

Notes on the Path Integral

Physics 305

In the canonical formulation of quantum mechanics, the time evolution of the wavefunction is governed by Schrödinger's Equation:

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle . \quad (1)$$

This equation was in fact one of our postulates, an unsatisfactory state of affairs for those of us who prefer axioms to be simple — a straight line segment can be drawn joining any two points, any straight line segment can be extended indefinitely in a straight line, etc. One can motivate the form of this equation from a careful consideration of plane waves, as Bransden and Joachain do in Chapter 3 of their book. But there is another powerful way of thinking of the origins of this equation.

Before getting to the path integral itself, I need to make a few preliminary remarks about time propagation and the Schrödinger and Heisenberg pictures of quantum mechanics. In the previous “Group Theory Remarks”, we discussed how, for a time independent Hamiltonian, one could write down a unitary operator $U(T) = e^{-iHT/\hbar}$ that propagated a wave function forward in time an amount T :

$$U(T)\psi(x, t) = e^{-iHT/\hbar}\psi(x, t) = \psi(x, t + T) . \quad (2)$$

To describe time evolution in quantum mechanics, one could in fact replace Schrödinger's equation with (2). To demonstrate this equivalence, take a derivative of $\psi(x, t) = U(t)\psi(x, 0)$ with respect to t . We find

$$\frac{d\psi}{dt} = \frac{dU}{dt}\psi(x, 0) = -\frac{iH}{\hbar}U(t)\psi(x, 0) = -\frac{iH}{\hbar}\psi(x, t) .$$

In this class, we have for the most part thought of states as being time dependent and operators as being time independent. This last paragraph suggests that there may well be circumstances in which this separation, often called the Schrödinger picture, is not useful and even confusing. There is an alternate version of quantum mechanics, the Heisenberg picture, in which states are time independent and operators are time dependent:

	Schrödinger	Heisenberg
states	time dependent	time independent
operators	time independent	time dependent

To translate between these two pictures is very simple using the unitary operator $U(t)$ given above. We use the subscript S to indicate Schrödinger picture and the subscript H to indicate Heisenberg picture. We have

$$|\psi(t)\rangle_S = e^{-iHt/\hbar}|\psi\rangle_H \quad \text{and} \quad \mathcal{O}_S = e^{-iHt/\hbar}\mathcal{O}_H(t)e^{iHt/\hbar} .$$

One way of thinking about a Heisenberg state is as a Schrödinger state at time $t = 0$: $|\psi(0)\rangle_S = |\psi\rangle_H$.

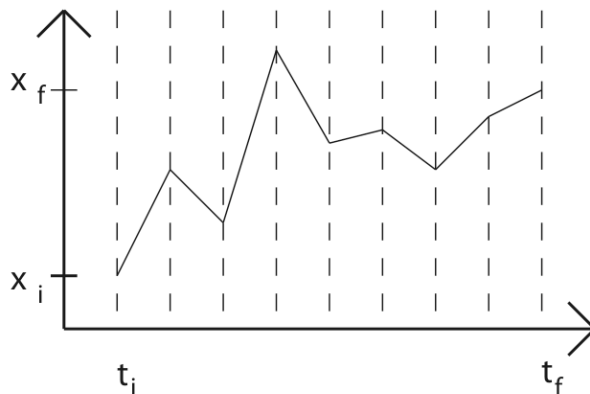


Figure 1: A particular path joining x_i and x_f .

The path integral formulation begins with a strange and beautiful result for the probability amplitude of a particle initially at position x_i at a time t_i to end up at a position x_f at time t_f . The claim is that

$$\langle x_f, t_f | x_i, t_i \rangle = N \int \mathcal{D}x \exp \left(\frac{i}{\hbar} \int_{t_i}^{t_f} L(x, \dot{x}) dt \right) . \quad (3)$$

To explain eq. (3), we first have to describe more precisely what we mean by the state $|x, t\rangle$. We are used to the definition of the wavefunction, that $\langle x | \psi(t) \rangle_S = \psi(x, t)$. In the Heisenberg picture, we would have $\langle x | e^{-iHt/\hbar} | \psi \rangle_H = \psi(x, t)$ which suggests defining

$$|x, t\rangle \equiv e^{iHt/\hbar} |x\rangle ,$$

such that $\langle x, t | \psi \rangle_H = \psi(x, t)$. Thus, we may write our probability amplitude in the form

$$\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | e^{-iHt_f/\hbar} e^{iHt_i/\hbar} | x_i \rangle = \langle x_f | e^{-iHT/\hbar} | x_i \rangle ,$$

where $T = t_f - t_i$.

The right hand side of eq. (3) is where the real conceptual meat lies. Here $L(x, \dot{x})$ is the classical Lagrangian for the particle, and thus $\int L dt = S$ is the classical action.¹ The factor N is a constant that turns out to be irrelevant for many physical questions. This funny integral over $\mathcal{D}x$ sums over all possible paths between x_i and x_f . It is an example of a functional integral, i.e. an integral over all possible functions $x(t)$ with the boundary conditions $x(t_i) = x_i$ and $x(t_f) = x_f$. Graphically, we can think of breaking up the integral into many short time segments τ and then summing over all x for each of these short time segments. A particular term in the sum is shown in Figure 1.

At the end of these notes, we will demonstrate the equivalence of Schrödinger's equation and this path integral formulation, but I want to show you first a beautiful feature of the path

¹Recall that the Hamiltonian is related to the Lagrangian via a Legendre transform $H = p\dot{x} - L$ where

$$p \equiv \frac{\partial L}{\partial \dot{x}} .$$

integral: The path integral provides a conceptually simple way of taking the classical limit of quantum mechanics. To set up this discussion, we begin with the method of stationary phase for evaluating oscillatory integrals. (It is a method with close connections to saddle point integration and the method of steepest descent.) Consider an ordinary integral

$$I = \int_{-\infty}^{\infty} e^{iS(x)} dx$$

where $S(x)$ is real and $e^{iS(x)}$ is a highly oscillatory function. Because of the oscillations, the integral cancels out almost everywhere except where $S'(x) = 0$, i.e. where the phase becomes stationary. Thus, we expect the largest contribution to the integral to come from x_0 where $S'(x_0)$ vanishes. We expand the exponent

$$S(x) = S(x_0) + \frac{1}{2}S''(x_0)(x - x_0)^2 + \dots$$

and approximate the integral as

$$I \approx e^{iS(x_0)} \int_{-\infty}^{\infty} \exp\left(\frac{i}{2}S''(x_0)(x - x_0)^2\right) dx .$$

This integral becomes Gaussian and can be carried out after the change of variables $x - x_0 = e^{i\pi/4}u$:

$$\begin{aligned} I &\approx e^{i\pi/4} e^{iS(x_0)} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}S''(x_0)u^2\right) du \\ &\approx e^{i\pi/4} \sqrt{\frac{2\pi}{S''(x_0)}} e^{iS(x_0)} . \end{aligned}$$

(This change of variables is a little bit of a cheat; we've been careless about the limits of integration and dropped a contour at $x = \infty$. The result can be justified with a little of complex analysis and a little bit of thought.)

We can treat the path integral in eq. (3) in an equivalent way. This condition $S'(x_0) = 0$ becomes in the path integral context that the variation of the action vanishes, $\delta S = 0$, under a variation in the path $x \rightarrow x + \delta x$. However, we know from classical mechanics that $\delta S/\delta x = 0$ is the condition that x be a solution to the classical equations of motion! Evaluating the path integral by the method of stationary phase yields the classical limit of quantum mechanics.

How does a quantum mechanical particle know where to go? It doesn't. It tries every possible path, but each path gets weighted by a phase $e^{iS/\hbar}$. Most of the paths interfere destructively with one another. The classical trajectory gives the dominant contribution to the path integral.

We calculate the action S for a solution to the equations of motion in order to figure out what the equivalent of the leading $e^{iS(x_0)}$ phase is in this functional integral context. For a simple mechanical system with a Lagrangian of the form

$$L = \frac{m}{2}\dot{x}^2 - V(x) ,$$

we know there is a conserved energy

$$E = \frac{m}{2}\dot{x}^2 + V(x) .$$

We can write the action in the form

$$\int_{t_i}^{t_f} L dt = \int_{t_i}^{t_f} \left(\frac{m}{2}\dot{x}^2 - V(x) \right) dt = \int_{t_i}^{t_f} (m\dot{x}^2 - E) dt = \int_{x_i}^{x_f} p dx - ET .$$

Thus, ignoring the equivalent of the $S''(x_0)$ dependent normalization, we find that

$$\langle x_f, t_f | x_i, t_i \rangle \sim \exp \left(\frac{i}{\hbar} \int_{x_i}^{x_f} p dx - \frac{iET}{\hbar} \right) .$$

This result should be familiar from the WKB approximation. For a particle of energy E , we have the usual time dependence $e^{-iET/\hbar}$ represented by the second term. But there is also the familiar WKB $\int p dx$ term in the exponent.

Deriving the path integral

To derive (3), we begin by splitting up the time propagation into n steps,

$$\langle x_f, t_f | x_i, t_i \rangle = \int \cdots \int dx_1 dx_2 \cdots dx_n \langle x_f, t_f | x_n, t_n \rangle \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \cdots \langle x_1, t_1 | x_i, t_i \rangle .$$

Next we consider the propagation over an infinitesimal time step $\tau = T/(n+1)$:

$$\begin{aligned} \langle x_{j+1}, t_{j+1} | x_j, t_j \rangle &= \langle x_{j+1} | e^{-iH\tau/\hbar} | x_j \rangle \\ &= \langle x_{j+1} | 1 - \frac{i}{\hbar} H\tau + \mathcal{O}(\tau^2) | x_j \rangle \\ &= \delta(x_{j+1} - x_j) - \frac{i\tau}{\hbar} \langle x_{j+1} | H | x_j \rangle + \mathcal{O}(\tau^2) \\ &= \frac{1}{2\pi\hbar} \int dp \exp \left[\frac{i}{\hbar} p(x_{j+1} - x_j) \right] - \frac{i\tau}{\hbar} \langle x_{j+1} | H | x_j \rangle + \mathcal{O}(\tau^2) . \end{aligned}$$

We now restrict to Hamiltonians of the form $H = \hat{p}^2/2m + V(x)$, and we evaluate $\langle x_{j+1} | H | x_j \rangle$. For the kinetic energy piece, we decompose the result into plane waves, using

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} .$$

We have

$$\begin{aligned} \frac{1}{2m} \langle x_{j+1} | \hat{p}^2 | x_j \rangle &= \frac{1}{2m} \int dp dp' \langle x_{j+1} | p' \rangle \langle p' | \hat{p}^2 | p \rangle \langle p | x_j \rangle , \\ &= \frac{1}{2m} \int \frac{dp dp'}{2\pi\hbar} \exp \left[\frac{i}{\hbar} (p'x_{j+1} - px_j) \right] p^2 \delta(p - p') \\ &= \int \frac{dp}{h} \exp \left[\frac{i}{\hbar} p(x_{j+1} - x_j) \right] \frac{p^2}{2m} . \end{aligned} \tag{4}$$

For the potential energy piece, we have

$$\begin{aligned}
\langle x_{j+1}|V(x)|x_j\rangle &= V\left(\frac{x_j+x_{j+1}}{2}\right)\langle x_{j+1}|x_j\rangle \\
&= V\left(\frac{x_j+x_{j+1}}{2}\right)\delta(x_{j+1}-x_j) \\
&= \int \frac{dp}{h} \exp\left[\frac{i}{\hbar}p(x_{j+1}-x_j)\right] V(\bar{x}_j), \tag{5}
\end{aligned}$$

where in the last line, we defined $\bar{x}_j \equiv (x_{j+1} + x_j)/2$. Putting the kinetic and potential energy pieces, (4) and (5), together, we find that

$$\langle x_{j+1}|H|x_j\rangle = \int \frac{dp}{h} \exp\left[\frac{i}{\hbar}p(x_{j+1}-x_j)\right] H(p, \bar{x}_j). \tag{6}$$

Note that the momentum p in $H(p, \bar{x}_j)$ is now interpreted as a number and not as an operator.

For the propagation over a short time interval τ , we thus find that

$$\langle x_{j+1}, t_{j+1}|x_j, t_j\rangle = \frac{1}{h} \int dp_j \exp\left[\frac{i}{\hbar}\left(p_j(x_{j+1}-x_j) - \tau H(p_j, \bar{x}_j)\right)\right] + \mathcal{O}(\tau^2).$$

We think of p_j as the momentum p between times t_j and t_{j+1} . In the limit $n \rightarrow \infty$, for the total amplitude, we find that

$$\langle x_f, t_f|x_i, t_i\rangle = \lim_{n \rightarrow \infty} \int \left(\prod_{j=1}^n dx_j\right) \left(\prod_{j=0}^n \frac{dp_j}{h}\right) \exp\left[\frac{i}{\hbar} \sum_{j=0}^n \left(p_j(x_{j+1}-x_j) - \tau H(p_j, \bar{x}_j)\right)\right] \tag{7}$$

where we think of $x_0 = x_i$ and $x_{n+1} = x_f$. Symbolically, we write this integral as a path integral:

$$\langle x_f, t_f|x_i, t_i\rangle = \int \frac{\mathcal{D}x \mathcal{D}p}{h} \exp\left[\frac{i}{\hbar} \int_{t_i}^{t_f} dt (p\dot{x} - H(p, x))\right].$$

When the Hamiltonian $H = p^2/2m + V(x)$, we can do the Gaussian integrals over the p_j . Consider the integral over just one of the p_j :

$$\int \frac{dp_j}{h} \exp\left[\frac{i}{\hbar} \left(p_j(x_{j+1}-x_j) - \tau \frac{p_j^2}{2m}\right)\right] = \sqrt{\frac{m}{ih\tau}} \exp\left[\frac{i\tau}{\hbar} \frac{m}{2} \left(\frac{x_{j+1}-x_j}{\tau}\right)^2\right].$$

Multiplying the $n+1$ of these p_j integrals together, we find that

$$\begin{aligned}
\langle x_f, t_f|x_i, t_i\rangle &= \lim_{n \rightarrow \infty} \left(\frac{m}{ih\tau}\right)^{(n+1)/2} \int \left(\prod_{j=1}^n dx_j\right) \exp\left[\frac{i\tau}{\hbar} \sum_{j=0}^n \left(\frac{m}{2} \left(\frac{x_{j+1}-x_j}{\tau}\right)^2 - V(\bar{x}_j)\right)\right] \\
&= N \int \mathcal{D}x \exp\left[\frac{i}{\hbar} \int_{t_i}^{t_f} L(x, \dot{x}) dt\right].
\end{aligned}$$