Phys 342 Lecture 36

Welcome back to more on the path integral! In the past two lectures, we derived the path integral, or position space transition amplitude, from the Schrödinger equation. In particular, we exploited the completeness of position and momentum eigenstates and used the time evolution operator, $\exp[-i\hat{H}t/\hbar]$. We found the path integral Z from this procedure to be:

$$Z = \langle x_f, t=T | x_i, t=0 \rangle = \int [dx]\, e^{i\frac{S[x]}{\hbar}} \text{, where } S[x]$$

is the classical action of the system,

$$S[x] = \int_0^T dt\, L(x,\dot{x}) = \int_0^T dt \left(\tfrac{1}{2}m\dot{x}^2 - V(x)\right),$$

and $L(x,\dot{x})$ is the Lagrangian of the system; the difference of the kinetic ($\frac{1}{2}m\dot{x}^2$) and potential ($V(x)$) energies of the system.

In this lecture, we will instead start from the path integral Z as our quantum mechanical axiom and construct the wavefunction $\Psi(x,t)$ and its time-evolution equation, the Schrödinger equation, from the path integral. Thus, we will demonstrate the equivalence of the path integral as a complete description of a quantum system and the Schrödinger equation (and vice versa).

To do this, we start with an arbitrary quantum state $|\psi\rangle \in \mathcal{H}$, the Hilbert space of our system. Recall that the state evolved from time $t=0$ to $t=T$ is just acted on by the exponentiated Hamiltonian:

$|\psi(T)\rangle = e^{-\frac{i\hat{H}T}{\hbar}} |\psi(0)\rangle$. Further, the wave function of this state is its representation in the position basis. To project to the position basis, we just act with the position eigenstate bra $\langle x|$ on our state $|\psi\rangle$:

$$\langle x|\psi(t)\rangle = \psi(x,t) = \langle x| e^{-\frac{i\hat{H}t}{\hbar}} |\psi\rangle,$$ the wavefunction

evaluated at time T in terms of the initial state $|\psi\rangle \equiv |\psi(0)\rangle$. Next, we insert a complete set of position eigenstates between our state $|\psi\rangle$ and the time evolution operator, where

$$1 = \int dx_0 \, |x_0\rangle\langle x_0|,$$ and so

$$\psi(x,t) = \int dx_0 \, \langle x| e^{-\frac{i\hat{H}t}{\hbar}} |x_0\rangle\langle x_0|\psi\rangle$$

Now, we recognize $\langle x_0|\psi\rangle = \psi(x_0)$ as the wavefunction at time $t=0$ and then the transition amplitude

$\langle x| e^{-\frac{i\hat{H}t}{\hbar}} |x_0\rangle$ is just the path integral for transition

from position eigenstate $|x_0\rangle$ to final position $|x\rangle$ over total time t. Thus, from our expression for the path integral, we can write:

$$\psi(x,t) = \int_{x_0}^{x} [dx'] \, e^{\frac{iS[x']}{\hbar}} \psi(x_0).$$

The integral here is a bit of a compact notation. By

$$\int_{x_0}^{x} [dx'] = \int \prod_{n=0}^{N-1} dx_n,$$ where $N \to \infty$ and $x_n \equiv x$, the final position (which we don't integrate over.).

Actually, we should be a bit more careful, too. With this choice of the integration measure of the path integral, we don't guarantee that the wavefunction is L^2-normalized. No worries; there's an easy fix: we just divide by the path integral Z:

$$\boxed{\psi(x,t) = \frac{1}{Z}\int_{x_0}^{x}[dx']\, e^{\frac{iS[x']}{\hbar}}\psi(x_0)}\ , \text{ where}$$

$$Z = \int [dx]\, e^{\frac{iS[x]}{\hbar}}.$$ In this sense, the path integral acts as a normalization factor, similar (actually, formally identical in the complexified time plane) to the partition function of statistical mechanics.

Now, if this is really the wave function, we should be able to derive the Schrödinger equation from the path integral representation. Our procedure for doing this will be similar as our operator derivation of the Schrödinger equation. We first only consider a time $t=\varepsilon$, as $\varepsilon \to 0$:

$$\psi(x,\varepsilon) = \frac{1}{Z}\int_{x_0}^{x}[dx']\, e^{\frac{iS[x']}{\hbar}}\psi(x_0).$$

For small enough ε, the particle can't take arbitrary paths from x_0 to x; this is to say that x_0 and x are near one another, and the continuity of quantum mechanical trajectories. Then, in the $\varepsilon \to 0$ limit, Z = constant (i.e., no paths to sum over) and the integrals that remain upstairs are just over x_0, the initial position:

$$\psi(x,\varepsilon) \approx \frac{1}{Z}\int dx_0\, e^{\frac{i}{\hbar}\int_0^{\varepsilon} dt\left[\frac{m\dot{x}^2}{2} - V(x)\right]}\psi(x_0).$$

Now, let's move on to the classical action in the exponent. As $\varepsilon \to 0$, the integral can be approximated by its integrand times ε, as it is assumed to not vary wildly over $t \in [0, \varepsilon]$ (again, by continuity). Additionally, note that the particle's velocity over time ε is:

$$\dot{x} \approx \frac{x(\varepsilon) - x(0)}{\varepsilon} = \frac{x - x_0}{\varepsilon},$$ by the assumption that $x(\varepsilon) = x$ and $x(0) = x_0$, the final and initial positions.

Using these observations, we have:

$$\lim_{\varepsilon \to 0} \int_0^{\varepsilon} dt \left(\frac{m}{2} \dot{x}^2 - V(x) \right) = \varepsilon \left[\frac{m}{2} \frac{(x - x_0)^2}{\varepsilon^2} - V(x) \right],$$

where, by continuity, we can just evaluate $V(x)$ at x, as we assume x and x_0 differ by $\mathcal{O}(\varepsilon)$, and so their difference is higher order in ε.

Thus, as $\varepsilon \to 0$, the wavefunction in the path integral formulation becomes:

$$\psi(x, \varepsilon) \approx \frac{1}{Z} \int dx_0 \exp\left[\frac{i\varepsilon}{\hbar} \left(\frac{m}{2} \frac{(x - x_0)^2}{\varepsilon^2} - V(x) \right) \right] \psi(x_0)$$

$$\approx \frac{e^{-\frac{i\varepsilon}{\hbar} V(x)}}{Z} \int_{-\infty}^{\infty} dx_0 \, e^{\frac{im}{2\hbar} \frac{(x - x_0)^2}{\varepsilon}} \psi(x_0),$$

where, to $\mathcal{O}(\varepsilon^2)$ corrections in the exponent, we can just pull out the potential factor. (We're also assuming that the potential is non-singular for any finite x; otherwise, we might not be able to claim that $\varepsilon V(x)$ is small.)

Now, we need to tackle the integral that remains. The exponential factor $\exp\left[\frac{im}{2\hbar} \frac{(x - x_0)^2}{\varepsilon} \right]$ becomes an extremely narrow spike in the limit that $\varepsilon \to 0$, centered at $x_0 = X$. Further, its integral is finite, and so, as $\varepsilon \to 0$, is proportional to a δ-function. If it were a δ-function, then evaluating the integral that remains would be easy. With this motivation, then, we want to expand the Gaussian in a series of δ-functions and its derivatives, centered about $x_0 = X$. That is, we want to write:

$$e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}} = a_0\,\delta(x-x_0) + a_1\,\delta'(x-x_0) + a_2\,\delta''(x-x_0) + \cdots,$$

where $a_0, a_1, a_2, \ldots$ are some coefficients we would like to determine. Now, the derivative of a δ-function looks scary, but using integration by parts it just acts on a function $f(x)$ as:

$$\int dx\,\delta'(x-x_0)\,f(x) = -\int dx\,\delta(x-x_0)\,f'(x),$$

and similar for higher-order derivatives. This demonstrates that the integral of a δ-function with any number $n>0$ derivatives on it is 0:

$$\int_{-\infty}^{\infty} dx\,\delta^{(n)}(x-x_0) = 0.$$ This immediately tells us that

$$a_0 = \int_{-\infty}^{\infty} dx_0\, e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}} = \frac{\sqrt{2\pi\hbar\varepsilon}}{\sqrt{-im}},$$ just evaluating the integral of a Gaussian.

Next, for the a_1 coefficient, we note that

$$\int_{-\infty}^{\infty} dx_0\,(x-x_0)\,\delta(x-x_0) = \int_{-\infty}^{\infty} dx_0\,(x-x_0)\,\delta^{(n)}(x-x_0), \text{ for } n>1,$$

because more than one derivative will kill the prefactor function. Further, note that

$$\int_{-\infty}^{\infty} dx_0\,(x_0 - x)\,\delta'(x - x_0) = -\int_{-\infty}^{\infty} dx_0\,(x_0 - x)\frac{d}{dx_0}\delta(x - x_0)$$

$$= \int_{-\infty}^{\infty} dx_0\left[\frac{d}{dx_0}(x_0 - x)\right]\delta(x - x_0) = 1,$$ and so the a_1

coefficient is:

$$a_1 = \int_{-\infty}^{\infty} dx_0\,(x_0 - x)\,e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}} = 0,$$ as the Gaussian is symmetric about $x_0 = x$.

Continuing to the a_2 coefficients, we note that

$$\int_{-\infty}^{\infty} dx_0\,(x_0 - x)^2\,\delta''(x_0 - x) = \int_{-\infty}^{\infty} dx_0\,2(x_0 - x)\,\delta'(x_0 - x)$$

$$= \int_{-\infty}^{\infty} dx_0\,2\,\delta(x_0 - x) = 2,$$ using integration by parts twice.

Then, the a_2 coefficient is

$$a_2 = \frac{1}{2}\int_{-\infty}^{\infty} dx_0\,(x - x_0)^2\,e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}} = \frac{\sqrt{2\pi}}{2}\left(-\frac{\hbar\varepsilon}{im}\right)^{3/2}.$$

Thus, this singular expansion of the very narrow Gaussian yields:

$$e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}} = \sqrt{-\frac{2\pi\hbar\varepsilon}{im}}\,\delta(x - x_0) + \sqrt{\frac{\pi}{2}}\left(-\frac{\hbar\varepsilon}{im}\right)^{3/2}\delta''(x - x_0) + \ldots$$

Now, this expansion can enable us to easily evaluate the integral over x_0 that remains. We have

$$\int_{-\infty}^{\infty} dx_0\,e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}}\,\psi(x_0) = \int_{-\infty}^{\infty} dx_0\left[\sqrt{-\frac{2\pi\hbar\varepsilon}{im}}\,\delta(x - x_0) + \sqrt{\frac{\pi}{2}}\left(-\frac{\hbar\varepsilon}{im}\right)^{3/2}\delta''(x - x_0) + \ldots\right]\psi(x_0)$$

$$= \sqrt{-\frac{2\pi\hbar\varepsilon}{im}}\,\psi(x) + \sqrt{\frac{\pi}{2}}\left(-\frac{\hbar\varepsilon}{im}\right)^{3/2}\psi''(x) + \dots$$

Now, putting this together and Taylor expanding the expression thus far, we have:

$$\psi(x,\varepsilon) = \psi(x) + \varepsilon\frac{d\psi(x)}{dt} + \dots = \frac{e^{-\frac{i\varepsilon V(x)}{\hbar}}}{Z}\int_{-\infty}^{\infty} dx_0\, e^{\frac{im}{2\hbar}\frac{(x-x_0)^2}{\varepsilon}}\psi(x_0)$$

$$= \frac{\sqrt{-\frac{2\pi\hbar\varepsilon}{im}}\,\psi(x) + \sqrt{\frac{\pi}{2}}\left(-\frac{\hbar\varepsilon}{im}\right)^{3/2}\psi''(x) - \frac{i\varepsilon}{\hbar}V(x)\sqrt{-\frac{2\pi\hbar\varepsilon}{im}}\,\psi(x) + \dots}{Z}$$

Now, to derive the Schrödinger equation, we would match terms at each order in ε on both sides of this equation. However, terms on the right side have half-integer powers of ε; not good, and not possible to match! However, we haven't yet accounted for the normalization "constant" Z in the denominator. Recall from last lecture that when we performed the integrals over momentum at time step n, we picked up a factor of:

$\sqrt{-\frac{im}{2\pi\hbar\varepsilon}}$, with $\Delta t = \varepsilon$, and we moved the factor of i from denominator to numerator. Now, because ε is sufficiently small, the path integral Z has no integrals over intermediate positions x_n, between x_0 and x, but does have one integral over momentum that allows travel from x_0 to x. That is, as $\varepsilon \to 0$, the path integral is just this normalization factor from integrating over p:

$Z = \left(\sqrt{-\frac{im}{2\pi\hbar\varepsilon}}\right)^{-1}$. This is exactly what we need!

Accounting for the normalization, we then find:

$$\Psi(x) + \varepsilon \frac{d\Psi(x)}{dt} + \cdots = \Psi(x) - \frac{1}{i}\frac{\hbar}{2m}\varepsilon \Psi''(x) - \frac{i\varepsilon}{\hbar} V(x)\Psi(x) + \mathcal{O}(\varepsilon^2).$$

Now, we can cancel $\Psi(x)$ from both sides and the $\mathcal{O}(\varepsilon)$ terms require:

$$\frac{d\Psi}{dt} = -\frac{1}{i}\frac{\hbar}{2m}\Psi''(x) - \frac{i}{\hbar}V(x)\Psi(x)$$, or, more familiarly

$$\boxed{i\hbar \frac{d\Psi}{dt} = -\frac{\hbar^2}{2m}\Psi'' + V\Psi}$$, which is just the Schrödinger equation!

Thus, we have shown that the Schrödinger equation implies the path integral, and vice-versa, thus one can start with either formulation to analyze quantum dynamics. While the Schrödinger equation seems nicer for the questions we have asked in this course, the path integral is a much more natural starting point for quantum field theory, when one harmonizes quantum mechanics and special relativity.

We have but scratched the surface of the path integral, but that's all the time we have now. Next week, we will re-visit the density matrix and see some of its consequences... Only three more lectures...