

THE PATH INTEGRAL IS EQUIVALENT TO THE SCHRÖDINGER EQUATION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.5.

We've seen that we can produce the propagator for the free particle by means of a complete path integral over all paths between some specified initial state at (x_0, t_0) and specified final state (x_N, t_N) . Here we'll show that the path integral approach is formally equivalent to the Schrödinger equation, even for an arbitrary potential V .

The Schrödinger equation is a differential equation that allows us to calculate the wave function as a function of position x and time t , when solved in the position basis. To find the same thing from the path integral, we'll consider an infinitesimal time interval ϵ and try to find $\psi(x, \epsilon)$ given the wave function at $t = 0$, that is, given $\psi(x', 0)$ for some arbitrary x' . To use a path integral in this way, we're effectively asking for the contribution to the propagator from all possible paths between $t = 0$ and $t = \epsilon$. That is, we're considering that the particle may have started at *any* position x' at $t = 0$ and still ended up at position x at $t = \epsilon$. In terms of the propagator, this is

$$\psi(x, \epsilon) = \int_{-\infty}^{\infty} U(x, \epsilon; x', 0) \psi(x', 0) dx' \quad (1)$$

Looking at our previous derivation of the propagator, we saw that there we fixed the initial and final states and integrated over all possible paths between these two states. In this case, all we're specifying is the final state so in principle, the particle could have been anywhere at $t = 0$.

The general form for the propagator is

$$U(t) = A \int_{\text{all paths}} e^{iS[x(t)]/\hbar} \quad (2)$$

where A is a scale factor and $S[x(t)]$ is the action for travelling along path $x(t)$:

$$S = \int_0^\epsilon L dt \quad (3)$$

We can approximate the action by taking the Lagrangian to be

$$L = T - V \quad (4)$$

$$= \frac{1}{2}mv^2 - V \quad (5)$$

$$= \frac{1}{2}m\frac{(x-x')^2}{\varepsilon^2} - V\left(\frac{x+x'}{2}, 0\right) \quad (6)$$

Here we take the velocity over the interval ε to be constant at $v = \frac{x-x'}{\varepsilon}$, and we take the potential to be constant, with its value at the midpoint between x and x' at time $t = 0$. The reason we can approximate V by its value at $t = 0$ is that in calculating the action 3, we will multiply L by ε , and we're interested only in terms of first order in ε . The action to this order is then

$$S = \varepsilon L = \frac{1}{2}m\frac{(x-x')^2}{\varepsilon} - \varepsilon V\left(\frac{x+x'}{2}, 0\right) \quad (7)$$

which gives a propagator of

$$U(x, \varepsilon; x', 0) = A \exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^2}{\varepsilon} - \varepsilon V\left(\frac{x+x'}{2}, 0\right)\right)\right] \quad (8)$$

We can try the same value for A that we had for the free particle

$$A = \left(\frac{m}{2\pi\hbar\varepsilon i}\right)^{N/2} \quad (9)$$

In this case, we have only one step so $N = 1$ and

$$U(x, \varepsilon; x', 0) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^2}{\varepsilon} - \varepsilon V\left(\frac{x+x'}{2}, 0\right)\right)\right] \quad (10)$$

We now need to do some approximating. The kinetic energy term is

$$\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^2}{\varepsilon}\right)\right] \quad (11)$$

The exponent is pure imaginary so for infinitesimal ε , it oscillates very rapidly away from the stationary point at $x = x'$. When this term is placed in the integral 1, it multiplies $\psi(x', 0)$ which we'll assume is a smooth function that doesn't oscillate much, at least over the scale at which 11 oscillates. We define

$$\eta \equiv x' - x \quad (12)$$

to be the distance from the minimum phase. Once the phase approaches π , the oscillations will be rapid enough that the contributions to the integral effectively cancel out, so we're looking at the region

$$\frac{m\eta^2}{2\hbar\varepsilon} \lesssim \pi \quad (13)$$

or

$$|\eta| \lesssim \sqrt{\frac{2\hbar\varepsilon\pi}{m}} \quad (14)$$

If we work to first order in ε we therefore must retain terms up to second order in η . In terms of η , 1 now becomes

$$\psi(x, \varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \exp\left(-\frac{i\varepsilon}{\hbar} V\left(x + \frac{\eta}{2}, 0\right)\right) \psi(x + \eta, 0) d\eta \quad (15)$$

We now expand the last two factors as a Taylor series in η and ε up to first order in ε or second order in η :

$$\exp\left(-\frac{i\varepsilon}{\hbar} V\left(x + \frac{\eta}{2}, 0\right)\right) = 1 - \frac{i\varepsilon}{\hbar} V\left(x + \frac{\eta}{2}, 0\right) + \dots \quad (16)$$

$$= 1 - \frac{i\varepsilon}{\hbar} V(x, 0) + \dots \quad (17)$$

We can drop terms in the expansion of $V\left(x + \frac{\eta}{2}, 0\right)$ beyond $V(x, 0)$ since they will be of order $\mathcal{O}(\varepsilon\eta) = \mathcal{O}(\varepsilon^{3/2})$ or higher.

For the second term, we have

$$\psi(x + \eta, 0) = \psi(x, 0) + \eta \frac{\partial \psi}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi}{\partial x^2} + \dots \quad (18)$$

where the partial derivatives are evaluated at $\eta = 0$.

Inserting these into the integral 15 we get

$$\psi(x, \varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \times \quad (19)$$

$$\left[\psi(x, 0) + \eta \frac{\partial \psi}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi}{\partial x^2} \right] \times \quad (20)$$

$$\left[1 - \frac{i\varepsilon}{\hbar} V(x, 0) \right] d\eta \quad (21)$$

Again, retaining only terms up to first order in ε or second order in η :

$$\psi(x, \varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \times \quad (22)$$

$$\left[\psi(x, 0) - \frac{i\varepsilon}{\hbar} V(x, 0) \psi(x, 0) + \eta \frac{\partial \psi}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi}{\partial x^2} \right] d\eta \quad (23)$$

Everything in the integrand is constant with respect to η except for the first exponential and the factors of η and η^2 in the last two terms. We are therefore faced with a couple of Gaussian integrals. We have

$$\int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) d\eta = \int_{-\infty}^{\infty} \exp\left(-\frac{m\eta^2}{2\hbar i\varepsilon}\right) d\eta \quad (24)$$

$$= \sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \quad (25)$$

$$\int_{-\infty}^{\infty} \eta \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) d\eta = 0 \quad (26)$$

$$\int_{-\infty}^{\infty} \eta^2 \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) d\eta = \int_{-\infty}^{\infty} \eta^2 \exp\left(-\frac{m\eta^2}{2\hbar i\varepsilon}\right) d\eta \quad (27)$$

$$= \frac{\hbar i\varepsilon}{m} \sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \quad (28)$$

$$= -\frac{\hbar\varepsilon}{im} \sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \quad (29)$$

Putting it all together, we have

$$\psi(x, \varepsilon) = \sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \sqrt{\frac{2\pi\hbar i\varepsilon}{m}} \left[\left(1 - \frac{i\varepsilon}{\hbar} V(x, 0)\right) - \frac{\hbar\varepsilon}{2im} \frac{\partial^2}{\partial x^2} \right] \psi(x, 0) \quad (30)$$

$$= \psi(x, 0) - \frac{i\varepsilon}{\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, 0) \right) \psi(x, 0) \quad (31)$$

Rearranging, we get

$$i\hbar \frac{\psi(x, \varepsilon) - \psi(x, 0)}{\varepsilon} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, 0) \right) \psi(x, 0) \quad (32)$$

In the limit $\varepsilon \rightarrow 0$, the LHS becomes $i\hbar \frac{\partial \psi}{\partial t}$ and we get the Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, 0) \right) \psi(x, 0) \quad (33)$$

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