PATH INTEGRALS IN QUANTUM MECHANICS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Anthony Zee, *Quantum Field Theory in a Nutshell*, 2nd edition (Princeton University Press, 2010) - Chapter I.2, Problem 1.

In all our posts on quantum mechanics, we never really addressed the question of how likely it is that a particle starting at some initial position ends up in a specified final position. One way of looking at this problem leads to the *path integral* formulation of quantum mechanics. The idea starts with the Schrödinger equation in its most general form (in one dimension)

$$H\Psi(q,t)=i\frac{\partial\Psi(q,t)}{\partial t} \tag{1}$$

[Here we're adopting Zee's conventions of defining the position coordinate as q instead of x, and of using 'natural' units in which $\hbar=1$.] H is, as usual, the Hamiltonian which, for now, we're assuming is time-independent.

We can formally integrate this equation over the time interval $t=0$ to $t=T$ to get

$$\Psi(q,T)=e^{-iHT}\Psi(q_I,0) \tag{2}$$

where q_I is the intial position of the particle.

Since H is an operator, the exponential has meaning only when we expand it in its Taylor series, but we won't need that in what follows. Using the bra-ket notation, this is

$$|q\rangle=e^{-iHT}|q_I\rangle \tag{3}$$

The probability amplitude that a particle starting in state $|q_I\rangle$ ends up in state $|q_F\rangle$ is therefore

$$\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle \tag{4}$$

Quantum mechanics, of course, doesn't specify an exact path by which the particle travels between the two locations. In fact, *any* intervening path is possible, even a path where the particle travels to the Andromeda galaxy and back to reach the final position. We can model this by breaking up the total time T into a large number N of short time intervals $\delta t\equiv\frac{T}{N}$, and then finding the amplitude for the particle moving from one point to another over each interval δt, with the condition that it ends up at location q_F. Formally, we can use the fact that the set of all position eigenstates is a complete set, so that

$$\int |q\rangle \langle q| \, dq = 1 \tag{5}$$

If you don't see this, use the fact that $\langle q' | q \rangle = \delta (q' - q)$ and then calculate as follows:

$$\begin{aligned}
\langle q'' | \int dq \, |q\rangle \langle q | q' \rangle &= \int dq \left\langle q'' | q \right\rangle \left\langle q | q' \right\rangle && (6)\\
&= \int dq \delta\left(q'' - q\right) \delta\left(q - q'\right) && (7)\\
&= \delta\left(q'' - q'\right) && (8)\\
&= \left\langle q'' | q' \right\rangle && (9)
\end{aligned}$$

Therefore, we can insert this unit operator anywhere we like without changing the result of a calculation. In particular, we could say

$$\left\langle q_F \left| e^{-iHT} \right| q_I \right\rangle = \left\langle q_F \left| e^{-iH\delta t} e^{-iH\delta t} \ldots e^{-iH\delta t} \right| q_I \right\rangle \tag{10}$$

where there are N factors of $e^{-iH\delta t}$ on the RHS. Now we can insert 5 between each pair of operators:

$$\left\langle q_F \left| e^{-iHT} \right| q_I \right\rangle = \left\langle q_F \left| e^{-iH\delta t} \left[\int |q_{N-1}\rangle \langle q_{N-1}| \, dq_{N-1} \right] e^{-iH\delta t} \ldots e^{-iH\delta t} \left[\int |q_1\rangle \langle q_1| \, dq_1 \right] e^{-iH\delta t} \right| q_I \right\rangle \tag{11}$$

We've inserted $N-1$ independent unit operators of the form $\int \left| q_j \right\rangle \left\langle q_j \right| dq_j$ in this expression, so we must integrate over $N-1$ separate q_j variables. We can condense the notation a bit by writing this as

$$\left\langle q_F \left| e^{-iHT} \right| q_I \right\rangle = \left[\prod_{j=1}^{N-1} \int dq_j \right] \left\langle q_F \left| e^{-iH\delta t} \right| q_{N-1} \right\rangle \left\langle q_{N-1} \left| e^{-iH\delta t} \right| q_{N-2} \right\rangle \ldots \left\langle q_1 \left| e^{-iH\delta t} \right| q_I \right\rangle \tag{12}$$

The product symbol $\prod_{j=1}^{N-1}$ applies to integrals that must be done, giving $N-1$ integrations.

Each term on the RHS has the form $\left\langle q_{j+1} \left| e^{-iH\delta t} \right| q_j \right\rangle$ which has the same form as the probability amplitude 4. Thus it represents the amplitude that the particle moves from location q_j to location q_{j+1} in time interval δt. However, because of the integrations over q_j and q_{j+1}, both these location variables range over all space, so we're adding up the amplitudes for the particle starting at every location in space and travelling to every other location in space, all in the time interval δt. The vast majority of these amplitudes will, of course, be zero (or as close to zero as makes no difference), but the idea is that we're considering all possible paths for the particle between the initial and final locations q_I and q_F.

We'll focus now on one of these amplitudes: $\left\langle q_{j+1}\left|e^{-iH\delta t}\right|q_j\right\rangle$. The most general time independent hamiltonian has the form

$$H=\frac{\hat{p}^2}{2m}+V\left(\hat{q}\right) \tag{13}$$

where $\hat{p}$ is the momentum operator, V is the potential energy and $\hat{q}$ is the position operator.

The eigenfunctions of the momentum operator are (recall that $\hat{p}=\frac{1}{i}\frac{\partial}{\partial q}$):

$$\left|p\right\rangle=e^{ipq} \tag{14}$$

Since the position eigenstate is

$$\left|q\right\rangle=\delta\left(q'-q\right) \tag{15}$$

we have

$$\begin{aligned}\left\langle q\right|p\rangle &= \int dq'\delta\left(q'-q\right)e^{ipq'} && (16)\\ &= e^{ipq} && (17)\end{aligned}$$

We can make a unit operator out of a complete set of momentum eigenstates in a similar way to that for the position eigenstates. It turns out that

$$\frac{1}{2\pi}\int\left|p\right\rangle\left\langle p\right|dp=1 \tag{18}$$

This can be verified by multiplying on the left by $\left\langle q'\right|$ and on the right by $\left|q\right\rangle$:

$$\frac{1}{2\pi}\left\langle q'\right|\int\left|p\right\rangle\left\langle p\left|q\right.\right\rangle dp = \frac{1}{2\pi}\int\left\langle q'\left|p\right.\right\rangle\left\langle p\left|q\right.\right\rangle dq \tag{19}$$
$$= \frac{1}{2\pi}\int e^{ipq'}e^{-ipq}dq \tag{20}$$
$$= \frac{1}{2\pi}\int e^{ip(q'-q)}dq \tag{21}$$
$$= \delta\left(q'-q\right) \tag{22}$$
$$= \left\langle q'\left|q\right.\right\rangle \tag{23}$$

where we used the definition of the delta function in the penultimate line. Returning to the hamiltonian 13 we have

$$\left\langle q_{j+1}\left|e^{-iH\delta t}\right|q_j\right\rangle = \left\langle q_{j+1}\left|e^{-i\hat{p}^2\delta t/2m}e^{-iV(\hat{q})\delta t}\right|q_j\right\rangle \tag{24}$$
$$= e^{-iV\left(q_j\right)\delta t}\left\langle q_{j+1}\left|e^{-i\hat{p}^2\delta t/2m}\right|q_j\right\rangle \tag{25}$$

The last line arises from the fact that $\left|q_j\right\rangle$ is an eigenstate of $\hat{q}$ with eigenvalue q_j so the potential energy $V(\hat{q})$ operating on $\left|q_j\right\rangle$ produces $V\left(q_j\right)\left|q_j\right\rangle$.

Zee does the calculation of the remaining amplitude $\left\langle q_{j+1}\left|e^{-i\hat{p}^2\delta t/2m}\right|q_j\right\rangle$ in detail, so we'll just summarize the method here. A unit operator 18 is inserted which results in the amplitude becoming a Gaussian integral involving an exponent which is a quadratic in p. The integral can be done by completing the square, with the result

$$\left\langle q_{j+1}\left|e^{-i\hat{p}^2\delta t/2m}\right|q_j\right\rangle = \left(\frac{-im}{2\pi\delta t}\right)^{1/2} e^{i\delta t(m/2)\left[\left(q_{j+1}-q_j\right)/\delta t\right]^2} \tag{26}$$

Putting this into 12 we get

$$\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle = \left(\frac{-im}{2\pi\delta t}\right)^{N/2}\left[\prod_{j=1}^{N-1}\int dq_j\right] e^{i\delta t(m/2)\sum_{j=0}^{N-1}\left[\left(q_{j+1}-q_j\right)/\delta t\right]^2} e^{-i\delta t\sum_{j=0}^{N-1}V\left(q_j\right)} \tag{27}$$

Taking the limit as $N\to\infty$ and $\delta t\to 0$ converts the sums in the exponents to integrals, giving

$$\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle = \lim_{N\to\infty}\left(\frac{-im}{2\pi\delta t}\right)^{N/2}\left[\prod_{j=1}^{N-1}\int dq_j\right] e^{i\int_0^T\left[\frac{1}{2}m\dot{q}^2-V(q)\right]dt} \tag{28}$$

Finally, defining

$$\int Dq(t) \equiv \lim_{N\to\infty}\left(\frac{-im}{2\pi\delta t}\right)^{N/2}\left[\prod_{j=1}^{N-1}\int dq_j\right] \tag{29}$$

we get the final path integral:

$$\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle = \int Dq(t)\,e^{i\int_0^T\left[\frac{1}{2}m\dot{q}^2-V(q)\right]dt} \tag{30}$$

This is certainly not something that can be easily computed, as the operator $\int Dq(t)$ involves an infinite number of integrals over an infinite number of paths.

PINGBACKS

Pingback: Steepest descent and the classical limit of quantum mechanics
Pingback: From mattress to field