Lecture 10

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1 Path integrals

We have so far presented the path integral as an alternative way to formulate quantum mechanics that can be derived from reasonable physical assumptions. We will now show that it is equivalent to the operator formulation. We will do this by first deriving it from the operator formalism, then using it to derive the Schrödinger equation. In the operator formalism, the probability amplitude $\langle x_f, t_f | x_i, t_i \rangle$ is given by:

$$\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | e^{-\frac{i}{\hbar}\mathcal{H}(t_f - t_i)} | x_i \rangle \tag{1}$$

This object is usually called the propagator which tells us what is the overlap of a state initially localized at x_i with a state localized at x_f after it is allowed to evolve for time $t_f - t_i$. We now divide the time-interval $T = t_f - t_i$ into N intervals with width $\Delta t = T/N$ and insert the resolution of unity

$$\int dx |x\rangle\langle x| = \mathbb{1} \tag{2}$$

$N - 1$ times to get

$$\langle x_f, t_f | x_i, t_i \rangle = \int dx_1 \dots dx_{N-1} \langle x_f | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x_{N-1} \rangle \langle x_{N-1} | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x_{N-2} \rangle \dots \\ \times \langle x_2 | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x_1, \rangle \langle x_1 | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x_i \rangle \tag{3}$$

This is the same as the expression (Eq. 2) we derived last lecture with the infinitesmal propagator $\langle x', t + \Delta t | x, t \rangle$ replaced by $\langle x' | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x \rangle$. We now consider the Hamiltonian $\mathcal{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$. The action of the potential energy operator $V(\hat{x})$ in the position basis is simple but not the kinetic energy operator. To simplify this expression, we use the Baker-Campbell-Haussdorff formula $e^{(X+Y)\Delta t} = e^{X\Delta t} e^{Y\Delta t} e^{-\frac{1}{2}[X,Y](\Delta t)^2} \dots$ where the dots contain exponential with higher powers of Δt. Since the Hamiltonian is multiplied by Δt and we are interested in the $\Delta t \to 0$ limit, we can write $e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} = e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(\hat{x})\Delta t}$. This leads to the simplification

$$\langle x' | e^{-\frac{i}{\hbar}\mathcal{H}\Delta t} | x \rangle = \langle x' | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(x)\Delta t} | x \rangle = \langle x' | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} | x \rangle e^{-\frac{i}{\hbar}V(x)\Delta t} \tag{4}$$

To simplify further, we insert another resolution of unity but using the momentum basis

$$\int dp |p\rangle\langle p| = \mathbb{1} \tag{5}$$

leading to

$$\langle x' | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} | x \rangle = \int dp \langle x' | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} | p \rangle \langle p | x \rangle = \int dp \langle x' | p \rangle \langle p | x \rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} \tag{6}$$

Using $\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px}$, we finally get

$$\langle x'|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\Delta t}|x\rangle = \frac{1}{2\pi\hbar}\int dp\, e^{-\frac{i\Delta t}{2m\hbar}[p^2+\frac{2mp}{\Delta t}(x'-x)]} = \frac{1}{2\pi\hbar}\int dp\, e^{-\frac{i\Delta t}{2m\hbar}[p+\frac{m}{\Delta t}(x'-x)]^2+i\frac{m}{2\hbar\Delta t}(x-x')^2}$$
$$= \sqrt{\frac{im}{2\pi\hbar\Delta t}} e^{i\frac{m}{2\hbar\Delta t}(x-x')^2} \tag{7}$$

This leads to

$$\langle x'|e^{-\frac{i}{\hbar}\mathcal{H}\Delta t}|x\rangle = \sqrt{\frac{im}{2\pi\hbar\Delta t}} e^{\frac{i}{\hbar}\Delta t[\frac{m(x-x')^2}{2(\Delta t)^2}-V(x)]} \tag{8}$$

Substituting in (8) yields the path integral expression

$$\langle x_f, t_f|x_i, t_i\rangle = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dtL[x,\dot{x}]} = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \mathcal{D}x(t)\, e^{\frac{i}{\hbar}S} \tag{9}$$

While the derivation above shows the equivalence of path integral and the probability amplitude defined in the operator formulation, it is instructive to show explicitly that the path integral representation of the amplitude also satisfied the Schrödinger equation, allowing us to "derive" the operator formalism from the path integral. However, before doing that we would like to emphasize some important conceptual distinctions between the path integral and operator formalisms. In the path integral formalism, the fundamental object in the path integral is the probability amplitude $\langle x_f, t_f|x_i, t_i\rangle$ which is usually called the propagator (since it gives us the probability of a particle to propagate from an initial position x_i at time t_i to a final position x_f at time t_f). Although the notation we use for propagators is inspired by the Dirac bra-ket notation, we did not really need to introduce a Hilbert space or the notion of state bras and kets to define the propagator. Instead, we are thinking of an experiment where the initial and final state can be characterized by classical variables and considering all possible trajectories between them.

1.1 Propagators and the Schrödinger equation

To make the connection to the operator formalism, we need to connect the wavefunction to the propagator defined above. This is straightforward since the wavefunction $\psi(x,t)$ is generally obtained by acting with the time evolution operator on some initial state $\psi(x,t_0) = \langle x|\psi, t_0\rangle$. This means that we can write the wavefunction in terms of the propagator $\langle x_f, t_f|x_i, t_i\rangle$ via

$$\psi(x,t) = \langle x|\psi,t\rangle = \langle x|e^{-\frac{i}{\hbar}\mathcal{H}\Delta t}|\psi,t_0\rangle = \int dx_0 \langle x|e^{-\frac{i}{\hbar}\mathcal{H}\Delta t}|x_0\rangle\psi(x_0,t_0) = \int dx_0\langle x,t|x_0,t_0\rangle\psi(x_0,t_0) \tag{10}$$

This means that the propagator can be interpreted as an integration Kernel that generates the action of the time evolution. Notice that the dependence on the Hamiltonian is fully contained in the propagator $\langle x,t|x_0,t_0\rangle$. If the energy eigenstates $|n\rangle$ and eigenvalues E_n are known for a given Hamiltonian, the propagator can be written as

$$\langle x,t|x_0,t_0\rangle = \langle x|e^{-\frac{i}{\hbar}\mathcal{H}(t-t_0)}|x_0\rangle = \sum_n e^{-\frac{i}{\hbar}E_n(t-t_0)}\langle x|n\rangle\langle n|x_0\rangle = \sum_n e^{-\frac{i}{\hbar}E_n(t-t_0)}\psi_n(x)\psi_n^*(x_0) \tag{11}$$

This implies that the propagator defined in the operator formalism satisfies the Schrödinger equation

$$i\hbar\frac{d}{dt}\langle x,t|x_0,t_0\rangle = \mathcal{H}(x)\langle x,t|x_0,t_0\rangle \tag{12}$$

Our goal now is to show that the propagator defined through the path integral (Eq. 9) satisfies the Schrödinger equation without referring to the operator formalism at all. Let us write

$$\langle x,t|x_0,t_0\rangle = \sqrt{\frac{im}{2\pi\hbar\Delta t}}\int dx_{N-1} e^{\frac{i}{\hbar}\Delta t[\frac{m(x-x_{N-1})^2}{2(\Delta t)^2}-V(x)]}\langle x_{N-1},t-\Delta t|x_0,t_0\rangle \tag{13}$$

Defining the variable $\xi = x_{N-1} - x$, we can rewrite this as

$$\langle x, t|x_0, t_0\rangle = \sqrt{\frac{im}{2\pi\hbar\Delta t}} \int d\xi e^{\frac{i}{\hbar}\Delta t[\frac{m\xi^2}{2(\Delta t)^2} - V(x)]} \langle x + \xi, t - \Delta t|x_0, t_0\rangle \tag{14}$$

The factor $e^{\frac{i}{\hbar}\frac{m\xi^2}{\Delta t}}$ cause the integral over ξ to be strongly peaked around $\xi = 0$ with width $\sqrt{\Delta t}$ so we can expand the integrand in power of ξ and Δt (noting that the $\xi^2 \sim \Delta t$)

$$\langle x, t|x_0, t_0\rangle = \sqrt{\frac{im}{2\pi\hbar\Delta t}} \int d\xi e^{\frac{i}{\hbar}\frac{m\xi^2}{2\Delta t}} [1 - \frac{i}{\hbar}V(x)\Delta t][1 - \Delta t\frac{d}{dt} + \xi\frac{d}{dx} + \frac{\xi^2}{2}\frac{d^2}{dx^2}]\langle x, t|x_0, t_0\rangle \tag{15}$$

Now we use the relations

$$\sqrt{\frac{\beta}{2\pi}} \int d\xi e^{-\frac{\beta}{2}\xi^2} = 1 \tag{16}$$

$$\sqrt{\frac{\beta}{2\pi}} \int d\xi \xi e^{-\frac{\beta}{2}\xi^2} = 0 \tag{17}$$

$$\sqrt{\frac{\beta}{2\pi}} \int d\xi \xi^2 e^{-\frac{\beta}{2}\xi^2} = \frac{1}{\beta} \tag{18}$$

Substituting in (15) yields

$$\langle x, t|x_0, t_0\rangle = [1 - \frac{i}{\hbar}V(x)\Delta t - \Delta t\frac{d}{dt} + \frac{i\hbar\Delta t}{2m}\frac{d^2}{dx^2}]\langle x, t|x_0, t_0\rangle \tag{19}$$

Setting the terms of order Δt on the right hand side to zero leads to

$$[-i\hbar\frac{d}{dt} + V(x) - \frac{\hbar^2}{2m}\frac{d^2}{dx^2}]\langle x, t|x_0, t_0\rangle = 0 \tag{20}$$

which is the Schrödinger wave equation.

1.2 Free particle and Harmonic oscillator from the path integral

I would like now to consider some examples of computing the propagators for some of the quantum mechanical problems we considered before and show that the path integral can reproduce these results. These calculations will help illustrate the mathematical structure of the path integral and show how it can be convenient to understand the quantum dynamics in the semiclassical limit. First consider the free particle example whose energy eigenstates are the momentum eigenstates $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$ and eigenvalues are $\frac{p^2}{2m}$. Substituting in (11), we get

$$\langle x_f, T|x_0, 0\rangle = \frac{1}{2\pi\hbar}\int dp\, e^{-\frac{i}{\hbar}[\frac{p^2}{2m}T - p(x_i - x_f)]} = \sqrt{\frac{m}{2\pi i\hbar T}} e^{\frac{im}{2\hbar}\frac{(x_f - x_i)^2}{T}} \tag{21}$$

Let us check if this expression satisfies all the properties we expect. First, in the limit of $T \to 0$, this expression approaches a delta function $\delta(x_f - x_i)$. This is expected since at the initial time, the particle was at x_i. As the time increases, we see that this expression is dominated by $x_f - x_i \sim \sqrt{T}$ [1] This is very similar to the behavior of a diffusing particle and can be understood in terms of a random walk where the particle turns left or right at each step at random. It is known that after n steps, the particle explores a region of size $\sqrt{n}$ around the starting position. The reason the propagator resembles a random walk is that it contains an

[1] The magnitude of the exponential is always one but its phase oscillates rapidly as the term in the exponential increases. Since we mainly use the propagator as an integration Kernel to generate time evolution (cf. Eq. 10), such rapidly oscillating phase leads to a neglegible contribution when integrating against any sufficiently smooth function.

equal superposition of left moving states with $p < 0$ and right moving states with $p > 0$. The normalization factor $\frac{1}{\sqrt{T}}$ precisely accounts for the fact that the probability is now spread over an 'area' proportional to $\sqrt{T}$.

The same expression can be computed in the path integral as follows. First, we write any trajectory connecting x_i to x_f as $x(t) = x_{\rm cl}(t) + y(t)$ where $x_{\rm cl}(t)$ is the classical trajectory which satisfies the classical equations of motion and the boundary condition $x(0) = x_i$ and $x(T) = x_f$. For a free particle, the classical equations of motion take the simple form $\ddot{x} = 0$. Thus, $x_{\rm cl}(t) = x_i + \frac{t}{T}(x_f - x_i)$. The action $S = \frac{m}{2}\int dt\dot{x}^2$ can be expended in terms of $x_{\rm cl}$ and y leading to

$$S = \frac{m}{2}\int_0^T dt\,\dot{x}_{\rm cl}^2 + \frac{m}{2}\int_0^T dt\,\dot{y}^2 + m\int_0^T dt\,\dot{x}_{\rm cl}\dot{y} \tag{22}$$

The last term vanishes after integrating by parts since $\ddot{x} = 0$ and $y(0) = y(T) = 0$. We note that this is a general feature that holds beyond the simple free particle problem. The linear term in $x_{\rm cl}$ always vanishes since $x_{\rm cl}$ satisfies the classical equations of motion. The first term is the classical action given by

$$S_{\rm cl} = \frac{m(x_f - x_i)^2}{2T} \tag{23}$$

This gives us the propagator

$$\langle x_f, T|x_i, 0\rangle = C(T)e^{\frac{im}{2\hbar}\frac{(x_f - x_i)^2}{T}}, \qquad C(T) = \int_{y(0)=0}^{y(T)=0}\mathcal{D}y\, e^{\frac{im}{2\hbar}\int_0^T dt\,\dot{y}^2} \tag{24}$$

The constant $C(T)$ is independent of the initial and final positions and only depends on T. The computation of such factors will be discussed in future problem sets and sections. However, for the time being let me emphasize that the dependence of the propagator on the variables x_f and x_i is more manifest in the path integral where the exponential is just given by the action of the classical path.

The same analysis can be performed for the harmonic oscillator. Here, we can also write $x(t) = x_{\rm cl}(t) + y(t)$. The classical trajectory satisfy $\ddot{x}_{\rm cl} = -\omega^2 x_{\rm cl}$ whose general solution is $x_{\rm cl} = A\cos\omega t + B\sin\omega t$. The boundary conditions $x(0) = x_i$ and $x(T) = x_f$ fix the coefficients to be $A = x_i$ and $B = \frac{x_f - x_i\cos\omega T}{\sin\omega T}$. After some tedious algebra, we get

$$S_{\rm cl} = \int_0^T dt[\frac{m}{2}\dot{x}_{\rm cl}^2 - \frac{m}{2}\omega^2 x_{\rm cl}^2] = \frac{m\omega}{2\sin\omega T}[(x_f^2 + x_i^2)\cos\omega T - 2x_f x_i] \tag{25}$$

Here, again the action decomposes into $S[x] = S[x_{\rm cl}] + S[y]$ so the propagator takes the form

$$\langle x_f, T|x_i, 0\rangle = C_{\rm HO}(T)e^{\frac{i}{\hbar}S_{\rm cl}} \tag{26}$$

where $C_{\rm HO}(T)$ is some normalization constant. I would like to emphasize here two things. First, computing the propagator by summing over all harmonic oscillator eigenstates, while doable, is more tedious than the above approach which only involved solving the classical equation of motion. Second notice that the action above reduces to the free particle classical action $\frac{m(x_i - x_f)^2}{2T}m$ in the limit of small T. This is in fact a general feature that holds for any potential $V(x)$. It can be seen from the observation that at short times T, the contribution of the kinetic term to the action goes as $1/T$ whereas the contribution from the potential term goes as T. Since the total kinetic term at short times will be at least equal to $\frac{m(x_i - x_f)^2}{2T}$, we can also employ the saddle point approximation whenever this value is large compared to $\hbar$. Thus, the propagator for any potential reduces to the free particle propagator at short times.

I would like to emphasize that in general, the propagator does not have the simple form of the exponent of the classical action times a factor that only depends on the time interval T. This was a particular simplification for the harmonic oscillator (the free particle can be thought as a harmonic oscillator with $\omega \to 0$). In general, the propagator will have the form $\langle x_f, T|x_i, 0\rangle = C(T, x_i, x_f)e^{\frac{i}{\hbar}S_{\rm cl}}$.