10 The Feynman Path Integral

In this chapter, we derive a convenient representation for the integral kernel of the Schrödinger evolution operator, $e^{-itH/\hbar}$. This representation, the "Feynman path integral", will provide us with a heuristic but effective tool for investigating the connection between quantum and classical mechanics. This investigation will be undertaken in the next section.

10.1 The Feynman Path Integral

Consider a particle in $\mathbb{R}^d$ described by a self-adjoint Schrödinger operator

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

Recall that the dynamics of such a particle is given by the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi.$$

Recall also that the solution to this equation, with the initial condition

$$\psi|_{t=0} = \psi_0,$$

is given in terms of the evolution operator $U(t) := e^{-iHt/\hbar}$ as

$$\psi = U(t)\psi_0.$$

Our goal in this section is to understand the evolution operator $U(t) = e^{-iHt/\hbar}$ by finding a convenient representation of its integral kernel. We denote the integral kernel of $U(t)$ by $U_t(y, x)$ (also called the *propagator* from x to y).

A representation of the exponential of a sum of operators is provided by the *Trotter product formula* (Theorem 10.2) which is explained in Section 10.3 at the end of this chapter. The Trotter product formula says that

$$e^{-iHt/\hbar} = e^{i(\frac{\hbar^2 t}{2m}\Delta - Vt)/\hbar} = \text{s-lim}_{n\to\infty} K_n^n$$

where $K_n := e^{\frac{i\hbar t}{2mn}\Delta} e^{-\frac{iVt}{\hbar n}}$. Let $K_n(x,y)$ be the integral kernel of the operator K_n. Then by Proposition 5.33,

$$U_t(y,x) = \lim_{n\to\infty} \int \cdots \int K_n(y, x_{n-1}) \cdots K_n(x_2, x_1) K_n(x_1, x) dx_{n-1} \cdots dx_1. \tag{10.1}$$

Now (see Section 5.7)

$$K_n(y,x) = e^{\frac{i\hbar t\Delta}{2mn}}(y,x) e^{-\frac{iV(y)t}{\hbar n}}$$

since V, and hence $e^{-iVt/n\hbar}$, is a multiplication operator (check this).

Using the expression (2.15), and plugging into (10.1) gives us

$$U_t(y,x) = \lim_{n\to\infty} \int \cdots \int e^{iS_n/\hbar} \left(\frac{2\pi i\hbar t}{mn}\right)^{-nd/2} dx_1 \cdots dx_{n-1}$$

where

$$S_n := \sum_{k=0}^{n-1} (mn|x_{k+1} - x_k|^2/2t - V(x_{k+1})t/n)$$

with $x_0 = x$, $x_n = y$. Define the piecewise linear function ϕ_n such that $\phi_n(0) = x$, $\phi_n(t/n) = x_1$, $\cdots$, $\phi_n(t) = y$ (see Fig. 10.1).

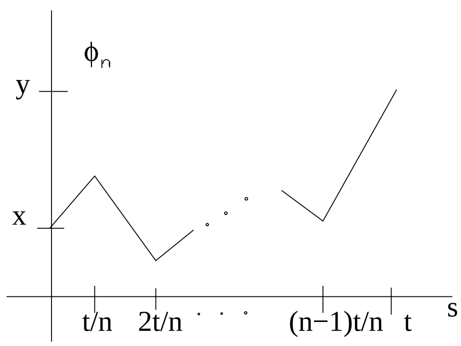

Fig. 10.1. Piecewise linear function.

Then

$$S_n = \sum_{k=0}^{n-1} \left\{ m \frac{|\phi_n((k+1)t/n) - \phi_n(kt/n)|^2}{2(t/n)^2} - V(\phi_n((k+1)t/n)) \right\} t/n.$$

Note that S_n is a Riemann sum for the classical action

$$S(\phi, t) = \int_0^t \left\{ \frac{m}{2} |\dot{\phi}(s)|^2 - V(\phi(s)) \right\} ds$$

of the path ϕ_n. So we have shown

$$U_t(y,x) = \lim_{n\to\infty} \int_{P^n_{x,y,t}} e^{iS_n/\hbar} D\phi_n \tag{10.2}$$

where $P^n_{x,y,t}$ is the $(n-1)$-dimensional space of paths ϕ_n with $\phi_n(0) = x$, $\phi_n(t) = y$, and which are linear on the intervals $(kt/n, (k+1)t/n)$ for $k = 0, 1, \ldots, n-1$, and $D\phi_n = (\frac{2\pi i\hbar t}{nm})^{-nd/2} d\phi_n(t/n) \cdots d\phi_n((n-1)t/n)$.

Heuristically, as $n \to \infty$ ϕ_n approaches a general path, ϕ, from x to y (in time t), and $S_n \to S(\phi)$. Thus we write

$$\boxed{U_t(y,x) = \int_{P_{x,y,t}} e^{iS(\phi,t)/\hbar} D\phi.} \tag{10.3}$$

Here $P_{x,y,t}$ is a space of paths from x to y, defined as

$$P_{x,y,t} := \{\phi : [0,t] \to \mathbb{R}^d | \int_0^t |\dot\phi|^2 < \infty, \quad \phi(0) = x, \quad \phi(t) = y\}.$$

This is the *Feynman path integral.* It is not really an integral, but a formal expression whose meaning is given by (10.2). Useful results are obtained non-rigorously by treating it formally as an integral. Answers we get this way are intelligent guesses which must be justified by rigorous tools.

Note that $P^n_{x,y,t}$ is an $(n-1)$-dimensional sub-family of the infinite-dimensional space $P_{x,y,t}$. It satisfies $P^n_{x,y,t} \subset P^{2n}_{x,y,t}$ and $\lim_{n\to\infty} P^n_{x,y,t} = P_{x,y,t}$ in some sense. We call such subspaces *finite dimensional approximations* of $P_{x,y,t}$. In (non-rigorous) computations, it is often useful to use finite-dimensional approximations to the path space other than the polygonal one above.

We can construct more general finite-dimensional approximations as follows. Fix a function $\phi_{xy} \in P_{x,y,t}$. Then

$$P_{x,y,t} = \phi_{xy} + P_{0,0,t}.$$

Note $P_{0,0,t}$ is a Hilbert space. Choose an orthonormal basis $\{\xi_j\}$ in $P_{0,0,t}$ and define

$$P^n_{0,0,t} := \text{ span } \{\xi_j\}^n_1$$

and

$$P^n_{x,y,t} := \phi_{xy} + P^n_{0,0,t}.$$

Then $P^n_{x,y,t}$ is a finite dimensional approximation of $P_{x,y,t}$. Typical choices of ϕ_{xy} and $\{\xi_j\}$ are

1. ϕ_{xy} is piecewise linear and $\{\xi_j\}$ are "splines". This gives the polygonal approximation introduced above.

2. ϕ_{xy} is a classical path (a critical point of the action functional $S(\phi)$) and $\{\xi_j\}$ are eigenfunctions of the Hessian of S at ϕ_{xy} (these notions are described in the following two chapters). In this case, if $\eta \in P^n_{0,0,t}$, then we can represent it as
$$\eta = \sum_{j=1}^{n} a_j \xi_j,$$
and we have
$$D\eta = \left(\frac{2\pi i t\hbar}{m}\right)^{-d/2} \left(\frac{2\pi n}{t}\sqrt{\frac{m}{\hbar}}\right)^n \prod_{j=1}^{n} da_j.$$

It is reasonable to expect that if
$$\lim_{n\to\infty} \int_{P^n_{x,y,t}} e^{iS(\phi,t)/\hbar} D\phi$$
exists, then it is independent of the finite-dimensional approximation, $P^n_{x,y,t}$, that we choose.

Problem 10.1

1. Compute (using (10.3) and a finite-dimensional approximation of the path space) U_t for
   a) $V(x) = 0$ (free particle)
   b) $V(x) = \frac{m\omega^2}{2}x^2$ (harmonic oscillator in dimension $d = 1$).
2. Derive a path integral representation for the integral kernel of $e^{-\beta H/\hbar}$.
3. Use the previous result to find a path integral representation for $Z(\beta) := \text{tr } e^{-\beta H/\hbar}$ (hint: you should arrive at the expression (11.10)).

10.2 Generalizations of the Path Integral

Here we mention briefly two extensions of the Feynman path integral we have just introduced.

1. Phase-space path integral:
$$U_t(y,x) = \int_{P_{x,y,t}\times \text{ anything}} e^{i\int_0^t (\dot\phi\pi - H(\phi,\pi))/\hbar} D\phi \,{D\!\!\!/}\pi$$
where ${D\!\!\!/}\pi$ is the *path measure*, normalized as
$$\int e^{-\frac{i}{2}\int_0^t \|\pi\|^2} {D\!\!\!/}\pi = 1$$
(in QM, ${d\!\!\!/}^3 p = d^3p/(2\pi)^{3/2}$). To derive this representation, we use the Trotter product formula, the expression $e^{-i\epsilon H} \approx 1 - i\epsilon H$ for ϵ small,

and the symbolic (pseudodifferential) composition formula. Unlike the representation $\int e^{iS/\hbar}D\phi$, this formula holds also for more complicated H, which are not quadratic in p!

2. A particle in a vector potential $A(x)$. In this case, the Hamiltonian is

$$H(x,p) = \frac{1}{2m}(p - eA(x))^2 + V(x)$$

and the Lagrangian is

$$L(x,\dot{x}) = \frac{m}{2}\dot{x}^2 - V(x) + e\dot{x}\cdot A(x).$$

The propagator still has the representation

$$U_t(y,x) = \int_{P_{x,y,t}} e^{iS(\phi)/\hbar}D\phi,$$

but with

$$S(\phi) = \int_0^t L(\phi,\dot{\phi})ds = \int_0^t (\frac{m}{2}\dot{\phi}^2 - V(\phi))ds + e\int_0^t A(\phi)\cdot\dot{\phi}ds.$$

Since $A(x)$ does not commute with ∇ in general, care should be exercised in computing a finite-dimensional approximation: one should take

$$\sum A(\frac{1}{2}(x_i + x_{i+1}))\cdot(x_{i+1} - x_i)$$

or

$$\sum \frac{1}{2}(A(x_i) + A(x_{i+1}))\cdot(x_{i+1} - x_i)$$

and not

$$\sum A(x_i)\cdot(x_{i+1} - x_i) \text{ or } \sum A(x_{i+1})\cdot(x_{i+1} - x_i).$$

10.3 Mathematical Supplement: the Trotter Product Formula

Let A, B, and $A + B$ be self-adjoint operators on a Hilbert space $\mathcal{H}$. If $[A,B] \neq 0$, then $e^{i(A+B)} \neq e^{iA}e^{iB}$ in general. But we do have the following.

Theorem 10.2 (Trotter product formula) Let either A and B be bounded, or A, B, and $A + B$ be self-adjoint and bounded from below. Then for $Re(\lambda) \leq 0$,

$$e^{\lambda(A+B)} = s - \lim_{n\to\infty}(e^{\lambda\frac{A}{n}}e^{\lambda\frac{B}{n}})^n$$

Remark 10.3 The convergence here is in the sense of the *strong operator topology*. For operators A_n and A on a Hilbert space $\mathcal{H}$, such that $D(A_n) = D(A)$, $A_n \to A$ in the strong operator topology (written $\text{s-lim}_{n\to\infty} A_n = A$) iff $\|A_n\psi - A\psi\| \to 0$ for all $\psi \in D(A)$. For bounded operators, we can take norm convergence. In the formula above, we used a uniform decomposition of the interval $[0,1]$. The formula still holds for a non-uniform decomposition.

Proof for A,B bounded: We can assume $\lambda = 1$. Let $S_n = e^{(A+B)/n}$ and $T_n = e^{A/n}e^{B/n}$. Now by "telescoping",

$$\begin{aligned} S_n^n - T_n^n &= S_n^n - T_n S_n^{n-1} + T_n S_n^{n-1} + \cdots - T_n^n \\ &= \sum_{k=0}^{n-1} T_n^k (S_n - T_n) S_n^{n-k-1} \end{aligned}$$

so

$$\begin{aligned} \|S_n^n - T_n^n\| &\leq \sum_{k=0}^{n-1} \|T_n\|^k \|S_n - T_n\| \|S_n\|^{n-k-1} \\ &\leq \sum_{k=0}^{n-1} (\max(\|T_n\|, \|S_n\|))^{n-1} \|S_n - T_n\| \\ &\leq n e^{\|A\|+\|B\|} \|S_n - T_n\|. \end{aligned}$$

Using a power series expansion, we see $\|S_n - T_n\| = O(1/n^2)$ and so $\|S_n^n - T_n^n\| \to 0$ as $n \to \infty$. □

A proof for unbounded operators can be found in [RSI].