

FREE PARTICLE PROPAGATOR FROM A COMPLETE PATH INTEGRAL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.4.

We've seen that the free-particle propagator can be obtained in the path integral approach by using only the classical path in the sum over paths. It turns out that it's not too hard to calculate the propagator for a free particle properly, by summing over all possible paths. The notation used by Shankar is as follows.

We want to evaluate the path integral

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathcal{D}[x(t)] \quad (1)$$

The notation $\mathcal{D}[x(t)]$ means an integration over all possible paths from x_0 to x_N in the given time interval. This includes paths where the particle might move to the right for a while, then jog back to the left, then back to the right again and so on. This might seem like a hopeless task, but we can make sense of this method by splitting the time interval between t_0 and t_N into N small intervals, each of length ε . Thus an intermediate time $t_n = t_0 + n\varepsilon$, and the final time is $t_N = t_0 + N\varepsilon$.

For a free particle, there is no potential energy so the Lagrangian is just the kinetic energy:

$$L = \frac{1}{2}m\dot{x}^2 \quad (2)$$

We can estimate the velocity in each time slice by

$$\dot{x}_i = \frac{x_{i+1} - x_i}{\varepsilon} \quad (3)$$

Note that this assumes that the velocity within each time slice is constant, but as we make ε smaller and smaller, this is increasingly accurate. Also note that it is possible for \dot{x}_i to be both positive (if the particle moves to the right in the interval) or negative (if it moves to the left).

The action for a given path is given by the integral of the Lagrangian:

$$S = \int_{t_0}^{t_N} L(t) dt \quad (4)$$

In our discretized approximation, we evaluate L within each time slice, and dt becomes the interval length ε , so the action becomes a sum:

$$S = \sum_{i=0}^{N-1} L(t_i) \varepsilon \quad (5)$$

$$= \frac{m}{2} \sum_{i=0}^{N-1} \left(\frac{x_{i+1} - x_i}{\varepsilon} \right)^2 \varepsilon \quad (6)$$

$$= \frac{m}{2} \sum_{i=0}^{N-1} \frac{(x_{i+1} - x_i)^2}{\varepsilon} \quad (7)$$

The key point here is to notice that we can label any given path by choosing values for all the x_i s between the two times, and that each x_i can vary independently of the others, over a range from $-\infty$ to $+\infty$. We can therefore implement the multiple integration required by $\mathfrak{D}[x(t)]$ by integrating over all the x_i variables separately. That is,

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathfrak{D}[x(t)] = A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp \left[\frac{im}{2\hbar} \sum_{i=0}^{N-1} \frac{(x_{i+1} - x_i)^2}{\varepsilon} \right] dx_1 dx_2 \dots dx_{N-1} \quad (8)$$

where A is some constant to make the scale come out right.

We don't integrate over x_0 or x_N since these are fixed as the end points of the path. To get the final version, we need to take the limit of this expression as $N \rightarrow \infty$ and $\varepsilon \rightarrow 0$. This still looks pretty scary, but in fact it is doable. We define the variable

$$y_i \equiv \sqrt{\frac{m}{2\hbar\varepsilon}} x_i \quad (9)$$

$$dx_i = \sqrt{\frac{2\hbar\varepsilon}{m}} dy_i \quad (10)$$

This gives us

$$A \left(\frac{2\hbar\varepsilon}{m} \right)^{(N-1)/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp \left[i \sum_{i=0}^{N-1} (y_{i+1} - y_i)^2 \right] dy_1 dy_2 \dots dy_{N-1} \quad (11)$$

We can do the integral in stages in order to spot a pattern. Consider first the integral over y_1 , which involves only two of the factors in the integrand:

$$\int_{-\infty}^{\infty} e^{i[(y_1-y_0)^2+(y_2-y_1)^2]} dy_1 \quad (12)$$

We first simplify the exponent

$$(y_1 - y_0)^2 + (y_2 - y_1)^2 = y_2^2 + y_0^2 + 2(y_1^2 - y_0 y_1 - y_1 y_2) \quad (13)$$

$$= y_2^2 + y_0^2 + 2y_1^2 - 2(y_0 + y_2)y_1 \quad (14)$$

We get

$$\int_{-\infty}^{\infty} e^{i[(y_1-y_0)^2+(y_2-y_1)^2]} dy_1 = e^{i(y_2^2+y_0^2)} \int_{-\infty}^{\infty} e^{2i[y_1^2-(y_0+y_2)y_1]} dy_1 \quad (15)$$

We can evaluate this using a standard Gaussian integral

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = e^{b^2/4a} \sqrt{\frac{\pi}{a}} \quad (16)$$

This gives

$$\int_{-\infty}^{\infty} e^{i[(y_1-y_0)^2+(y_2-y_1)^2]} dy_1 = e^{i(y_2^2+y_0^2)} e^{4(y_0+y_2)^2/8i} \sqrt{-\frac{\pi}{2i}} \quad (17)$$

$$= e^{i(y_2^2+y_0^2)} e^{(y_0+y_2)^2/2i} \sqrt{\frac{\pi i}{2}} \quad (18)$$

To simplify the exponents on the RHS:

$$i(y_2^2 + y_0^2) + \frac{(y_0 + y_2)^2}{2i} = \frac{1}{2i} [(y_0 + y_2)^2 - 2y_2^2 - 2y_0^2] \quad (19)$$

$$= -\frac{1}{2i} (y_0 - y_2)^2 \quad (20)$$

Thus we have

$$\int_{-\infty}^{\infty} e^{i[(y_1-y_0)^2+(y_2-y_1)^2]} dy_1 = \sqrt{\frac{\pi i}{2}} e^{-(y_0-y_2)^2/2i} \quad (21)$$

Having eliminated y_1 we can now do the integral over y_2 :

$$\sqrt{\frac{\pi i}{2}} \int_{-\infty}^{\infty} e^{-(y_3-y_2)^2/i-(y_2-y_0)^2/2i} dy_2 \quad (22)$$

Again, we can simplify the exponent:

$$-\frac{(y_3 - y_2)^2}{i} - \frac{(y_2 - y_0)^2}{2i} = \frac{1}{2i} [-(2y_3^2 + y_0^2) - 3y_2^2 + y_2(4y_3 + 2y_0)] \quad (23)$$

The integral now becomes

$$\sqrt{\frac{\pi i}{2}} \int_{-\infty}^{\infty} e^{-(y_3 - y_2)^2/i - (y_2 - y_0)^2/2i} dy_2 = \sqrt{\frac{\pi i}{2}} e^{-(2y_3^2 + y_0^2)/2i} \int_{-\infty}^{\infty} e^{(-3y_2^2 + y_2(4y_3 + 2y_0))/2i} dy_2 \quad (24)$$

Doing the Gaussian integral on the RHS using 16:

$$\int_{-\infty}^{\infty} e^{(-3y_2^2 + y_2(4y_3 + 2y_0))/2i} dy_2 = e^{-(4y_3 + 2y_0)^2 i/24} \sqrt{\frac{2\pi i}{3}} \quad (25)$$

$$= e^{(2y_3 + y_0)^2/6i} \sqrt{\frac{2\pi i}{3}} \quad (26)$$

Thus the combined integral over y_1 and y_2 is

$$\sqrt{\frac{\pi i}{2}} e^{-(2y_3^2 + y_0^2)/2i} e^{(2y_3 + y_0)^2/6i} \sqrt{\frac{2\pi i}{3}} = \sqrt{\frac{(\pi i)^2}{3}} e^{(-6y_3^2 - 3y_0^2 + (2y_3 + y_0)^2)/6i} \quad (27)$$

$$= \sqrt{\frac{(\pi i)^2}{3}} e^{-(y_3 - y_0)^2/3i} \quad (28)$$

The general pattern after $N - 1$ integrations is (presumably this could be proved by induction, but we'll accept the result):

$$\frac{(\pi i)^{(N-1)/2}}{\sqrt{N}} e^{-(y_N - y_0)^2/Ni} = \frac{(\pi i)^{(N-1)/2}}{\sqrt{N}} e^{-m(x_N - x_0)^2/2\hbar\varepsilon Ni} \quad (29)$$

where we reverted back to x_i using 9.

Going back to 11, we must multiply the result by $A \left(\frac{2\hbar\varepsilon}{m}\right)^{(N-1)/2}$ to get the final expression for the propagator:

$$U = A \left(\frac{2\hbar\varepsilon}{m}\right)^{(N-1)/2} \frac{(\pi i)^{(N-1)/2}}{\sqrt{N}} e^{-m(x_N - x_0)^2/2\hbar\varepsilon Ni} \quad (30)$$

$$= A \left(\frac{2\pi\hbar\varepsilon i}{m}\right)^{N/2} \sqrt{\frac{m}{2\pi\hbar i N \varepsilon}} e^{im(x_N - x_0)^2/2\hbar\varepsilon N} \quad (31)$$

In the limit as $N \rightarrow \infty$ and $\varepsilon \rightarrow 0$, $N\varepsilon = t_N - t_0$ so we have

$$U = A \left(\frac{2\pi\hbar\varepsilon i}{m} \right)^{N/2} \sqrt{\frac{m}{2\pi\hbar i(t_N - t_0)}} e^{im(x_N - x_0)^2 / 2\hbar(t_N - t_0)} \quad (32)$$

The expression we got earlier using the Schrödinger method is

$$U(x, t; x', t') = \sqrt{\frac{m}{2\pi\hbar i(t - t')}} e^{im(x - x')^2 / 2\hbar(t - t')} \quad (33)$$

Thus the full path integral gives the same result, with $t' = t_0$ and $t = t_N$ (similarly for x), provided that we can set

$$A = \left(\frac{m}{2\pi\hbar\varepsilon i} \right)^{N/2} \equiv B^{-N} \quad (34)$$

Shankar then says that it is conventional to associate one factor of B^{-1} with each integration over an x_i , and the remaining factor with the overall process. This seems to overlook a basic problem, in that as $N \rightarrow \infty$ and $\varepsilon \rightarrow 0$, $A \rightarrow \infty$, so we seem to be cancelling two infinities when we multiply the path integral by A .

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