Lecture 10 (Oct. 11, 2017)

10.1   Path Integral Formulation of Quantum Mechanics

10.1.1   The Propagator

In the last lecture, we introduced the propagator,

$$K\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big) = \sum_{a'}\langle\boldsymbol{x}|a'\rangle e^{-iE_{a'}(t-t_0)/\hbar}\langle a'|\boldsymbol{x}'\rangle = \langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}'\rangle\,. \tag{10.1}$$

In terms of the propagator, we can write the wavefunction in the form

$$\psi(\boldsymbol{x},t) = \int_{-\infty}^{\infty}\mathrm{d}^d x'\,K\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big)\psi\big(\boldsymbol{x}',t_0\big)\,, \tag{10.2}$$

From the Schrödinger equation, assuming a Hamiltonian of the form

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})\,, \tag{10.3}$$

the propagator must satisfy the differential equation

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{x})\right)K\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big) = 0\,. \tag{10.4}$$

Furthermore, it must satisfy

$$\lim_{t\to t_0} K\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big) = \delta^{(d)}\big(\boldsymbol{x}-\boldsymbol{x}'\big)\,. \tag{10.5}$$

A convenient related quantity is the *retarded propagator*

$$K_{\mathrm{ret}}\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big) = \theta(t-t_0)K\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big)\,. \tag{10.6}$$

The retarded propagator satisfies

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{x})\right)K_{\mathrm{ret}}\big(\boldsymbol{x},t;\boldsymbol{x}',t'\big) = i\hbar\delta^{(d)}(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t')\,, \tag{10.7}$$

i.e., it is a Green's function for the Schrödinger equation (a solution of the Schrödinger equation with a delta function source or forcing term).

Alternatively, we can think of the propagator as

$$K\big(\boldsymbol{x},t;\boldsymbol{x}',t_0\big) = \langle\boldsymbol{x},t|\boldsymbol{x}',t_0\rangle\,, \tag{10.8}$$

which follows from its definition.

As an example, consider the free particle in one dimension, with Hamiltonian

$$H = \frac{p^2}{2m}\,. \tag{10.9}$$

The propagator in this case is given by

$$\begin{aligned}
K\big(x,t;x',t'\big) &= \int \mathrm{d}p\,\langle x|p\rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}(t-t')}\langle p|x'\rangle \\
&= \int \frac{\mathrm{d}p}{2\pi\hbar}\,e^{ip(x-x')-\frac{i}{\hbar}\frac{p^2}{2m}(t-t')} \\
&= \sqrt{\frac{m}{2\pi i\hbar(t-t')}}e^{i\frac{m(x-x')^2}{2\hbar(t-t')}}\,.
\end{aligned} \tag{10.10}$$

The propagator has a number of properties that make it useful to calculate. The first is related to quantum statistical mechanics. We define the partition function as

$$G(t) = \int \mathrm{d}^d x \, K(\boldsymbol{x}, t; \boldsymbol{x}, 0) = \sum_{a'} e^{-iE_{a'}t/\hbar} \,. \tag{10.11}$$

If we analytically continue to imaginary time, $t = -i\hbar\beta$, then this yields the familiar partition function of statistical mechanics:

$$G(-i\hbar\beta) = \sum_{a'} e^{-\beta E_{a'}} := Z \,. \tag{10.12}$$

Another useful quantity is the Fourier transform of the partition function,

$$\tilde{G}(E) = -i \int \mathrm{d}t \, G_{\mathrm{ret}}(t) e^{iEt/\hbar} = -i \sum_{a'} \int_0^\infty \mathrm{d}t \, e^{i(E-E_{a'})t/\hbar} \,, \tag{10.13}$$

where $G_{\mathrm{ret}}(t) = \theta(t)G(t)$. In order to make this integral converge, we take $E \to E + i\epsilon$, which then yields

$$\tilde{G}(E) = \sum_{a'} \frac{\hbar}{E - E_{a'} + i\epsilon} \,. \tag{10.14}$$

The poles of $\tilde{G}$ in the limit $\epsilon \to 0$ describe the energy spectrum of the system.

We can also use the Fourier transform of the partition function to find the density of states. The density of states is defined as

$$\rho(E) = \sum_{a'} \delta(E - E_{a'}) \,. \tag{10.15}$$

Using the property

$$\lim_{\epsilon \to 0} \mathrm{Im} \, \frac{1}{E - E' + i\epsilon} = \lim_{\epsilon \to 0} \frac{-\epsilon}{(E - E')^2 + \epsilon^2} \tag{10.16}$$
$$= -\pi\delta(E - E') \,,$$

we see that we can write the density of states as

$$\rho(E) = -\frac{1}{\pi\hbar} \mathrm{Im} \, \tilde{G}(E) \,. \tag{10.17}$$

10.1.2 Path Integrals

From the composition property of time evolution,

$$U(t, t_0) = U(t, t')U(t', t_0) \,, \quad t > t' > t_0 \,, \tag{10.18}$$

we see that the propagator satisfies a similar composition property,

$$K(\boldsymbol{x}, t; \boldsymbol{x}', t_0) = \int \mathrm{d}^d \tilde{x} \, K(\boldsymbol{x}, t; \tilde{\boldsymbol{x}}, \tilde{t}) K(\tilde{\boldsymbol{x}}, \tilde{t}; \boldsymbol{x}', t_0) \,. \tag{10.19}$$

We can break the interval $[t_0, t]$ into N equal time intervals of width

$$\Delta t = \frac{t - t_0}{N} \,, \tag{10.20}$$

with endpoints

$$t_0 < t_1 < \cdots < t_N = t \,. \tag{10.21}$$

Iterating the composition rule then gives us

$$K(x_N, t_N; x_0, t_0) = \int \prod_{k=1}^{N-1} K(x_N, t_N; x_{N-1}, t_{N-1}) \cdots K(x_2, t_2; x_1, t_1) K(x_1, t_1; x_0, t_0) \,. \tag{10.22}$$

Feynman proposed that

$$K(x, t; x', t_0') = \int [\mathcal{D}x] e^{iS[x(t)]/\hbar} \,, \tag{10.23}$$

where the right-hand side is a sum over all possible paths from (x', t_0) to (x, t) (including those that do not satisfy the equations of motion), and S is the classical action of the trajectory. Recall that in classical mechanics, the Lagrangian is given by

$$L = \frac{1}{2}m\dot{x}^2 - V(x) \,, \tag{10.24}$$

and the action is given by $S = \int \mathrm{d}t\, L$. (Here, we have assumed that the kinetic energy is of the form $m\dot{x}^2/2$.) The classical trajectory between two spacetime points is obtained by extremizing this action, $\frac{\delta S}{\delta x} = 0$. This is known as the principle of least action. This requirement leads to the Euler–Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0 \,. \tag{10.25}$$

For the Lagrangian given above, this gives Newton's force law,

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{\partial V}{\partial x} \,. \tag{10.26}$$

Note that Feynman's proposed expression for the propagator,

$$K(x, t; x', t_0') = \int [\mathcal{D}x] e^{iS[x(t)]/\hbar} \,, \tag{10.27}$$

clearly satisfies the composition property. It also gives a very simple connection to classical mechanics: in the $\hbar \to 0$ limit, we expect the sum over paths is dominated by the path for which the phase is stationary (this is the stationary phase approximation, which we will discuss more thoroughly later), i.e., the path for which S is extremized. Thus, Feynman's path integral expression yields the principle of least action in the classical limit.

8.321 Quantum Theory I
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