13 Feb 2019

SCPY 323

Quantum Mechanics II

Read Sakurai 2.5.

Feynman Path Integrals.

First consider the relationship between propagators and Feynman Path Integrals.

Consider a propagator in x-basis.

$$\langle x''|U(t;t_0)|x'\rangle \equiv U(x'',t;x',t_0)$$
$$= \sum_a \langle x''|a\rangle\langle a|x'\rangle \exp\left[\frac{-iE_a(t-t_0)}{\hbar}\right]$$

Properties of propagator.

1) $U(x'',t;x',t_0)$ satisfies Schrödinger's time-dependent ware equation in variable x'' and t.

2). $\lim_{t\to t_0} U(x'',t;x',t_0) = \delta^3(x''-x')$ for 3D.

Note that $\lim_{t\to t_0} \langle x''|U(t;t_0)|x'\rangle = \langle x''|x'\rangle = \delta^3(x''-x')$

If we want to find time evolution of $\psi(x',t_0)$, we can multiply $\psi(x',t_0)$ by $U(x'',t;x',t_0)$ and integrate over all x'.

$\Rightarrow$ We add various contributions from different positions x'

This procedure is the same as the calculation of electric potential in electrostatics, where we add the contribution of charge $\rho(x')$. We can first find the contribution of a point-charge, multiply the point-charge solution with the charge distribution and integrate.

$$\Rightarrow \quad \phi(\vec{x}) = \int d^3\vec{x}' \frac{\rho(\vec{x}')}{|\vec{x} - \vec{x}'|}$$

In this sense, the propagator is simply the Green's function for the time-dependent wave-function equation

$$\left(-\left(\frac{\hbar^2}{2m}\right)\nabla''^2 + V(x'') - i\hbar\frac{\partial}{\partial t}\right) U(x'', t; x', t_0) = -i\hbar\,\delta^3(x''-x')\,\delta(t-t_0)$$

with the boundary condition.

$$U(x'', t; x', t_0) = 0 \quad \text{for } t < t_0.$$

Consider a free particle

$$\mathcal{H} = \frac{p^2}{2m}.$$

$$\mathcal{H}|p\rangle = \frac{p^2}{2m}|p\rangle \quad \text{where } |p\rangle \text{ is the momentum eigenstate.}$$

From homework we know that.

$$U(x'', t; x', t_0) = \left(\frac{1}{2\pi\hbar}\right)\int_{-\infty}^{\infty} dp' \exp\left[\frac{ip'(x''-x')}{\hbar} - \frac{ip'^2(t-t_0)}{2m\hbar}\right]$$

$$= \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\exp\left[\frac{im(x''-x')^2}{2\hbar(t-t_0)}\right]$$

Consider the case where $x'' = x'$ and let $t_0 = 0$. and integrate over all space.

$$G(t) \equiv \int d^3x' \, U(x',t;x',0)$$

$$= \int d^3x' \sum_a |\langle x'|a\rangle|^2 \exp\left(\frac{-iE_a t}{\hbar}\right)$$

$$= \sum_a \exp\left(\frac{-iE_a t}{\hbar}\right)$$

Note that by setting $x'' = x'$ and integrating over all space, we calculater the trace of the time-evolution operator in x-basis. However, since the trace does not depend on a basis, we can calculate the trace using the basis $|a\rangle$ where we can right away get the result.

Interestingly, if we Let $\beta = \frac{it}{\hbar}$. the.

$$G(\beta) \equiv Z = \sum_a \exp(-\beta E_a),$$

which is the partition function.

Consider the Laplace-Fourier transform of $G(t)$.

$$\tilde{G}(E) = \frac{-i}{\hbar}\int_0^\infty dt \, G(t) \, e^{iEt/\hbar} = -\frac{i}{\hbar}\int_0^\infty dt \sum_a \exp\left(-i\frac{E_a t}{\hbar}\right)\exp\left(\frac{+iEt}{\hbar}\right)$$

Let $E \to E + i\varepsilon$ and let $\varepsilon \to 0$.

$$\Rightarrow \quad \tilde{G}(E) = \sum_a \frac{1}{E - E_a}.$$

The complete energy spectrum E_a is given by poles of $\tilde{G}(E)$

Propagator as a transition amplitude.

Consider.

$$U(x'',t\,;x',t_0) = \sum_a \langle x''|a\rangle\langle a|x'\rangle \exp\left[\frac{-iE_a(t-t_0)}{\hbar}\right]$$

$$= \sum_a \langle x''|\exp\left(\frac{-iHt}{\hbar}\right)|a'\rangle\langle a'|\exp\left(\frac{iHt_0}{\hbar}\right)|x'\rangle$$

$$= \underbrace{\left[\langle x''|\exp\left(\frac{-iHt}{\hbar}\right)\right]}_{\langle x''(t)|}\underbrace{\left[\exp\left(\frac{iHt_0}{\hbar}\right)|x'\rangle\right]}_{|x'(t_0)\rangle}$$

where $\langle x''(t)|$ $\cancel{|x''(t)\rangle}$ and $|x'(t_0)\rangle$ are eigenbra and eigenket of the position operator in the Heisenberg picture, Note that the basis "rotate in an opposite sense" compared to the wavefunction.

$$\Rightarrow \quad U(x'',t\,;x',t_0) = \langle x''(t)|x'(t_0)\rangle$$

We can identify $\langle x''(t)|x'(t_0)\rangle$ as the probability amplitude for the particle at position x' and time t_0 to be at position x'' at time t.

Now consider the time evolution from t' to t'''

$$t' \to t''' \quad = \quad t' \to t'' \quad + \quad t'' \to t'''$$

We have the composition property.

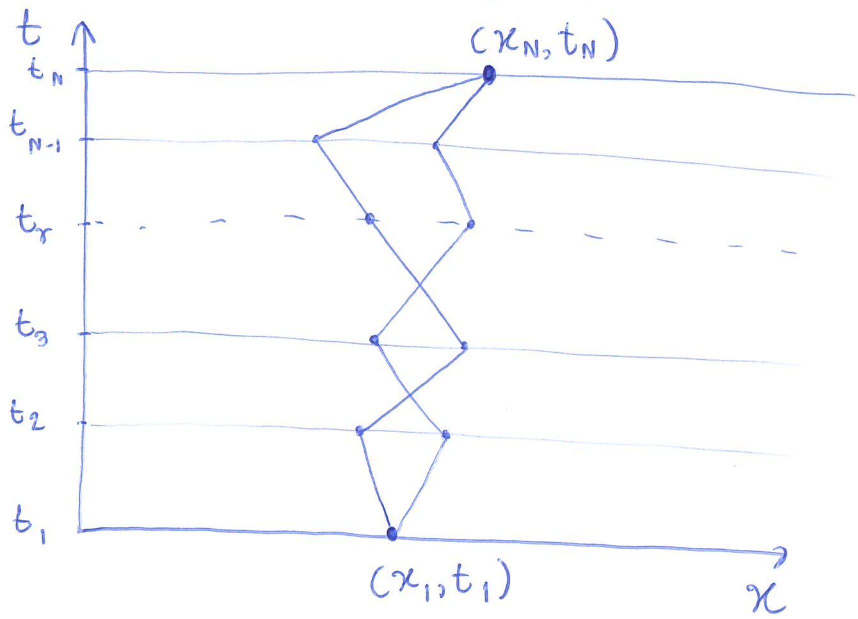
$$\langle x'''(t''') | x'(t') \rangle = \int d^3x'' \langle x'''(t''') | x''(t'') \rangle \langle x''(t'') | x'(t') \rangle$$

for $t''' > t'' > t'$

For N-1 intervals, we have.

$$\langle x_N, t_N | x_1, t_1 \rangle = \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \langle x_N, t_N | x_{N-1}, t_{N-1} \rangle$$
$$\times \langle x_{N-1}, t_{N-1} | x_{N-2}, t_{N-2} \rangle \cdots \langle x_2, t_2 | x_1, t_1 \rangle$$

Paths in the x-t plane.



Since we integrate over $x_2, \ldots, x_{N-1}$, we must sum over all paths. while fixing two endpoints.

Feynman's Formulation

Difference between classical and quantum mechanics is that in classical mechanics a definite path in the x-t plane is taken by a particle but in quantum mechanics all possible paths play roles.

And quantum mechanics reduces to classical mechanics in the limit $h \to 0$.

Feynman was motivated by a remark in Dirac's book. that states.

$$\exp\left[i \int_{t_1}^{t_2} dt \, L_{\text{classical}}(x, \dot{x}) / \hbar \right]$$

corresponds to $\langle x_2, t_2 | x_1, t_1 \rangle$

Let $S(n, n-1) \equiv \int_{t_{n-1}}^{t_n} dt \, L_{\text{classical}}(x, \dot{x})$

Consider a small segment along one particular path between (x_{n-1}, t_{n-1}) and (x_n, t_n). We can write down

$\exp\left[i S(n, n-1)/\hbar \right]$ to associate with this segment.

We can then add all segment along this path.

$$\prod_{n=2}^{N} \exp\left[\frac{i S(n, n-1)}{\hbar} \right] = \exp\left[\left(\frac{i}{\hbar}\right) \sum_{n=2}^{N} S(n, n-1) \right] = \exp\left[\frac{i S(N, 1)}{\hbar} \right]$$

but this is not yet $\langle x_N, t_N | x_1, t_1 \rangle$, since this expression is only for one path.

To obtain $\langle x_N, t_N | x_1, t_1 \rangle$, we have to add up the contribution from all paths.

$$\Rightarrow \quad \langle x_N, t_N | x_1, t_1 \rangle \sim \sum_{\text{all path}} \exp\left[\frac{iS(N,1)}{\hbar}\right]$$

where the sum is taken over an infinite numbers of paths.

Now let us consider the limit $\hbar \to 0$.

$\exp\left[\frac{iS(N,1)}{\hbar}\right]$ will oscillate and the contribution from different paths will cancel one another out.

However, if the path satisfies

$$\delta S(N,1) = 0$$

then the phase around this path will not cancel out since this path is an extremum. Note that. This path is a classical path. where $S = S_{min}$. and the phase of $\exp[iS/\hbar]$ does not change much if we slightly deviate from this path.

$\Rightarrow$ classical path dominates in the limit $\hbar \to 0$.

More precisely,

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \left[\frac{1}{W(\Delta t)}\right] \exp\left[\frac{iS(n,n-1)}{\hbar}\right]$$

where thweight factor $1/w(\Delta t)$ depends only on Δt and not on $V(x)$.

Evaluate $S(n, n-1)$ in the limit $\Delta t \to 0$

Since Δt is small, the segment can be taken to be a straight line joining (x_{n-1}, t_{n-1}) and (x_n, t_n)

$$S(n, n-1) = \int_{t_{n-1}}^{t_n} dt \left[\frac{m\dot{x}^2}{2} - V(x) \right]$$

$$= \Delta t \left[\left(\frac{m}{2}\right) \left[\frac{(x_n - x_{n-1})}{\Delta t} \right]^2 - V\left(\frac{(x_n + x_{n-1})}{2} \right) \right]$$

Consider a free particle where $V = 0$.

$$\Rightarrow \langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \left[\frac{1}{W(\Delta t)} \right] \exp\left[\frac{im(x_n - x_{n-1})^2}{2\hbar \Delta t} \right]$$

Note the expression of the exponential which is the same as that propagator for a free particle.

Evaluate $\frac{1}{W(\Delta t)}$

Since it is independent of $V(x)$, we can evaluate it in the case of free particle.

Note that.

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle \Big|_{t_n = t_{n-1}} = \delta(x_n - x_{n-1})$$

Normalization:

$$\int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar\Delta t} \right) = \sqrt{\frac{2\pi i \hbar \Delta t}{m}}$$

$$\Rightarrow \frac{1}{W(\Delta t)} = \sqrt{\frac{m}{2\pi i \hbar \Delta t}}.$$

And

$$\lim_{\Delta t \to 0} \sqrt{\frac{m}{2\pi i\hbar \Delta t}} \exp\left(\frac{im\xi^2}{2\hbar \Delta t}\right) = \delta(\xi)$$

So, as $\Delta t \to 0$, we have.

$$\langle x_n, t_n | x_{n-1}, t_{n-1}\rangle = \sqrt{\frac{m}{2\pi i\hbar \Delta t}} \exp\left[\frac{iS(n,n-1)}{\hbar}\right]$$

Therefore, between t_N and t_1 $(t_1 \to t_N)$, we have.

$$\langle x_N, t_N | x_1, t_1\rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar \Delta t}\right)^{(N-1)/2} \times \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2 \prod_{n=2}^{N} \exp\left[\frac{iS(n,n-1)}{\hbar}\right]$$

Define

$$\int_{x_1}^{x_N} \mathcal{D}[x(t)] \equiv \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar \Delta t}\right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2.$$

So, we have.

$$\boxed{\langle x_N, t_N | x_1, t_1\rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)] \exp\left[i\int_{t_1}^{t_N} dt \frac{L_{\text{classical}}(x,\dot{x})}{\hbar}\right]}$$

This expression is known as <u>Feynman's path integral</u>.

Next we will show that Feynman's path integral satisfies Schrödinger equation.

$$\langle x_N, t_N | x_1, t_1\rangle = \int dx_{N-1} \langle x_N, t_N | x_{N-1}, t_{N-1}\rangle \langle x_{N-1}, t_{N-1} | x_1, t_1\rangle$$

$$= \int_{-\infty}^{\infty} dx_{N-1} \sqrt{\frac{m}{2\pi i\hbar \Delta t}} \exp\left[\left(\frac{im}{2\hbar}\right) \frac{(x_N - x_{N-1})^2}{\Delta t} - \frac{iV\Delta t}{\hbar}\right]$$

$$\times \langle x_{N-1}, t_{N-1} | x_1, t_1\rangle$$

where $t_N - t_{N-1}$ is infinitesimally small.

Let $\xi = x_N - x_{N-1}$. and $x_N \to x$, $t_N \to t + \Delta t$.

$$\Rightarrow \langle x, t+\Delta t | x_1, t_1\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar\Delta t} - \frac{iV\Delta t}{\hbar}\right) \langle x-\xi, t | x_1, t_1\rangle$$

Note that as $\Delta t \to 0$ the major contribution is from $\xi = 0$ so we can expand $\langle x-\xi, t | x_1, t_1\rangle$ around $\xi = 0$ in powers of ξ. and expand $\langle x, t+\Delta t | x_1, t_1\rangle$ in powers of Δt

$$\Rightarrow \langle x, t | x_1, t_1\rangle + \Delta t \frac{\partial}{\partial t} \langle x, t | x_1, t_1\rangle$$

$$= \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar\Delta t}\right) \left(1 - \frac{iV\Delta t}{\hbar} + \cdots\right)$$

$$\times \left[\langle x, t | x_1, t_1\rangle + \left(\frac{\xi^2}{2}\right) \frac{\partial^2}{\partial x^2} \langle x, t | x_1, t_1\rangle + \cdots\right]$$

Note that the linear term of ξ vanishes when $\int d\xi$.

Use. $\displaystyle\int_{-\infty}^{\infty} d\xi\, \xi^2 \exp\left(\frac{im\xi^2}{2\hbar\Delta t}\right) = \sqrt{2\pi}\left(\frac{i\hbar\Delta t}{m}\right)^{3/2}$.

$$\Rightarrow \Delta t \frac{\partial}{\partial t}\langle x,t|x_1,t_1\rangle = \left(\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\right)(\sqrt{2\pi})\left(\frac{i\hbar\Delta t}{m}\right)^{3/2}\cdot\frac{1}{2}\frac{\partial^2}{\partial x^2}\langle x,t|x_1,t_1\rangle$$

$$-\left(\frac{i}{\hbar}\right)\Delta t\, V\langle x,t|x_1,t_1\rangle$$

$$\Rightarrow i\hbar\frac{\partial}{\partial t}\langle x,t|x_1,t_1\rangle = -\left(\frac{\hbar^2}{2m}\right)\frac{\partial^2}{\partial x^2}\langle x,t|x_1,t_1\rangle + V\langle x,t|x_1,t_1\rangle.$$

So $\langle x,t|x_1,t_1\rangle$ satisfies the Schrödinger equation ∎