Lecture 29: The Path Integral

Friday, April 03, 2020

When we last left off, we were discussing the propagator

$$k(x_f, t_f; x_i, t_i) = \sum_n u_n(x_f) u_n^*(x_i) e^{-\imath E_n \Delta t/\hbar}$$

We did this by starting with $\langle x_f t_f | x_i t_i \rangle$ and inserting a complete set f states. Notice the boundary condition, where $t_i \to t_f$ gives us

$$k(x_f, t_f; x_i, t_i) = \delta(x_i - x_f)$$

Physically, this is just saying that the probability of moving from x_i to x_f instantaneously is zero unless they're the same. If we consider

$$\int \mathrm{d}x \lim_{x' \to x} \sum_n e^{-E_n t/\hbar} \langle x|n\rangle \langle n|x'\rangle = \sum_n e^{-\imath E_n t/\hbar} \equiv G(t)$$

If we take $t \to -\imath\tau$, then

$$G(-\imath\tau) = \sum_n e^{-\tau E_n/\hbar} \sim \sum_n e^{-\beta H}$$

There seems to be some connection between quantum mechanics in real time and statistical mechanics in imaginary time. Last time we were working through calculating the propagator for a free particle.

$$\begin{aligned}
k(x, x'; \delta t) &= \int \frac{\mathrm{d}p}{2\pi} \langle x|p\rangle \langle p|x'\rangle e^{-\frac{\imath p^2 \delta t}{2m\hbar}} \\
&= \int \frac{\mathrm{d}p}{2\pi} e^{\imath p(x-x')/\hbar} e^{-\frac{\imath p^2 \Delta t}{2m\hbar}} \\
&= \sqrt{\frac{m}{2\pi\imath\hbar\Delta t}} e^{\frac{\imath m(x-x')^2}{2\hbar\Delta t}}
\end{aligned}$$

0.0.1 The Propagator as a Green's Function of the Wave Equation

If we have some differential operator O where $O\varphi(x) = J(x)$. We can solve this by calculating the Green's function, which is defined as

$$OG(x, x') = \delta(x' - x)$$

Once we have this,

$$O[\varphi(x) = \int \mathrm{d}x'\, G(x - x')J(x')] = \int \mathrm{d}x'\, \delta(x - x')J(x') = J(x)$$

The Schrödinger equation can be written as

$$\left(\imath\hbar\frac{\partial}{\partial t} - H_0\right)|\psi\rangle = V|\psi\rangle$$

where $H = H_0 + V$. The Green's function is the propagator, so we want to find

$$\left(\imath\hbar\frac{\partial}{\partial t} - H_0\right) k(\vec{\mathbf{x}}_i, t_i; \vec{\mathbf{x}}_f, t_f) = \delta^3(xvece - \vec{\mathbf{x}}')\delta(t_i - \delta_f)$$

which would mean that

$$\psi(x, t) = \int \mathrm{d}^3x'\, k(x, x'; \Delta t)V$$

Now if we operate with the differential operator, we see that the Schrödinger equation is satisfied. We can find k by solving the equation with the δ function, and the easiest way to do this is in momentum space, where the equation we want to solve is

$$\left(\hbar\omega - \frac{\vec{\mathbf{p}}^2}{2m}\right) K(\vec{\mathbf{p}}, \omega) = \frac{1}{(2\pi)^4}$$

so

$$k(\vec{\mathbf{p}}, \omega) = \frac{1}{(2\pi)^4} \frac{1}{\left(\hbar\omega - \frac{\vec{\mathbf{p}}^2}{2m}\right)}$$

However, this equation has a pole in it, so the inverse Fourier transform is not well-defined. We have to do this in a careful way:

$$k(x_f - x_i; t_f - t_i) = \int \frac{\mathrm{d}^3p \, \mathrm{d}\omega}{(2\pi)^4} \frac{e^{\imath \frac{\vec{\mathbf{p}} \cdot \Delta x}{\hbar} - \imath\omega\Delta t}}{\hbar\omega - \frac{\vec{\mathbf{p}}^2}{2m} \pm \imath\epsilon}$$

We need to integrate around the pole in either the lower half-plane or the upper half=plane. If $t_f < t_i$, the probability should be zero, so if $\Delta t < 0$, $k = 0$ to preserve causality. By the Jordan curve theorem, we want to close in the lower half-plane.

$$k = -\frac{2\pi i}{(2\pi)^4} \int \mathrm{d}^3p \, e^{\frac{\imath\vec{\mathbf{p}} \cdot \Delta\vec{\mathbf{x}}}{\hbar} + \frac{\imath\vec{\mathbf{p}}^2}{2m\hbar}\Delta t}$$

which gives us the same result as when we calculated the free-particle propagator before.

0.0.2 The Path Integral

Dirac said that the probability amplitude should be related to the integral of the Lagrangian due to the time difference:

$$\langle x_f, t_f | x_i, t_i \rangle \sim e^{\imath \int L \mathrm{d}t}$$

We can do this by breaking up the path in $x - t$ space into many infinitesimal steps:

$$\langle x_f, t_f | \int \mathrm{d}^3x \, |x, t_f - \epsilon\rangle \, \langle x, t_f - \epsilon| \cdots |x_i, t_i\rangle$$

or

$$\langle x_f, t_f | x_i t_i \rangle = \lim_{n\to\infty} \int \mathrm{d}^3x_1 \cdots \mathrm{d}^3x_n \, \langle x_1, t_f | x_1, t_f - \epsilon\rangle \, \langle x_1, t_f - \epsilon | x_2, t_2 - 2\epsilon\rangle \cdots$$

where $n\epsilon = t_f - t_i$. Each one of these steps can be written as

$$\langle x_m | x_{m+1} \rangle - \frac{\imath\epsilon}{\hbar} \langle x_m | H | x_{m+1} \rangle$$

We know that

$$\langle x_m | f(x) | x_{m+1} \rangle = f(x_m)\delta(x_m - x_{m+1}) \equiv \frac{f(x_m + x_{m+1})}{2} \int \frac{\mathrm{d}p}{(2\pi)\hbar} e^{\frac{\imath p(x_m - x_{m+1})}{\hbar}}$$

If we do this as a function of p, we get

$$\langle x_m | f(p) | x_{m+1} \rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} f(p) e^{\imath p(x_m - x_{m+1})/\hbar}$$

so that

$$\langle x_m + 1 | e^{-\imath\epsilon H/\hbar} | x_m \rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} e^{-\imath\epsilon H\left(\frac{x_m - x_{m+1}}{2}, p\right)}$$

We then have to repeat this over an over for each small step:

$$\left[\prod_{k=1}^{N} \int \mathrm{d}x_k \frac{\mathrm{d}p_k}{2\pi\hbar}\right] e^{\imath \sum_k p_k(x_{k+1} - x_k) - \imath\epsilon H\left(\frac{x_{k+1} - x_k}{2}, p_k\right)}$$

In the limit as $N \to \infty$, $\epsilon \to 0$ and $N\epsilon = t_f - t_i$, we can write this as

$$\int Dx(t)Dp(t)e^{\imath \int_{t_i}^{t_f} p\dot{x}-H} = \langle x_f, t_f | x_i, t_i \rangle$$

as long as $x(t_i) = x_i$ and $x(t_f) = x_f$. This is what's known as a functional integral. We are integrating over all possible functions of time (that's what $Dx(t)$ refers to, rather than $\mathrm{d}x$). You can recognize the exponential as the Lagrangian.