Path Integral in Quantum Mechanics

particle in time-dependent potential $V(x,t)$

Hamiltonian operator: $\hat{H}(t) = \frac{1}{2m}\hat{P}^2 + V(\hat{X},t)$

coordinate eigenstate: $|x\rangle$

$$\langle x|p\rangle = e^{ipx}$$

momentum eigenstate: $|p\rangle$

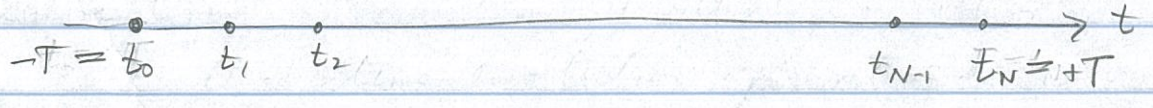
completeness relations:

$$\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = \mathbb{1} = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\, |p\rangle\langle p|$$

amplitude for particle that is at position x_i at time $t=-T$ to be at position x_f at time $t=T$:

$$\langle x_f|U(T,-T)|x_i\rangle = \langle x_f|\,T\exp\left(-i\int_{-T}^{T} dt\, \hat{H}(t)\right)|x_i\rangle$$

Break time interval $2T$
into N subinterval of length δt: $2T = N\delta t$



express transition operator as product of N factors.

$$\langle x_f | U(T,-T) | x_i \rangle = \langle x_f | U(T, t_{N-1})\, U(t_{N-1}, t_{N-2}) \cdots U(t_2, t_1)\, U(t_1, -T) | x_i \rangle$$

Insert complete set of coordinate eigenstates
between each pair of operators

$$1 = \int_{-\infty}^{\infty} dx_j \; |x_j\rangle \langle x_j|$$

$$\langle x_f | U(T,-T) | x_i \rangle = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_{N-1} \; \langle x_f | U(t_N, t_{N-1}) | x_{N-1} \rangle$$

$$\times \cdots \langle x_2 | U(t_2, t_1) | x_1 \rangle \langle x_1 | U(t_1, t_0) | x_i \rangle$$

make approximations in each factor
that have an error of order $(\delta t)^2$
then the product will have an error of order $N(\delta t)^2$

$$N(\delta t)^2 = N\left(\frac{2T}{N}\right)^2 = \frac{4T^2}{N} \longrightarrow 0 \quad \text{as} \quad N \to \infty$$

$$\text{operator}: \; U(t_j, t_{j+1}) = T\exp\left(-i \int_{t_j}^{t_{j+1}} \hat{H}(t)\, dt\right)$$

$$= \exp\left(-i\, \hat{H}(t_j)\, \delta t + O((\delta t)^2)\right)$$

$$= \mathbb{1} - i\, \hat{H}\, \delta t + O((\delta t)^2)$$

matrix element

$$\langle x_{j+1} | U(t_{j+1}, t_j) | x_j \rangle = \langle x_{j+1} | \left(\mathbb{1} - i H(t_j) \delta t \right) | x_j \rangle + O((\delta t)^2)$$

$$= \langle x_{j+1} | \left(\mathbb{1} - i \left[\tfrac{1}{2m} \hat{P}^2 + V(\hat{X}, t_j) \right] \delta t \right) | x_j \rangle + O((\delta t)^2)$$

insert complete set of momentum eigenstates after $\langle x_{j+1}|$

$$\mathbb{1} = \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} |p_j\rangle \langle p_j|$$

$$\langle x_{j+1} | \left(\mathbb{1} - i \left[\tfrac{1}{2m} \hat{P}^2 + V(\hat{X}) \right] \delta t \right) | x_j \rangle$$

$$= \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} \langle x_{j+1} | p_j \rangle \langle p_j | \left(\mathbb{1} - i \left[\tfrac{1}{2m} \hat{P}^2 + V(\hat{X}, t_j) \right] \delta t \right) | x_j \rangle$$

$$= \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} \langle x_{j+1} | p_j \rangle \left(1 - i \left[\tfrac{1}{2m} p_j^2 + V(x_j, t) \right] \delta t \right) \langle p_j | x_j \rangle$$

$$= \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} e^{i p_j x_{j+1}} e^{-i p_j x_j} \left(1 - i \left[\tfrac{1}{2m} p_j^2 + V(x_j, t) \right] \delta t \right)$$

$$= \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} e^{i p_j (x_{j+1} - x_j)} e^{-i \left[\frac{1}{2m} p_j^2 + V(x_j, t) \right] \delta t} + O((\delta t)^2)$$

The integral over p_j is a Gaussian integral that can be evaluated analytically

$$\int_{-\infty}^{\infty} \frac{dp_j}{2\pi} e^{-i \frac{p_j^2}{2m} \delta t + i p_j (x_{j+1} - x_j)}$$

$$= \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} e^{-\frac{i}{2m} \left(p_j - \frac{m(x_{j+1} - x_j)}{\delta t} \right)^2 \delta t + \frac{im}{2} \frac{(x_{j+1} - x_j)^2}{\delta t}} = \sqrt{\frac{m}{2\pi i \delta t}}\, e^{i \frac{m}{2} (x_{j+1} - x_j)^2 / \delta t}$$

The matrix element is therefore

$$\langle x_{j+1} | U(t_{j+1}, t_j) | x_j \rangle$$

$$= \sqrt{\frac{m}{2\pi i \delta t}} \exp\left(i \frac{m}{2} \frac{(x_{j+1}-x_j)^2}{\delta t} \right) \exp\left(-i V(x_j, t_j) \delta t \right) + O((\delta t)^2)$$

$$= \sqrt{\frac{m}{2\pi i \delta t}} \exp\left(i \left[\frac{1}{2} m \left(\frac{x_{j+1}-x_j}{\delta t} \right)^2 - V(x_j, t_j) \right] \delta t \right) + O((\delta t)^2)$$

$$= \sqrt{\frac{m}{2\pi i \delta t}} \exp\left(i L\left(x_j, \frac{x_{j+1}-x_j}{\delta t}, t\right) \delta t \right) + O((\delta t)^2)$$

In the complete matrix element, there are N such factors

$$\langle x_f | U(T, -T) | x_i \rangle$$

$$= \left(\sqrt{\frac{m}{2\pi i \delta t}} \right)^N \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp\left(i \sum_{j=1}^{N} L\left(x_j, \frac{x_{j+1}-x_j}{\delta t}, t\right) \delta t \right) + O\left(N (\delta t)^2\right)$$

In the limit $N \to \infty$, the error goes to 0

The discretized path $(x_0, x_1, \ldots, x_{N-1}, x_N)$

approaches a continuous path $x(t)$

with boundary values $x(-T) = x_i$, $x(T) = x_f$

The integral over $x_1, \ldots, x_{N-1}$

approaches an integral over the function $x(t)$

$$\langle x_f | U(T, -T) | x_i \rangle$$

$$\longrightarrow \mathcal{N} \int_{\substack{x(T)=x_f \\ x(-T)=x_i}} \mathcal{D}x \exp\left(i \int_{-T}^{+T} dt\, L(x(t), \dot{x}(t), t) \right)$$

The prefactor $\mathcal{N}$ does not have a well-behaved limit as $N \to \infty$.

matrix element of time ordered product of evolution operator and coordinate operator

$$\langle x'| \mathcal{T} \exp\left(-i\int_{-T}^{+T} dt\, \hat{H}(t)\right) \hat{X}(t_0) |x\rangle$$

$$= \langle x'| U(+T, t_0)\, \hat{X}\, U(t_0, -T) | x\rangle \qquad \text{if } -T < t_0 < +T$$

insert complete set of coordinate eigenstates

$$= \langle x'| U(+T, t_0) \Big(\int_{-\infty}^{\infty} dx_0 \underbrace{|x_0\rangle\langle x_0|\big) \hat{X}}_{x_0 \langle x_0|}\, U(t_0, -T) | x\rangle$$

$$= \int_{-\infty}^{\infty} dx_0\; x_0\, \langle x'| U(+T, t_0) | x_0\rangle \langle x_0 | U(t_0, -T) | x\rangle$$

$$= \int_{-\infty}^{\infty} dx_0\; x_0\, N(T, t_0) \int \mathcal{D}x\, e^{i\int dt\, L(t)}\, N(t_0, -T) \int \mathcal{D}x\, e^{i\int dt\, L(t)}$$

$$= \underbrace{N(T, t_0)\, N(t_0, -T)}_{N(T, -T)} \int \mathcal{D}x\; e^{i\int_{-T}^{+T} dt\, L(t)}\; x(t_0)$$

generalization to two coordinate operators

$$\langle x'| \mathcal{T}\left(\exp\left(-i\int_{-T}^{+T} dt\, \hat{H}(t)\right) \hat{X}(t_1) \hat{X}(t_2)\right) | x\rangle$$

$$= N \int \mathcal{D}x\; e^{i\int_{-T}^{T} dt\, L(t)}\; \underbrace{X(t_1)\, X(t_2)}$$

no explicit time ordering
time ordering provided automatically by path integral

Suppose $V(x,t) \longrightarrow V_0(x)$ as $t \longrightarrow \pm\infty$

The Hamiltonian $H_0 = \frac{1}{2}m\dot{x}^2 + V_0(x)$

has a ground state $|E_0\rangle$ with energy E_0

wavefunction $\langle x|E_0\rangle$

transition amplitude from $|x_i\rangle$ at time $-T$

to $|x_f\rangle$ at time $+T$

$$\langle x_f|\,U(+T,-T)\,|x_i\rangle = \mathcal{N}\int_{\substack{x(-T)=x_i\\ x(+T)=x_f}} \mathcal{D}x\ \exp\left(i\int_{-T}^{+T} dt\, L(x,\dot{x},t)\right)$$

analytically continue in initial and final time

$$+T \longrightarrow +T(1-i\epsilon)$$

$$-T \longrightarrow -T(1-i\epsilon)$$

Time evolution operator $e^{-iH_0T(1-i\epsilon)}$

includes factor $e^{-\epsilon H_0 T}$ that suppresses all other energy eigenstates relative to the ground state as $T\to\infty$

$$\langle x_f|\,U(+T,-T)\,|x_i\rangle \longrightarrow \langle x_f|E_0\rangle\langle E_0|\,U(+T,-T)\,|E_0\rangle\langle E_0|x_i\rangle$$

Limit $T\to\infty$ followed by $\epsilon\to 0$

gives ground-state-to-ground-state amplitude

multiplied by ground-state wavefunctions extra factors cancel out in ratio of matrix element

$$\frac{\langle E_0 | T\, U(+\infty,-\infty)\, \hat{X}(t_1)\, \hat{X}(t_2) | E_0 \rangle}{\langle E_0 | T\, U(+\infty,-\infty) | E_0 \rangle}$$

$$= \frac{\int \mathcal{D}x \, \exp\left(i \int_{-\infty}^{\infty} dt\, L(x,\dot{x},t) \right) x(t_1)\, x(t_2)}{\int \mathcal{D}x \, \exp\left(i \int_{-\infty}^{\infty} dt\, L(x,\dot{x},t) \right)}$$

where $\int_{-\infty}^{\infty} dt \equiv \lim_{\epsilon \to 0} \lim_{T \to \infty} \int_{-T(1-i\epsilon)}^{+T(1-i\epsilon)} dt$