Lecture 11 (Oct. 16, 2017)

11.1 Path Integrals

As we have seen, the amplitude for a state to "propagate" from coordinates (x, t) to (x', t') is given by the propagator,

$$K(x', t'; x, t) = \int [\mathcal{D}x] \; e^{iS[x(t)]/\hbar} \,, \tag{11.1}$$

where $S[x(t)]$ is the classical action of the path $x(t)$,

$$S[x(t)] = \int \mathrm{d}t' \; L(x, \dot{x}, t') \,, \tag{11.2}$$

for L the classical Lagrangian. The integration in the path integral is over all possible paths $x(t)$.

We need to define this precisely. In particular, we need to write a measure on the space of paths in order to know how to properly integrate over all paths. The strategy will be to start with the definition of K, and then derive the path integral and the appropriate definition of the measure. Then we will go back and recompute K for a free particle.

The starting point of deriving the path integral is to use the composition law for K, which comes from the composition law for the time-evolution operator. Recall that the propagator K is the matrix element

$$K(x, t; x', t') = \langle x|U(t', t)|x\rangle \,. \tag{11.3}$$

From the composition law, we have

$$\begin{aligned} K(x_N, t_N; x_0, t_0) &= \int \prod_{k=1}^{N-1} \mathrm{d}x_k \; K(x_N, t_N; x_{N-1}, t_{N-1}) \cdots K(x_1, t_1; x_0, t_0) \\ &= \int \prod_{k=1}^{N-1} \mathrm{d}x_k \; \langle x_N|U(t_N, t_{N-1})|x_{N-1}\rangle \cdots \langle x_1|U(t_1, t_0)|x_0\rangle \\ &= \int \prod_{k=1}^{N-1} \mathrm{d}x_k \; \langle x_N|e^{-i\epsilon H/\hbar}|x_{N-1}\rangle \cdots \langle x_1|e^{-i\epsilon H/\hbar}|x_0\rangle \,, \end{aligned} \tag{11.4}$$

where $\epsilon = t/N$. This expression holds in general for time-dependent Hamiltonians, if we understand each occurrence of H in the expression above to be a function of the time.

We now consider a single matrix element in this expression,

$$\langle x_{j+1}|e^{-i\epsilon H/\hbar}|x_j\rangle = \langle x_{j+1}|e^{-i\epsilon(T+V)/\hbar}|x_j\rangle \,, \tag{11.5}$$

where

$$T = \frac{p^2}{2m} \,, \quad V = V(x) \,. \tag{11.6}$$

Note that

$$e^{-i\epsilon(T+V)/\hbar} = 1 - \frac{i\epsilon(T+V)}{\hbar} - \frac{\epsilon^2(T+V)^2}{2\hbar^2} + \cdots = e^{-i\epsilon T/\hbar} e^{-i\epsilon V/\hbar} + O(\epsilon^2) \,. \tag{11.7}$$

Thus, if we take $\epsilon \to 0, N \to \infty$ with $N\epsilon$ fixed, then we can use

$$e^{-i\epsilon(T+V)/\hbar} \xrightarrow{\epsilon \to 0} e^{-i\epsilon T/\hbar} e^{-i\epsilon V/\hbar} \,. \tag{11.8}$$

We can only make this replacement legally in this limit, as these two expressions differ at higher orders.

We now choose ϵ small so that we can safely omit the $O(\epsilon^2)$ terms above. We then have

$$\begin{aligned}\langle x_{j+1}|e^{-i\epsilon H/\hbar}|x_j\rangle &\xrightarrow{\epsilon\to 0} \langle x_{j+1}|e^{-i\epsilon p^2/2m\hbar}e^{-i\epsilon V/\hbar}|x_j\rangle \\ &= \langle x_{j+1}|e^{-i\epsilon p^2/2m\hbar}|x_j\rangle e^{-i\epsilon V(x_j)/\hbar}\,.\end{aligned} \tag{11.9}$$

We see then that we only have to evaluate the matrix element for a free particle. We can evaluate this by inserting the resolution of the identity in the momentum basis, which results in taking a Fourier transform:

$$\begin{aligned}\langle x_{j+1}|e^{-i\epsilon p^2/2m\hbar}|x_j\rangle &= \int \mathrm{d}p_j\ \langle x_{j+1}|p_j\rangle\langle p_j|e^{-i\epsilon p^2/2m\hbar}|x_j\rangle \\ &= \int \frac{\mathrm{d}p_j}{2\pi\hbar}e^{ip_j(x_{j+1}-x_j)/\hbar}e^{-i\epsilon p_j^2/2m\hbar} \\ &= \sqrt{\frac{m}{2\pi i\hbar\epsilon}}e^{\frac{im(x_{j+1}-x_j)^2}{2\hbar\epsilon}}\,.\end{aligned} \tag{11.10}$$

This is the same result we found in the last lecture.

Thus, we have

$$\langle x_{j+1}|e^{-i\epsilon H/\hbar}|x_j\rangle \xrightarrow{\epsilon\to 0} \sqrt{\frac{m}{2\pi i\hbar\epsilon}}e^{i\left[\frac{m(x_{j+1}-x_j)^2}{2\hbar\epsilon}-\frac{\epsilon V(x_j)}{\hbar}\right]}\,. \tag{11.11}$$

We then have

$$K(x_N,t_N;x_0,t_0) = \lim_{\substack{\epsilon\to 0\\ N\to\infty\\ N\epsilon=t_N-t_0}} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int\prod_{k=1}^{N-1}\mathrm{d}x_k\ e^{i\sum_{j=0}^{N-1}\left[\frac{m(x_{j+1}-x_j)^2}{2\hbar\epsilon}-\frac{\epsilon V(x_j)}{\hbar}\right]}\,. \tag{11.12}$$

In the limit $\epsilon \to 0$, we have

$$x_{j+1}-x_j \approx \epsilon\frac{\mathrm{d}x}{\mathrm{d}t}\,, \tag{11.13}$$

which gives us

$$\frac{(x_{j+1}-x_j)^2}{\epsilon} \approx \epsilon\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2. \tag{11.14}$$

Thus,

$$\begin{aligned}\sum_{j=0}^{N-1}\left[\frac{m(x_{j+1}-x_j)^2}{2\hbar\epsilon}-\frac{\epsilon V(x_j)}{\hbar}\right] &\xrightarrow{\epsilon\to 0}\frac{1}{\hbar}\int \mathrm{d}t\ \left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x)\right] \\ &= \frac{1}{\hbar}\int_{t_0}^{t_N}\mathrm{d}t\ L(x,\dot{x},t)\,,\end{aligned} \tag{11.15}$$

where L is the classical Lagrangian. This is the desired result. We now define the path integral formally through the limiting process

$$\int[\mathcal{D}x]\ e^{iS[x(t)]/\hbar} := \lim_{\substack{\epsilon\to 0\\ N\to\infty\\ N\epsilon=t_N-t_0}} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int\prod_{k=1}^{N-1}\mathrm{d}x_k\ e^{i\sum_{j=0}^{N-1}\left[\frac{m(x_{j+1}-x_j)^2}{2\hbar\epsilon}-\frac{\epsilon V(x_j)}{\hbar}\right]}\,. \tag{11.16}$$

The factor in front of the product of integrals is required to make sure that the limit exists.

Now we will recalculate the free particle propagator. Let us choose the number of steps to be a power of two, $N = 2^n$, and let us define

$$K_N = \left(\frac{mN}{2\pi i\hbar t}\right)^{N/2} \int \prod_{k=0}^{N-1} \mathrm{d}x_k \; e^{\frac{imN}{2\hbar t}\sum_j (x_{j+1}-x_j)^2} . \tag{11.17}$$

Again, we have $\epsilon = t/N$. Expanding all of the squares, we see that

$$\sum_j (x_{j+1}-x_j)^2 = x_0^2 + 2x_1^2 + 2x_2^2 + \cdots + 2x_{N-1}^2 + x_N^2 - 2x_0x_1 - 2x_1x_2 - \cdots - 2x_{N-1}x_N . \tag{11.18}$$

We now carry out all of the odd integrals first, which will cause the problem to simplify. We find

$$\begin{aligned} K_N &= \int \prod_{j \text{ even}} \mathrm{d}x_j \int \prod_{k \text{ odd}} \mathrm{d}x_k \left(\frac{m2^n}{2\pi i\hbar t}\right) e^{\frac{im2^n}{2\hbar t}\left[2x_k^2 + x_{k-1}^2 + x_{k+1}^2 - 2x_k(x_{k-1}+x_{k+1})\right]} \\ &= \int \prod_{j \text{ even}} \mathrm{d}x_j \int \prod_{k \text{ odd}} \mathrm{d}x_k \left(\frac{m2^n}{2\pi i\hbar t}\right) e^{\frac{im2^n}{2\hbar t}\left[2\left(x_k - \frac{x_{k-1}+x_{k+1}}{2}\right)^2 + \frac{1}{2}\left(x_{k+1}^2 + x_{k-1}^2\right) - x_{k+1}x_{k-1}\right]} \\ &= \left(\frac{m2^{n-1}}{2\pi i\hbar t}\right)^{2^{n-2}} \int \prod_{\ell=0}^{2^{n-1}-1} \mathrm{d}x_{2\ell} \; e^{\frac{im2^{n-1}}{2\hbar t}\sum_{\ell=0}^{2^{n-1}-1}(x_{2\ell+2}-x_{2\ell})^2} \\ &= K_{N/2} . \end{aligned} \tag{11.19}$$

We see then that

$$K_{2^n} = K_{2^{n-1}} = K_{2^{n-2}} = \cdots = K_1 = \sqrt{\frac{m}{2\pi i\hbar t}} e^{\frac{im}{2\hbar t}(x_N - x_0)^2} . \tag{11.20}$$

Thus, we have recovered the expected result.

We can explicitly evaluate the path integral for any system in which the potential is at most quadratic in $x, \dot{x}$. We will see several examples on the homework.

The path integral formulation seems unwieldy. Why does anyone bother with this? This is a completely different way of formulating quantum mechanics than we have seen previously, but it is completely equivalent to our other formulations, so what is the use? Feynman emphasized that different formulations, even though they are mathematically equivalent, may each be useful for describing different systems. Furthermore, we can use a given formulation to generalize quantum mechanics, and the different formalisms may not be equivalent in these generalizations. Finally, as Feynman says, it feels psychologically different to be thinking about the same physics from a completely different perspective. In practice, path integrals are not usually a practical way of solving problems. However, the path integral gives us quantum intuition, which allows us to say many things about how systems will behave, even if we cannot solve them exactly.

11.1.1 Technical Details

For each time step, we wrote

$$\langle x_{j+1}| e^{-i\epsilon H/\hbar} |x_j\rangle = e^{-\frac{i\epsilon m}{2\hbar}\left(\frac{x_{j+1}-x_j}{2}\right) - \frac{i\epsilon}{\hbar}V(x_j)} . \tag{11.21}$$

It seems arbitrary that we wrote

$$e^{-i\epsilon(T+V)/\hbar} \approx e^{-i\epsilon T/\hbar} e^{-i\epsilon V/\hbar} \tag{11.22}$$

instead of

$$e^{-i\epsilon(T+V)/\hbar} \approx e^{-i\epsilon V/\hbar} e^{-i\epsilon T/\hbar}, \tag{11.23}$$

in which case we would have had $V(x_{j+1})$ in the exponent of Eq. (11.21) instead of $V(x_j)$. Either is a perfecetly good choice to the order at which we are working. A more symmetric choice is to use $V\left(\frac{x_j+x_{j+1}}{2}\right)$.

This choice is very important for the particle in a magnetic field described by a vector potential $\boldsymbol{A}$ (through $\boldsymbol{B} = \nabla \times \boldsymbol{A}$). In this system, the Lagrangian is

$$L = \frac{1}{2} m\dot{\boldsymbol{x}}^2 + e\boldsymbol{A} \cdot \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} - V(\boldsymbol{x})\,. \tag{11.24}$$

Here, in the quantum mechanical path integral we must use

$$\boldsymbol{A} \to \boldsymbol{A}\left(\frac{x_j + x_{j+1}}{2}\right). \tag{11.25}$$

See the homework for more on this.