1 Feynman Path Integral.

The version of quantum mechanics:

1. Schrödinger's wavefuction (operator form):

$$\hat{H}|\psi\rangle = \mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle \tag{1}$$

2. Feynman's Path Integral (Common number form):

$$\mathrm{i}G(\text{Green's function}) \propto \int \mathcal{D}(x,t)\mathrm{e}^{\mathrm{i}\int \mathcal{L}\mathrm{d}t} \tag{2}$$

There are many advantages of Feynman Path Integral:

1. Make the double-slit experiment more understandable.
2. The classical limit "$\hbar \to 0$" is "tractable": quantum $\xrightarrow{\hbar\to 0}$ classical.
3. Provide a semi-classical picture. for. quantum mechanics.
4. "Quantum fluctuations" are more "understandable".
5. A natural route. to low energy effective theory of quantum many-body systems.
6. A natural language for describing topological properties of quantum many-body systems.

But the practical calculation in the path-integral representation of simple quantum mechanical problem many be notoriously difficult and lengthy.

1.1 Propagators.

Consider a quantum partical confined in a one-dimensional space:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{3}$$

and the canonical pair: $[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = \mathrm{i}\hbar$

The Schrödinger's equation is:

$$\mathrm{i}\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle \tag{4}$$

This first-order nature allows us to define a time evolution operator $\hat{U}(t,t_0)$ which propagates the state vector from an initial time t_0 to a final time t:

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \tag{5}$$

Assuming the Hamiltonian H is not explicitly depend on time, the formal solution of $\hat{U}$ is:

$$\hat{U} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)} \tag{6}$$

A crucial property of $\hat{U}$ is the "chain-like" rule, or composition property. For any intermediate time t' such that $t > t' > t_0$:

$$\hat{U}(t, t_0) = \hat{U}(t, t')\hat{U}(t', t_0) \tag{7}$$

This property is the key to the entire path integral derivation. And $\hat{U}(t, t_0)$ is unitary:

$$\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = \hat{\mathbb{I}} \tag{8}$$

where $\hat{\mathbb{I}}$ is the identity operator.

In the position representation, we can obtain matrix elements:

$$\begin{aligned} U(x, t; x_0, t_0) &= \langle x|\hat{U}(t, t_0)|x_0\rangle \\ &= \langle x|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)}|x_0\rangle \end{aligned} \tag{9}$$

We can define a propagators (Green's function) of the quantum system by using the matrix elements:

$$\mathrm{i}G(x, t; x_0, t_0) = U(x, t; x_0, t_0) \tag{10}$$

Using the matrix elements, $\psi(x, t)$ can be reformulated as:

$$\begin{aligned} \psi(x, t) &= \langle x|\hat{U}(t, t_0)|\psi(t_0)\rangle \\ &= \int \mathrm{d}x_0 \langle x|\hat{U}(t, t_0)|x_0\rangle\langle x_0|\psi(t_0)\rangle \\ &= \int \mathrm{d}x_0 U(x, t; x_0, t_0)\psi(x_0, t_0) \end{aligned} \tag{11}$$

Also, the propagator also satisfies the Schrödinger's equation:

$$\boxed{\mathrm{i}\hbar\frac{\partial}{\partial t}G(x, t; x_0, t_0) = \hat{H}G(x, t; x_0, t_0)} \tag{12}$$

And the initial condition is:

$$G(x, t_0; x_0, t_0) = -\mathrm{i}\langle x|\hat{U}(t_0, t_0)|x_0\rangle = -\mathrm{i}\delta(x - x_0) \tag{13}$$

$\delta(x - x_0)$ is Dirac function.

Example 1.1. For free particle: $\hat{H} = \frac{1}{2m}\hat{p}^2$, in position representation:

$$\hat{p} \longrightarrow -\mathrm{i}\hbar\frac{\partial}{\partial x} \tag{14}$$

So the PDE is:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}G(x, t; x_0, t_0) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}G(x, t; x_0, t_0) \tag{15}$$

Solve the PDE:

Use Fourier Transform: (we use $G(x,t)$ instead of $G(x,t;x_0,t_0)$). We solve the free-particle Green's function by transforming to momentum space:

$$\begin{cases} G(x,t) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int \mathrm{d}k \cdot \tilde{G}(k,t)\mathrm{e}^{\mathrm{i}kx} \\ \tilde{G}(k,t) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int \mathrm{d}x\, G(x,t)\mathrm{e}^{-\mathrm{i}kx} \end{cases} \tag{16}$$

With these conventions, spatial derivatives become algebraic in k-space while the time derivative remains unchanged:

$$\begin{cases} \mathcal{F}\left\{\mathrm{i}\hbar \dfrac{\partial G(x,t)}{\partial t}\right\} = \mathrm{i}\hbar \dfrac{\partial \tilde{G}(k,t)}{\partial t} \\ \mathcal{F}\left\{-\dfrac{\hbar^2}{2m}\dfrac{\partial^2 G}{\partial x^2}\right\} = -\dfrac{\hbar^2}{2m}[-k^2\tilde{G}(k,t)] = \dfrac{\hbar^2 k^2}{2m}\tilde{G}(k,t) \end{cases} \tag{17}$$

Applying the transform to the PDE yields an ordinary differential equation in time for each k:

$$\begin{cases} \mathrm{i}\hbar \dfrac{\partial}{\partial t}\tilde{G}(k,t) = \dfrac{\hbar^2 k^2}{2m}\tilde{G}(k,t) \\ \dfrac{\mathrm{d}\tilde{G}}{\tilde{G}} = -\mathrm{i}\dfrac{\hbar k^2}{2m}\mathrm{d}t \end{cases} \tag{18}$$

Integrating in time gives the logarithm of the solution up to a k-dependent constant:

$$\ln \tilde{G} = -\mathrm{i}\frac{\hbar k^2}{2m}t + C(k) \tag{19}$$

So we can get the solution:

$$\tilde{G}(k,t) = A(k)\mathrm{e}^{-\mathrm{i}\frac{\hbar k^2}{2m}t}, \quad A(k) = \mathrm{e}^{C(k)} \tag{20}$$

To determine $A(k)$, impose the initial condition at time t_0 in position space:

$$\begin{aligned} \tilde{G}(k,t_0) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x G(x,t_0)\mathrm{e}^{-\mathrm{i}kx} \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x \delta(x-x_0)\mathrm{e}^{-\mathrm{i}kx} \end{aligned} \tag{21}$$

Using the Fourier transform of the Dirac delta, we find:

$$\tilde{G}(k,t_0) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-\mathrm{i}kx_0} \tag{22}$$

Matching at t_0 fixes the k-space amplitude:

$$A(k) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-\mathrm{i}kx_0} \cdot \mathrm{e}^{\mathrm{i}\frac{\hbar k^2}{2m}t_0}. \tag{23}$$

Therefore, for general time t we have:

$$\tilde{G}(k,t) = \frac{1}{\sqrt{2\pi}} e^{-ikx_0} e^{-i\frac{\hbar k^2}{2m}(t-t_0)} \tag{24}$$

Finally, inverse-transform back to position space to obtain the integral representation of the propagator:

$$\begin{aligned} G(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \cdot \tilde{G}(k,t) e^{ikx} \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x-x_0)} \cdot e^{-i\frac{\hbar(t-t_0)}{2m}k^2} \end{aligned} \tag{25}$$

This is a standard Gaussian integral of the form:

$$\int_{-\infty}^{\infty} dk\, e^{-ak^2+bk} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}. \tag{26}$$

Let's identify the coefficients:

$$\begin{cases} a = i\dfrac{\hbar(t-t_0)}{2m} \\ b = i(x-x_0) \end{cases} \tag{27}$$

So we can get the solution:

$$iG(x,t) = \left[\frac{m}{2\pi\hbar i(t-t_0)}\right]^{\frac{1}{2}} \cdot e^{\frac{i}{\hbar}\cdot\frac{m(x-x_0)^2}{2(t-t_0)}} \tag{28}$$

Also, we can solve this PDE via definition:

$$\begin{aligned} iG &= \langle x| e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} |x_0\rangle \\ &= \int \langle x| e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} |p\rangle\langle p|x_0\rangle\, dp \\ &= \int dp\, e^{-\frac{i(t-t_0)p^2}{2m\hbar}} \langle x|p\rangle\langle p|x_0\rangle \\ &= \frac{1}{2\pi\hbar} \int dp\, e^{-\frac{i(t-t_0)p^2}{2m\hbar} + i\frac{(x-x_0)}{\hbar}p}. \end{aligned} \tag{29}$$

we use $P = \hbar k$ and can get the same equation as the Fourier Transform Method.

1.2 Path-Integral

When $t > t_1 > t_0$, and t_1 is an arbitrarily selected intermediate time, we can write:

$$\begin{aligned} \mathrm{i}G(x,t;x_0,t_0) &= \langle x|\hat{U}(t,t_0)|x_0\rangle \\ &= \langle x|\hat{U}(t,t_1)\hat{U}(t_1,t_0)|x_0\rangle \\ &= \int \mathrm{d}x_1 \langle x|\hat{U}(t,t_1)|x_1\rangle\langle x_1|\hat{U}(t_1,t_0)|x_0\rangle \\ &= \int \mathrm{d}x_1\, \mathrm{i}G(x,t;x_1,t_1)\cdot \mathrm{i}G(x_1,t_1;x_0,t_0) \end{aligned} \tag{30}$$

This intergral over x_1 means "superposition" of all possible "path" that connect x and x_0. Next, we try to "smooth" the path along time directly. We can insert more time slices between x and x_0. If we insert infinite time slices, the path become smooth.

Firstly, let's discretize time. domain $[t_0, t]$ into N pieces of equal length $\Delta t = \frac{t-t_0}{N}$:

$$\begin{aligned} \mathrm{i}G(x,t;x_0,t_0) &= \langle x|\hat{U}(t,t_{N-1})\hat{U}(t_{N-1},t_{N-2})\cdots\hat{U}(t_1,t_0)|x_0\rangle \\ &= \int \mathrm{d}x_{N-1}\cdots\mathrm{d}x_1 \prod_{l=1}^{N} \mathrm{i}G(x_l,t_l;x_{l-1},t_{l-1}) \end{aligned} \tag{31}$$

let $\mathcal{D}_x = \prod_{l=1}^{N-1}\mathrm{d}x_l$. Consider $N\to\infty$, so $\Delta t = \frac{t-t_0}{N} \to 0$, which means $t_l - t_{l-1} = \Delta t$.

$$\mathrm{i}G(x_l,t_l;x_{l-1},t_{l-1}) = \langle x_l|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t}|x_{l-1}\rangle \tag{32}$$

Because Δt is small, we can approximate the exponential function by its Taylor series:

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \approx \hat{\mathbb{I}} - \frac{\mathrm{i}}{\hbar}\hat{H}\Delta t = \hat{\mathbb{I}} - \frac{\mathrm{i}}{\hbar}\Delta t\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right] \tag{33}$$

Substitute (33) into (32):

$$\begin{aligned} \mathrm{i}G(x_l,t_l;x_{l-1},t_{l-1}) &= \int \mathrm{d}p_l \langle x_l|p_l\rangle\langle p_l|\hat{\mathbb{I}} - \frac{\mathrm{i}}{\hbar}\Delta t\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]|x_{l-1}\rangle \\ &= \int \mathrm{d}p_l \langle x_l|p_l\rangle\langle p_l|x_{l-1}\rangle \left[1 - \frac{\mathrm{i}}{\hbar}\left(\frac{p_l^2}{2m} + V(x_{l-1})\right)\Delta t\right] \end{aligned} \tag{34}$$

With the approximations $V(x_l) \approx V(x_{l-1})$:

$$\left[1 - \frac{\mathrm{i}}{\hbar}\left(\frac{p_l^2}{2m} + V(x_{l-1})\right)\Delta t\right] \approx \left(1 - \frac{\mathrm{i}}{\hbar}H_l\Delta t\right) \approx \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_l\Delta t} \tag{35}$$

So $\mathrm{i}G(x_l,t_l;x_{l-1},t_{l-1})$ can be written as:

$$\begin{aligned} \mathrm{i}G(x_l,t_l;x_{l-1},t_{l-1}) &= \int \mathrm{d}p_l \frac{1}{2\pi\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_l(x_l-x_{l-1})}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_{cl}\Delta t} \\ &= \frac{1}{2\pi\hbar}\int \mathrm{d}p_l e^{\frac{\mathrm{i}}{\hbar}[p_l(x_l-x_{l-1})-H_l\Delta t]} \\ &= \frac{1}{2\pi\hbar}\int \mathrm{d}p_l \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[p_l(\frac{x_l-x_{l-1}}{\Delta t})-H_l]\Delta t} \end{aligned} \tag{36}$$

where, H_l is the classical Hamiltonion as a function of p_l and x_l.

When $\Delta t \to 0$:

$$\frac{x_l - x_{l-1}}{\Delta t} = \dot{x}_l \tag{37}$$

So we can get:

$$p_l \dot{x}_l - H_l = \mathcal{L}_l. \tag{38}$$

where, $\mathcal{L}_l$ is the classical Lagrangian.

So $\mathrm{i}G(x_l, t_l; x_{l-1}, t_{l-1})$ can be written as the form with Lagrangian:

$$\mathrm{i}G(x_l, t_l; x_{l-1}, t_{l-1}) = \int \mathrm{d}p_l \cdot \frac{1}{2\pi\hbar} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{L}_l \Delta t}. \tag{39}$$

Substitute $\mathrm{i}G(x_l, t_l; x_{l-1}, t_{l-1})$ into the path integral:

$$\prod_{l=1}^{N} \mathrm{i}G(x_l, t_l; x_{l-1}, t_{l-1}) = \int \frac{\mathrm{d}p_N}{2\pi\hbar} \cdots \frac{\mathrm{d}p_1}{2\pi\hbar} \cdot \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sum_{l=1}^{N} \mathcal{L}_l \cdot \Delta t} \tag{40}$$

let $\mathcal{D}_p = \prod_{l=1}^{N} \frac{\mathrm{d}p_l}{2\pi\hbar}$, when $\Delta t \to 0$, which means:

$$\sum_{l=1}^{N} \mathcal{L}_l \Delta t = \int_{t_0}^{t} \mathrm{d}\tau \cdot \mathcal{L}[p(\tau), x(\tau)] \tag{41}$$

Finally, we can get the propagators by the path integral:

Theorem 1.1. *The propagators path integral:*

$$\mathrm{i}G(x, t; x_0, t_0) = \int \mathcal{D}_x \mathcal{D}_p \cdot \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} \mathrm{d}\tau \cdot \mathcal{L}[p(\tau), x(\tau)]} \tag{42}$$

where, the pair of $p(t)$ and $\dot{x}(t)$ characterizes a path in the px phase space.