Phys 342 Lecture 35

Welcome back to more about the path integral! If you recall from last time, we were working on calculating the transition amplitudes from one position eigenstate at time 0, $|x_i, t=0\rangle$, to another position eigenstate at time T, $|x_f, t=T\rangle$. This transition amplitude is just the inner product of these two states:

$$\mathcal{A}(x_i \to x_f) = \langle x_f, t=T | x_i, t=0\rangle = \langle x_f | e^{-\frac{i\hat{H}T}{\hbar}} | x_i \rangle,$$

where, on the right, we have just inserted the time evolution operator so that the states are evaluated at the same time. Our procedure established in the previous lecture to make sense of this amplitude was to divide up the total time T into N steps, and calculate the amplitude for taking each little time step and multiplying them all together. This is thus the "time-slicing" derivation of this transition amplitude, or path integral. By the end of the previous lecture, we had found that we could write:

$$\langle x_f, t=T | x_i, t=0\rangle = \int \frac{dp_1}{2\pi\hbar} dx_1 \frac{dp_2}{2\pi\hbar} dx_2 \cdots \frac{dp_{N-1}}{2\pi\hbar} dx_{N-1}$$

$$\times \exp\left[\frac{i}{\hbar}\sum_{n=1}^{N-1}\left[p_n(x_{n+1}-x_n) - H(p_n, x_n)\Delta t\right]\right],$$

where each time step is size Δt and x_n and p_n are the position and momentum, respectively of the particle at time $t_n = n\Delta t$. In this lecture, we are going to complete the derivation and make some sense out of the final result.

As you might have expected, whenever we break some

interval up into N parts, we want to take the $N\to\infty$ limit, in which things (hopefully!) simplify. Let's first look at the exponent:

$$\sum_{n=1}^{N-1}\left[p_n(x_{n+1}-x_n) - H(p_n,x_n)\,\Delta t\right].$$

To the first term, we can multiply and divide by Δt, which means that there is an overall Δt in the sum:

$$\Rightarrow \sum_{n=1}^{N-1}\Delta t\left[p_n\frac{x_{n+1}-x_n}{\Delta t} - H(p_n,x_n)\right].$$

Recall that $\Delta t = T/N$, so as $N\to\infty$, $\Delta t\to 0$. Correspondingly, $x_n = x(t_n) = x(n\Delta t)$, and so the difference $x_{n+1}-x_n$ is just the difference of positions of the particle at sequential times. As $\Delta t\to 0$ ($N\to\infty$), this becomes the time derivative of position:

$\lim_{\Delta t\to 0}\frac{x_{n+1}-x_n}{\Delta t} = \dot{x}(t_n)$, and the sum transmogrifies into an integral (i.e., a continuous sum):

$$\lim_{N\to\infty}\sum_{n=1}^{N-1}\Delta t\left[p_n\frac{x_{n+1}-x_n}{\Delta t} - H(p_n,x_n)\right] = \int_0^T dt\left(p\dot{x} - H(p,x)\right),$$

where x and p are implicit functions of time t. Using this result the transition amplitude is then:

$$\langle x_f, t=T \mid x_i, t=0\rangle = \int\prod_{n=1}^{\infty}\left[\frac{dp_n}{2\pi\hbar}\,dx_n\right]\exp\left[\frac{i}{\hbar}\int_0^T dt\left(p\dot{x} - H(p,x)\right)\right]$$

This is called the Hamiltonian path integral. We'll massage it a bit more in a second, but I want to point out the somewhat awkward infinity of integrals that we

have to do: $\int \prod_{n=1}^{\infty} \frac{dp_n}{2\pi\hbar} dx_n$. Recall that at every time step $0 < t_n < T$, we have to allow for the possibility of the particle to have any position x_n and any momentum p_n. As time is continuous, this means that we have to do a continuous number of integrals! This may sound like a bad trade-off, like we're getting swindled in our deal for manipulating the transition amplitude. However, in many cases this "infinity of integrals" can be re-interpreted and evaluated rather straightforwardly.

Let's see one example of this now. In this course, we have only considered Hamiltonians for which the kinetic energy is quadratic in momentum:

$H(p,x) = \frac{p^2}{2m} + V(x)$, where $V(x)$ is a purely position-dependent potential. Note that this Hamiltonian is just a function of the phase space variables p and x, and not an operator. If this form of the Hamiltonian is assumed, then the path integral is:

$$\langle x_f, t=T | x_i, t=0 \rangle = \int \prod_{n=1}^{\infty} \left[\frac{dp_n}{2\pi\hbar} dx_n \right] \exp\left[\frac{i}{\hbar} \int_0^T dt \left(p\dot{x} - \frac{p^2}{2m} - V(x) \right) \right].$$

Next, we would like to perform all of the integrals over momentum p, as we know its explicit dependence in the exponent. The first thing we will do is to complete the square in the exponent. Note that:

$$-\frac{p^2}{2m} + \dot{x}p = -\frac{1}{2m}\left(p^2 - 2m\dot{x}p\right) = -\frac{1}{2m}\left[(p - m\dot{x})^2 - m^2\dot{x}^2 \right]$$

so that: $-\frac{p^2}{2m} + \dot{x}p = \frac{1}{2}m\dot{x}^2 - \frac{(p-m\dot{x})^2}{2m}$

Then, the transition amplitude is:

$$\langle x_f, t=T | x_i, t=0\rangle = \int \prod_{n=1}^{\infty} \left[\frac{dp_n}{2\pi\hbar}\, dx_n\right] \exp\left[\frac{i}{\hbar}\int_0^T dt \left(\frac{1}{2}m\dot{x}^2 - \frac{(p-m\dot{x})^2}{2m} - V(x)\right)\right]$$

So, to completely integrate over momentum, we just have to integrate:

$$\int \prod_{n=1}^{\infty} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\int_0^T dt\, \frac{(p-m\dot{x})^2}{2m}\right].$$

Note that each integral over momentum extends over all real values: $\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar}$, so we can make the change of variables that: $p_n \to p_n - m\dot{x}$, for which the Jacobian is 1 and the bounds of integration are unaffected. Thus, the momentum integral is:

$$\int \prod_{n=1}^{\infty} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\int_0^T dt\, \frac{p^2}{2m}\right].$$

To continue, note that $p^2 = p(t)\cdot p(t)$ and the integral is a sum over all time $t \in [0,T]$. Thus, the integral is just a dot product of momenta with itself at every time t_n:

$\int_0^T dt\, p^2 = \Delta t \sum_{n=1}^{\infty} p(t_n)\, p(t_n) = \Delta t \sum_{n=1}^{\infty} p_n^2$, and the Δt just makes the dot product sensible. Then, with this identification, the integrals over momentum break up into a product of one-dimensional integrals:

$$\int \prod_{n=1}^{\infty} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\int_0^T dt\, \frac{p^2}{2m}\right] = \int \prod_{n=1}^{\infty} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i\Delta t}{2m\hbar}\sum_{n=1}^{\infty} p_n^2\right]$$

$$= \int \prod_{n=1}^{\infty}\left[\frac{dp_n}{2\pi\hbar}\exp\left[-\frac{i\Delta t}{2m\hbar}p_n^2\right]\right]$$

$$= \left[\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\exp\left[-\frac{i\Delta t}{2m\hbar}p^2\right]\right]^{N-1}, \text{ as } N-1\to\infty.$$

The integral that remains is a Gaussian form, and so we immediately know its value. This integral is

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\exp\left[-\frac{i\Delta t}{2m\hbar}p^2\right] = \sqrt{\frac{m}{2\pi\hbar\Delta t i}}, \text{ which is just some value.}$$

We get this integral for <u>each</u> momentum p_n, so the transition amplitude can be expressed as:

$$\langle x_5, t=T \mid x_i, t=0\rangle = \int \prod_{n=1}^{\infty}\left[\sqrt{\frac{m}{2\pi\hbar\Delta t i}}\, dx_n\right]\exp\left[\frac{i}{\hbar}\int_0^T dt\left(\tfrac{1}{2}m\dot{x}^2 - V(x)\right)\right].$$

In practice, this factor from integrating over momentum is typically ignored, or "absorbed" into the integration measure for positions, dx_n. Another way to justify ignoring this factor is noting that it is just some constant, and we can always divide by normalization at the end, or ask questions that are independent of normalization (e.g., eigenvalues or eigenvectors appropriately defined). Going forward, we will just denote the infinite integration measure as:

$$[dx] \equiv \prod_{n=1}^{\infty}\sqrt{\frac{m}{2\pi\hbar\Delta t i}}\, dx_n, \text{ so that}$$

the transition amplitude or <u>the</u> path integral is:

$$\langle x_f, t=T \,|\, x_i, t=0\rangle \equiv Z(x_i, x_f) = \int [dx]\, e^{\frac{i}{\hbar}\int_0^T dt\left[\frac{1}{2}m\dot{x}^2 - V(x)\right]}.$$

Now, the factor in the exponent is the classical action of the quantum system. The Lagrangian $L(t)$ is the difference of kinetic and potential energy:

$$L(t) = \tfrac{1}{2}m\dot{x}^2 - V(x) \equiv L(x, \dot{x}),$$

and its time integral is the action for a given trajectory $x(t)$:

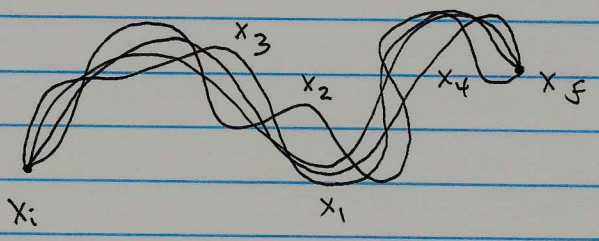
$$S[x(t)] = \int_0^T dt\, L(x, \dot{x}).$$

The action is a functional as its argument is a complete trajectory $x(t)$, and not just some independent variable. Then, the most compact expression for the path integral is:

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

I could teach an entire course on the path-integral formulation of quantum mechanics, but I'm just giving you a flavor for it here. We'll make some connections to other quantum aspects next lecture; I want to finish this lecture by making the connection to classical mechanics. The classical mechanics limit, as we have stated many times before, is the limit in which $\hbar \to 0$. Now, staring at the path integral's integrand, you might think that as $\hbar \to 0$, the exponential factor wildly oscillates, and so would just evaluate to 0. Indeed, this would be the case for an arbitrary trajectory, $x(t)$. The action $S[x]$ evaluated on an arbitrary trajectory $x_1(t)$ is, say,

$S_1 \equiv S[x_1]$. A nearby trajectory, a path that differs by only a small amount in space will in general have an action that differs significantly. Let's consider nearby trajectories $x_2(t)$, $x_3(t)$, $x_4(t)$, ... to $x_1(t)$, visualized as:

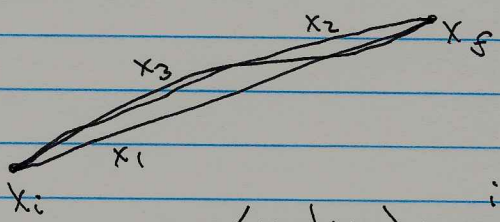


The path integral sums up their exponentiated actions:

$$\langle x_f | x_i \rangle \sim e^{i\frac{S_1}{\hbar}} + e^{i\frac{S_2}{\hbar}} + e^{i\frac{S_3}{\hbar}} + e^{i\frac{S_4}{\hbar}} + \dots,$$

and in general $S_1, S_2, S_3, S_4, \dots$ will all be significantly different values of the action. $e^{iS/\hbar}$ is a sinusoidal function, and summing up sinusoidal functions with essentially arbitrary phases produces 0, in the limit that $\hbar \to 0$. Thus, as $\hbar \to 0$, an arbitrary trajectory from x_i to x_f does not contribute to the path integral.

However, nearby trajectories <u>will</u> contribute to the path integral if the value of the action doesn't vary significantly. That is, for trajectories x_1, x_2, x_3, etc., illustrated as



contribute to the path integral as:

$$\langle x_f | x_i \rangle \sim e^{i\frac{S_1}{\hbar}} + e^{i\frac{S_2}{\hbar}} + e^{i\frac{S_3}{\hbar}} + \dots$$

and the values of these actions are all extremely close to one another:

$S_4[x_1] \sim S[x_2] \sim S[x_3] \sim \dots$, then the contribution to the path integral is non-zero. As we assume that the trajectories x_1 and x_2 (say) are close to one another, we can write:

$x_2(t) = x_1(t) + \varepsilon(t)$, for some small difference, $\varepsilon(t) \ll x_1(t)$.

Now, demanding that the values of the actions differ only slightly, we take the difference:

$$S[x_2] - S[x_1] = S[x_1+\varepsilon] - S[x_1] = S[x_1] + \varepsilon \frac{\delta S}{\delta x_1} + \theta(\varepsilon^2) - S[x_1]$$

$$= \varepsilon \frac{\delta S}{\delta x_1} + \dots, \text{ where we have Taylor expanded in the small trajectory } \varepsilon(t).$$

Thus, if a trajectory is to contribute to the path integral for $\hbar \to 0$, then that path must be a trajectory for which the action is <u>stationary</u> or <u>extremized</u>:

$\frac{\delta S}{\delta x} = 0$. This, however, is just the principle of least action from classical mechanics. In the limit as $\hbar \to 0$, only classical paths, those for which $\delta S/\delta x = 0$, contribute to the path integral. If that isn't a beautiful manifestation of the correspondence principle, then I don't know what is.

More next time...