PATH INTEGRAL FORMULATION OF QUANTUM MECHANICS: FREE PARTICLE PROPAGATOR

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8.

Although all the non-relativistic quantum mechanics we've done so far has started with the Schrödinger equation, a different approach was devised by Richard Feynman in the 1940s. The Schrödinger method requires us to find the eigenvalues (allowed energies) and eigenstates of the hamiltonian H and then use these to construct the unitary operator known as the propagator. For discrete energies, this propagator is

$$U(t)=\sum e^{-iEt/\hbar}\left|E\right\rangle \left\langle E\right| \tag{1}$$

and for continuous energies, we have

$$U(t)=\int e^{-iEt/\hbar}\left|E\right\rangle \left\langle E\right|dE \tag{2}$$

Given the state of the system at an initial time $t=0$, the general solution as a function of time is then

$$\left|\psi(t)\right\rangle =U(t)\left|\psi(0)\right\rangle \tag{3}$$

Feynman's method allows us to compute the propagator directly, without first solving the Schrödinger equation. It is known as the *path integral forumulation*.

The idea is based on the observation that the exponential $e^{-iEt/\hbar}$ that appears in the propagator contains the ratio of two quantities with the dimensions of action, that is, energy times time. In classical mechanics, the actual trajectory of a particle is found by minimizing the action S over all possible paths available to the particle. The path integral formulation of quantum mechanics works in a similar way, although at first sight, it looks like a completely impractical method.

The formulation works like this, for a single particle:

(1) Find all paths available for the particle to travel between its initial point (x',t') and its final point (x,t). This is actually similar to what we do in classical mechanics, where S is defined as $S=\int L\,dt$ where L is the Lagrangian. We then use the functional derivative

to minimize S over all these paths and find the path that gives the minimum action.

(2) For each path, calculate the action S. (This is where things sound terribly impractical, since there are an infinite number of paths of all possible shape, so how can we find the action for all these paths? It turns out that, in most cases, we don't need to.)

(3) Calculate the propagator as

$$U\left(x,t;x',t'\right)=A\sum_{all\ paths}e^{iS[x(t)]/\hbar} \tag{4}$$

The notation $S[x(t)]$ indicates that S is a functional of the path $x(t)$.

The key to the success of this method is that since the action is real, the exponential $e^{iS[x(t)]/\hbar}$ is an oscillatory function, so we can expect contributions from the actions for different paths to cancel each other to some extent. Although the quantum path of a particle can't be defined precisely due to the uncertainty principle, we expect that the particle is much more likely to be found following a path that is close to the classical path, and the classical path occurs when $S[x(t)]$ is a minimum. Paths sufficiently far from this minimum will tend to cancel each other, so for practical purposes, we need calculate 4 only for paths near to the classical path.

The example given by Shankar is of a particle of mass 1 gram moving from $(x,t)=(0,0)$ to $(1,1)$ by two different paths. In the first path, the particle moves with constant speed so $x=t$. The action is

$$\begin{aligned}
S &= \int_0^1 L\,dt && (5)\\
&= \int_0^1 (T-V)\,dt && (6)\\
&= \int_0^1 \frac{1}{2}mv^2dt && (7)\\
&= \frac{m}{2}\int_0^1\left(\frac{dx}{dt}\right)^2dt && (8)\\
&= \frac{m}{2}\int_0^1 dt && (9)\\
&= \frac{m}{2} && (10)
\end{aligned}$$

In the second path, we have $x=t^2$, so the velocity is

$$v=\frac{dx}{dt}=2t \tag{11}$$

with associated action

$$\begin{aligned} S &= \int_0^1 \frac{1}{2}mv^2 dt && (12)\\ &= 2m\int_0^1 t^2 dt && (13)\\ &= \frac{2m}{3} && (14)\end{aligned}$$

The guideline for when the phases of the paths start to cancel each other is when $S/\hbar$ is about π out of phase with $S_{cl}/\hbar$. In this example, the second path is πout of phase with the first when

$$\left(\frac{2m}{3}-\frac{m}{2}\right)=\pi\hbar\approx 3\times 10^{-34}\ \mathrm{m^2 kg\ s^{-1}} \tag{15}$$

Thus for any mass larger than about $6\pi\hbar\approx 1.8\times 10^{-33}$ kg the second path will contribute essentially nothing to 4 and can be ignored. This mass is smaller than the mass of the electron.

For the free particle, we worked out the propagator earlier and found that (where we've generalized the earlier result for an arbitrary initial time t'):

$$U\left(t,t'\right)=\int_{-\infty}^{\infty} e^{-ip^2(t-t')/2m\hbar}\left|p\right\rangle\left\langle p\right| dp \tag{16}$$

The matrix elements of U in the x basis are worked out by evaluating a Gaussian integral

$$\begin{aligned} U\left(x,t;x',t'\right) &= \int_{-\infty}^{\infty} e^{-ip^2(t-t')/2m\hbar}\left\langle x\left|p\right.\right\rangle\left\langle p\left|x'\right.\right\rangle dp && (17)\\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-x')/\hbar}e^{-ip^2(t-t')/2m\hbar}dp && (18)\\ &= \sqrt{\frac{m}{2\pi\hbar i\left(t-t'\right)}}e^{im(x-x')^2/2\hbar(t-t')} && (19)\end{aligned}$$

We can try to estimate U using the path integral approach by assuming that only the classical path contributes to the propagator. For a free particle travelling between (x',t') to (x,t), the constant velocity is

$$v=\frac{x-x'}{t-t'} \tag{20}$$

The Lagrangian is a constant

$$L=\frac{mv^{2}}{2}=\frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^{2} \tag{21}$$

The classical action is thus

$$\begin{aligned}
S_{cl} &= \int_{t'}^{t}L\,dt'' && (22)\\
&= \frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^{2}\int_{t'}^{t}dt'' && (23)\\
&= \frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^{2}\left(t-t'\right) && (24)\\
&= \frac{m}{2}\frac{\left(x-x'\right)^{2}}{t-t'} && (25)
\end{aligned}$$

The propagator in this approximation is

$$U\left(x,t;x',t'\right)=A\exp\left[\frac{im}{2\hbar}\frac{\left(x-x'\right)^{2}}{\left(t-t'\right)}\right] \tag{26}$$

Comparing with 19 we see that the exponential factors match; all that is left is to determine the constant A. To do this, we require $\lim_{t\to t'}U\left(x,t;x',t'\right)=\delta\left(x-x'\right)$, since if the time interval $t'-t$ goes to zero, the particle cannot move so must be in the same place. By comparing 26 with the form of a delta function as the limit of a gaussian integral, which is

$$\lim_{\Delta^{2}\to0}\frac{1}{\left(\pi\Delta^{2}\right)^{1/2}}\int_{-\infty}^{\infty}e^{-(x-x')/\Delta^{2}}dx=\delta\left(x-x'\right) \tag{27}$$

we see that

$$\Delta^{2}=\frac{2\hbar i\left(t-t'\right)}{m} \tag{28}$$

so the final propagator is the same as 19.

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