation to obtain physical results.

An equivalent approach is to perform the analytic continuation by evaluating the time evolution kernel at initial and final times with a small negative imaginary part:

$$\langle q_f | \hat{U}(t_f(1-i\epsilon), t_i(1-i\epsilon)) | q_i \rangle = \langle q_f | e^{-i\hat{H} \cdot (t_f - t_i)(1-i\epsilon)} | q_i \rangle.$$
(1.29)

Here ϵ is a positive quantity that is taken to zero at the end of the calculation. The quantity ϵ is therefore treated as an infinitesimal that is relevant only when it is

¹This action also appears in the variational formulation of classical Hamiltonian dynamics.

needed to make expressions well-defined. For example, in this approach the transfer matrix becomes

$$T_{q',q'} = \int \frac{dp}{2\pi} \exp\left\{ i(q'-q)p - i\Delta t(1-i\epsilon) \left[\frac{p^2}{2m} + V(q)\right] \right\}.$$
 (1.30)

This integral is well-defined as long as $\epsilon > 0$ because the coefficient of p^2 in the exponent has a negative real part that suppresses the integrand as $p \to \pm \infty$.

We now perform the integral over p in Eq. (1.30). The integral has the form of a generalized Gaussian integral

$$\int_{-\infty}^{\infty} dp \, e^{-\frac{1}{2}Ap^2 + Bp}, \qquad \text{Re}(A) > 0.$$
 (1.31)

We can evaluate this integral by completing the square in the exponent

$$-\frac{1}{2}Ap^{2} + Bp = -\frac{1}{2}A\left(p - \frac{B}{A}\right)^{2} + \frac{B^{2}}{2A}$$
(1.32)

and shifting the variable of integration to p' = p - B/A:

$$\int_{-\infty}^{\infty} dp \, e^{-\frac{1}{2}Ap^2 + Bp} = e^{B^2/(2A)} \int_{-\infty}^{\infty} dp' \, e^{-\frac{1}{2}Ap'^2} = e^{B^2/(2A)} \left(\frac{2\pi}{A}\right)^{1/2}.$$
 (1.33)

This trick for doing Gaussian integrals will be used repeatedly. Applying this formula, we obtain

$$T_{q',q} = \left(\frac{m}{2\pi i \Delta t}\right)^{1/2} \exp\left\{i\Delta t(1-i\epsilon) \left[\frac{m}{2} \left(\frac{q'-q}{\Delta t(1-i\epsilon)}\right)^2 - V(q)\right]\right\}.$$
 (1.34)

Note that the time always appears with a small negative imaginary part. Omitting the $i\epsilon$ factors for brevity, the time-evolution kernel is

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \int dq_{N-1} \cdots \int dq_1$$

$$\times \exp\left\{ i \sum_{n=0}^{N-1} \Delta t \left[\frac{m}{2} \left(\frac{q_{n+1} - q_n}{\Delta t} \right)^2 - V(q_n) \right] \right\}.$$

$$(1.35)$$

Note that there is one factor

$$C = \left(\frac{m}{2\pi i \Delta t}\right)^{1/2} \tag{1.36}$$

for each q integral, with one factor left over. We therefore define the path integral measure to be

$$d[q] \stackrel{\text{def}}{=} \prod_{n=1}^{N-1} \left(C dq_n \right). \tag{1.37}$$

Taking the continuum limit $\Delta t \to 0$, we obtain

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = C \int_{q(t_i) = q_i}^{q(t_f) = q_f} d[q] e^{iS[q]},$$
(1.38)

where

$$S[q] = \int_{t_i}^{t_f} dt \left[\frac{m}{2} \dot{q}^2(t) - V(q(t)) \right]$$
(1.39)

is the **Lagrangian action**, the integral of the Lagrangian over the path q(t). Note that the measure factor C is highly divergent in the continuum limit. However, this divergence is in the overall normalization of the path integral, and we will see that it drops out of physical quantities.

One immediate consequence of the path integral is that it gives a different way of looking at the classical limit of quantum mechanics. Suppose that there is a solution q(t) to the classical equations of motion with $q(t_i) = q_i$, $q(t_f) = q_f$. The fact that it is a classical solution means that the action is stationary, *i.e.*

$$\frac{\delta S}{\delta q} = 0 \tag{1.40}$$

evaluated along the path. The path integral is over all paths, not just the classical path. However, paths that are close to the classical one have an action close to the classical path, and therefore add coherently, while paths that are far from the classical path tend to interfere destructively.

Exercise: Show that the classical equation of motion for the Lagrangian

$$L = \frac{1}{2}m(q)\dot{q}^2 - V(q).$$
(1.41)

is given by

$$m\ddot{q} + \frac{1}{2}m'\dot{q}^2 + V' = 0, \qquad (1.42)$$

where m' = dm/dq, etc. (This shows that a position-dependent mass for a particle gives rise to a frictional force.) If you have difficulty with this problem, you may want to review the classical variational principle.

We can use the path integral to give an expression for the ground state wavefunction of the system. Consider

$$\langle q_f | \hat{U}(0, -T(1-i\epsilon)) | q_i \rangle = \langle q_f | e^{-i\hat{H}T} e^{-\epsilon\hat{H}T} | q_i \rangle, \qquad (1.43)$$

where $\epsilon > 0$ is taken to zero at the end of the calculation. Note that this is equivalent to the $i\epsilon$ prescription that was used to make the path integral well-defined above. Inserting a complete set of energy eigenstates, we get

$$\langle q_f | \hat{U}(0, -T(1-i\epsilon)) | q_i \rangle = \sum_n e^{-iE_n T} e^{-\epsilon E_n T} \langle q_f | n \rangle \langle n | q_i \rangle.$$
(1.44)

Taking $T \to \infty$, the ϵ -dependent term suppresses the contribution of all excited states, leaving only the contribution from the ground state n = 0:

$$\langle q|\hat{U}(0, -T(1-i\epsilon))|q_i\rangle \to e^{iE_0T}\psi_0(q_f)\psi_0^*(q_i).$$
 (1.45)

Viewed as a function of q_f , this gives the ground state of the system up to a (singular) normalization factor. Therefore, we can write

$$\psi_0(q_f) = \mathcal{N} \int d[q] \, e^{iS[q]}.$$
(1.46)

Here, the integral is over all paths from $t_i \to -\infty$ with the $i\epsilon$ prescription is understood, and \mathcal{N} is a (singular) normalization factor. The fact that the $i\epsilon$ prescription projects out the ground state will be used frequently in the following.

The singular normalization factors should not bother you too much. Conceptually, they arise for the same reason as non-normalizable states in quantum mechanics, and we will see how to deal with them when we start using the path integral to compute physical quantities.

2 From Path Integrals to Quantum Mechanics

We now reverse the procedure above and show how to reconstruct the operator form of quantum mechanics from the path integral. That is, we attempt to *define* a quantum-mechanical evolution operator by the path integral with a given action.

There is one generalization of the previous section that will be needed here. In the discussion above, the path integral measure is independent of q (see Eq. (1.36)). A simple example of a quantum-mechanical system with a nontrivial path integral measure is given by a particle with a position-dependent mass, defined by the Lagrangian

$$L = \frac{1}{2}m(q)\dot{q}^2 - V(q).$$
(2.1)

The canonical momentum is

$$p = \frac{\partial L}{\partial \dot{q}} = m(q)\dot{q}, \qquad (2.2)$$

so the classical Hamiltonian is

$$H = \frac{p^2}{2m(q)} + V(q).$$
 (2.3)

There is an ambiguity in writing the quantum Hamiltonian arising from the fact that \hat{q} and \hat{p} do not commute. There are infinitely many Hermitian operator generalizations of the classical kinetic term, *e.g.*

$$\hat{p}\frac{1}{2m(\hat{q})}\hat{p}, \quad \frac{1}{4m(\hat{q})}\hat{p}^2 + \hat{p}^2\frac{1}{4m(\hat{q})}, \quad \frac{1}{2}\left(\frac{1}{m(\hat{q})}\right)^{1/2}\hat{p}^2\left(\frac{1}{m(\hat{q})}\right)^{1/2}, \quad (2.4)$$

etc. All of these have the same classical limit, but they differ at the quantum level. This situation is referred to as an **operator ordering ambiguity**. There is nothing deep going on here: different operator orderings give different theories, so we just have to pick one (or let experiment decide). We will choose the theory defined by the quantum Hamiltonian

$$\hat{H} = \hat{p} \frac{1}{2m(\hat{q})} \hat{p} + V(\hat{q}).$$
(2.5)

The path integral for this system can be derived following the steps of the previous section. It is convenient to order the operators in \hat{H} so that \hat{p} is always to the left of \hat{q} ('Weyl ordering'). Using the canonical commutation relations, we obtain

$$\hat{H} = \frac{1}{2}\hat{p}^2 m(\hat{q}) - \frac{i}{2}\hat{p}\frac{m'(\hat{q})}{m^2(\hat{q})} + V(\hat{q}).$$
(2.6)

This is not look Hermitian, but of course it is. We can now write the transfer matrix as

$$T_{q',q} = \langle q'|e^{-i\hat{H}\Delta t}|q\rangle = \int dp \,\langle q'|p\rangle e^{-i\hat{H}\Delta t}|q\rangle$$
$$= \int \frac{dp}{2\pi} e^{ip(q'-q)-i\tilde{H}(p,q)\Delta t},$$
(2.7)

where

$$\tilde{H}(p,q) = \frac{p^2}{2m(q)} - \frac{i}{2} \frac{m'(q)}{m^2(q)} p + V(q).$$
(2.8)

The 'extra' term compared to Eq. (2.3) is a result of the operator ordering we have chosen. Performing the p integral, we obtain

$$T_{q',q} = C(q) \exp\left\{i\Delta t L\left(q, \frac{q'-q}{\Delta t}\right)\right\},\tag{2.9}$$

where

$$\tilde{L}(q,\dot{q}) = \frac{1}{2}m(q)\dot{q}^2 + \frac{i}{2}\frac{m'(q)}{m(q)}\dot{q} - \frac{(m'(q))^2}{8m^3(q)} + V(q).$$
(2.10)

Again, the 'extra' terms come from the operator ordering. The measure factor is

$$C(q) = \left(\frac{m(q)}{2\pi i \Delta t}\right)^{1/2}.$$
(2.11)

The Lagrangian appearing in the path integral is not the same as the classical Lagrangian we started with. This should not worry us, since we should *a priori* allow all possible terms consistent with symmetries (and restricted by experimental data if we are attempting to describe the real world).

Another feature of this example is the fact that the measure factor depends on q. The path integral for this system can then be written

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = C(q_i) \int_{q_i}^{q(t_f) = q_f} d[q] e^{iS[q]}.$$

$$(2.12)$$

Here the measure is defined by

$$d[q] = \lim_{N \to \infty} \prod_{n=1}^{N-1} C(q_n) dq_n,$$
(2.13)

where the time interval from t_i to t_f is discretized into N steps as before. The fact that the measure factor in Eq. (2.12) involves q_i rather than q_f originates in the fact that we chose to order the quantum Hamiltonian so that \hat{p} is to the left of \hat{q} , rather than the other way around. It is clear that physical quantities should not depend on this choice, and we will see that indeed the measure factor C(q) cancels out when we compute physical quantities.

We want to see if we can *define* the time evolution operator using the right-hand side of the path integral Eq. (2.12) with the generalized measure. (Eq. (2.12) defines the matrix elements of the time evolution operator for a complete set of states, which is the same as defining the operator.) In order to define a consistent time evolution, the operator $\hat{U}(t_f, t_i)$ defined by the path integral must be unitary, and it must satisfy the 'time composition rule'

$$\hat{U}(t_f, t_i) = \hat{U}(t_f, t)\hat{U}(t, t_i)$$
(2.14)

for any t. This just says that the result of evolving from t_i to t_f can be split into a time evolution from t_i to t, followed by time evolution from t to t_f . In terms of matrix elements, Eq. (2.14) is equivalent to

$$\langle q_f | \hat{U}(t_f, t_i) | q_i \rangle = \int dq \, \langle q_f | \hat{U}(t_f, t) | q \rangle \langle q | \hat{U}(t, t_i) | q_i \rangle.$$
(2.15)

To check this, we write the left-hand side using the transfer matrix

$$\langle q_N | \hat{U}(t_N, t_0) | q_0 \rangle \stackrel{\text{def}}{=} \int dq_{N-1} \cdots dq_1 T_{q_N, q_{N-1}} C(q_{N-1}) \cdots T_{q_1, q_0} C(q_0)$$
(2.16)

$$= \int dq_n \left(\int dq_{N-1} \cdots dq_{n+1} T_{q_N, q_{N-1}} C(q_{N-1}) \cdots T_{q_{n+1}, q_n} C(q_n) \right)$$

$$\times \left(\int dq_{n-1} \cdots dq_1 T_{q_n, q_{n-1}} C(q_{n-1}) \cdots T_{q_1, q_0} C(q_0) \right) . (2.17)$$

Note that the measure factors simply pair up with the transfer matrices. With the identification Eq. (2.12), this shows that the path integral definition satisfies the time composition rule Eq. (2.15). It works just because the integral over all paths from q_i to q_f is equal to the integral over all paths from q_i to q_i followed by the integral over all paths from q all paths from q to q_f , provided that we integrate over all intermediate positions q.

The last thing we need to show is that the time evolution operator is unitary. This is far from obvious from the definition Eq. (2.12). Even though the measure factor e^{iS} is a phase, the path integral is a *sum* of phases, which not in general unitary. Once again, our starting point is the formulation of the time evolution operator in terms of the transfer matrix, Eq. (2.16), where the transfer matrix is given by

$$T_{q',q} = \exp\left\{i\Delta t L\left(q, \frac{q'-q}{\Delta t}\right)\right\}.$$
(2.18)

We make the connection to the operator formalism by looking for an operator \hat{T} with the property that

$$\langle q'|\hat{T}|q\rangle = T_{q',q}.\tag{2.19}$$

Note that the operator \hat{T} is not diagonal in q space, so it must be a function of both \hat{q} and \hat{p} . To find \hat{T} , we use the fact that \hat{p} acts as a translation operator for q, *i.e.*

$$\langle q'|e^{-i\Delta q\hat{p}}|q\rangle = \langle q'|q + \Delta q\rangle = \delta(q' - q - \Delta q).$$
 (2.20)

From this, we can see that we can write

$$\hat{T} = \int d(\Delta q) \, e^{-i\Delta q \hat{p}} e^{i\Delta t L(\hat{q}, \, \Delta q/\Delta t)}.$$
(2.21)

To check this, we compute

$$\langle q' | \hat{T} | q \rangle = \int d(\Delta q) \, \langle q' | e^{-i\Delta q \hat{p}} e^{i\Delta t L(\hat{q}, \, \Delta q/\Delta t)} | q \rangle$$

$$= \int d(\Delta q) \, \langle q' | q + \Delta q \rangle e^{i\Delta t L(q, \, \Delta q/\Delta t)}$$

$$= e^{i\Delta t L(q, \, (q'-q)/\Delta t)}.$$

$$(2.22)$$

Note that this defines the matrix elements of \hat{T} in a complete set of states, so the solution is unique.

With this result, we can write the path integral as an integral (sum) over intermediate states:

$$\langle q_N | \hat{U}(t_N, t_0) | q_0 \rangle = \int dq N - 1 \cdots dq_1 \langle q_N | \hat{T} \hat{C} | q_{N-1} \rangle \cdots \langle q_1 | \hat{T} \hat{C} | q_0 \rangle, \quad (2.23)$$

where $\hat{C} = C(\hat{q})$. This can be written much more compactly as the operator statement

$$\hat{U}(t_N, t_0) = (\hat{T}\hat{C})^N.$$
 (2.24)

That is, $\hat{T}\hat{C}$ is the infinitesmal time evolution operator. We see that \hat{U} is unitary if and only if the operator $\hat{T}\hat{C}$ is unitary.

The operator \hat{T} defined by Eq. (2.21) is not unitary by itself, since it is an integral (sum) of unitary operators. Unitarity of $\hat{T}\hat{C}$ is equivalent to

$$\langle q'|(\hat{T}\hat{C})^{\dagger}(\hat{T}\hat{C})|q\rangle \rightarrow \langle q'|q\rangle = \delta(q'-q).$$
 (2.25)

A short calculation analogous to Eq. (2.22) gives

$$\begin{split} \langle q' | (C\hat{T})^{\dagger} (C\hat{T}) | q \rangle &= C^{*}(q') C(q) \int d(\Delta q) \\ & \times \exp\left\{ i \Delta t \left[L\left(q, \frac{\Delta q}{\Delta t}\right) - L\left(q', \frac{q-q' + \Delta q}{\Delta t}\right) \right] \right\}. \end{split}$$

The integral on the right-hand side is a function of q and q' that is sharply peaked at q = q' for small Δt . The reason is that for $q' \neq q$, the phase of the integrand oscillates wildly, suppressing the value of the integral. The integral becomes more and more sharply peaked as $\Delta t \to 0$, and we have

$$\langle q'|(C\hat{T})^{\dagger}(C\hat{T})|q\rangle \to |C(q)|^2 \times \text{(sharply peaked function of } q'-q\text{)}.$$
 (2.26)

We can choose C(q) (as a function of Δt) so that this has unit area in the limit $\Delta t \to 0$, *i.e.* the integral is equal to $\delta(q - q')$.

If the measure factor depends on q, it can be rewritten as a correction to the action:

$$\prod_{t} C(q(t)) = \exp\left\{\sum_{t} C(q(t))\right\} \to \exp i\Delta S,$$
(2.27)

where

$$\Delta S = -\frac{i}{\Delta t} \int dt \,\ln C. \tag{2.28}$$

This is a very peculiar contribution to the action: it is imaginary, and diverges in the continuum limit $\Delta t \rightarrow 0$. We will be able to understand the significance of this factor only after we have properly discussed the issue of the continuum limit ('renormalization'). The bottom line is that this factor is not present in all reasonable definitions of the continuum limit.

These arguments are rather formal, since they deal with highly divergent quantities. However, I believe that these considerations capture the reason that path integrals automatically give rise to unitary time evolution. Later, we will give a rigorous argument that the path integral gives rise to unitary time evolution, at least to all orders in perturbation theory.

3 Generalization to Field Theory

The generalization from 1-dimensional quantum mechanics to quantum field theory is in principle straightforward: we just have more degrees of freedom! We will illustrate this with the example of a real scalar field $\phi(x)$. The classical Lagrangian is

$$\mathcal{L} = \frac{1}{2} \partial^{\mu} \phi \partial_{\mu} \phi - V(\phi) \tag{3.1}$$

$$= \frac{1}{2}\dot{\phi}^2 - (\vec{\nabla}\phi)^2 - V(\phi).$$
(3.2)

To pass to the quantum system we must construct the Hamiltonian. The dynamical variables at a fixed time are the scalar fields $\phi(\vec{x})$, with canonically conjugate momenta $\phi(\vec{x})$. The canonical momentum is $\pi = \dot{\phi}$, and the quantum Hamiltonian is

$$\hat{H} = \int d^3x \, \left[\frac{1}{2} \hat{\pi}^2 + \frac{1}{2} (\vec{\nabla} \hat{\phi})^2 + V(\hat{\phi}) \right].$$
(3.3)

Note that Lorentz invariance is not manifest in the Hamiltonian, since we implicitly made a choice of Lorentz frame in defining the canonical momenta. Note that there are independent quantum operators $\hat{\phi}(\vec{x})$ and $\hat{\pi}(\vec{x})$ at each spatial point \vec{x} . To make this well-defined, we can replace the spatial continuum with a discrete square lattice of points with spacing a:

$$\vec{x} = a \cdot (n_1, n_2, n_3),$$
 (3.4)

where n_1, n_2, n_3 are integers. We then have independent operators $\hat{\phi}_{\vec{x}}$ and $\hat{\pi}_{\vec{x}}$ at each lattice site. The quantum Hamiltonian then

$$\hat{H} = \sum_{\vec{x}} a^3 \left[\frac{1}{2} \hat{\pi}_{\vec{x}}^2 + \frac{1}{2} \sum_{\vec{j}} \left(\frac{\hat{\phi}_{\vec{x}+\vec{j}} - \hat{\phi}_{\vec{x}}}{a} \right)^2 + V(\hat{\phi}_{\vec{x}}) \right],$$
(3.5)

where \vec{j} runs over the unit lattice vectors (a, 0, 0), (0, a, 0), (0, 0, a).

We now retrace the steps leading up to the path integral. We want to evaluate the time evolution kernel

$$\langle \phi_f | \hat{U}(t_f, t_i) | \phi_i \rangle = \langle \phi_f | e^{-iH(t_f - t_i)} | \phi_i \rangle, \qquad (3.6)$$

where $|\phi\rangle$ is an eigenstate of the field operator:

$$\hat{\phi}_{\vec{x}}|\phi\rangle = \phi_{\vec{x}}|\phi\rangle. \tag{3.7}$$

(That is, $|\phi\rangle$ is a simultaneous eigenstate of all of the operators $\hat{\phi}_{\vec{x}}$.) We again break the time interval into N intervals of length $\Delta t = (t_f - t_i)/N$, and insert a complete set of states $|\phi\rangle$ between each interval. In this way, we obtain the Hamiltonian path integral

$$\begin{array}{l} & \phi(\vec{x},t_f) = \phi_f(\vec{x}) \\ \langle \phi_f | \hat{U}(t_f,t_i) | \phi_i \rangle = \int d[\pi] d[\phi] \, e^{iS_{\mathrm{H}}[\phi,\pi]}, \\ & \phi(\vec{x},t_i) = \phi_i(\vec{x}) \end{array}$$
(3.8)

with Hamiltonian action

$$S_{\rm H}[\phi,\pi] = \sum_{n=0}^{N-1} \Delta t \sum_{\vec{x}} a^3 \left[\pi_{\vec{x},n} \frac{\phi_{\vec{x},n+1} - \phi_{\vec{x},n}}{\Delta t} - \frac{1}{2} \pi_{\vec{x},n}^2 - \frac{1}{2} \sum_{\vec{j}} \left(\frac{\phi_{\vec{x}+\vec{j},n} - \phi_{\vec{x},n}}{a} \right)^2 - V(\phi_{\vec{x},n}) \right]$$
(3.9)

$$\longrightarrow \int_{t_i}^{t_f} dt \int d^3x \left[\pi \dot{\phi} - \frac{1}{2} \pi^2 - \frac{1}{2} \left(\vec{\nabla} \phi \right)^2 - V(\phi) \right], \tag{3.10}$$

where we have taking the continuum limit $\Delta t \to 0$, $a \to 0$ in the last line. The measure is

$$d[\phi] = \prod_{n=1}^{N-1} \prod_{\vec{x}} d\phi_{\vec{x},n}, \qquad d[\pi] = \prod_{n=0}^{N-1} \prod_{\vec{x}} \frac{d\pi_{\vec{x},n}}{2\pi}.$$
 (3.11)

We can now do the π (functional!) integral. This is easy because it amounts to a Gaussian integral for each $\pi_{\vec{x}}$. The result is the Lagrangian path integral

$$\langle \phi_f | \hat{U}(t_f, t_i) | \phi_i \rangle = C \int_{\phi(\vec{x}, t_i) = \phi_i(\vec{x})}^{\phi(\vec{x}, t_f) = \phi_f(\vec{x})} d[\phi] e^{iS[\phi]}, \qquad (3.12)$$

where the action is

$$S[\phi] = \sum_{n=0}^{N-1} \Delta t \sum_{\vec{x}} a^3 \left[\frac{1}{2} \left(\frac{\phi_{\vec{x},n+1} - \phi_{\vec{x},n}}{\Delta t} \right)^2 - \frac{1}{2} \sum_{\vec{j}} \left(\frac{\phi_{\vec{x}+\vec{j},n} - \phi_{\vec{x},n}}{a} \right)^2 - V(\phi_{\vec{x},n}) \right]$$
(3.13)

$$\longrightarrow \int_{t_i}^{t_f} dt \int d^3x \left[\frac{1}{2} \dot{\phi}^2 - \frac{1}{2} (\vec{\nabla} \phi)^2 - V(\phi) \right].$$
(3.14)

This is exactly the classical action that we started with. The path integral measure is

$$d[\phi] = \prod_{n} \left(C \prod_{\vec{x}} d\phi_{\vec{x},n} \right), \qquad C = \prod_{\vec{x}} \left(\frac{1}{2\pi i \Delta t} \right)^{1/2}.$$
(3.15)

Some comments:

- Eq. (3.12) tells us to sum over all evolutions of the field configuration from the initial field configuration ϕ_i at time t_i to the final field configuration ϕ_f at time t_f . The formula Eq. (3.12) is completely Lorentz invariant (in the continuum limit) except for the specification of the initial and final states. This manifest Lorentz invariance is one of the main reasons for using the path integral formulation of quantum field theory.
- The path integral contains an infinite number of degrees of freedom in the limit $\Delta t \rightarrow 0, a \rightarrow 0$. This gives rise to the ultraviolet divergences, which we will study in detail later. Note however that the path integral for nonzero Δt and a is completely well-defined. If we put the system in a finite spatial box (by imposing periodic boundary conditions, for example), the number of integrals

is finite, and the integrals can be approximated numerically. This approach is called 'lattice field theory,' and there is currently a major research effort underway to perform quantum field theory calculations using this approach.