Path Integrals and semiclassical Propagator

Path Integral for single particle QM:

Propagator $K = \langle x_N | e^{-iHt} | x_0 \rangle$

$$= \langle x_N | e^{-i\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]t} | x_0 \rangle$$

$\hat{p}$ and $\hat{x}$ don't commute $\rightarrow$ Trotterize

$$= \langle x_N | \left[e^{-i\epsilon\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]}\right]^N | x_0 \rangle$$

$N \rightarrow \infty$
$\epsilon \rightarrow 0$ s.t.
$N\epsilon = t$

$$= \langle x_N | e^{-i\epsilon\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]} | x_{N-1} \rangle$$
$$\langle x_{N-1} | e^{-i\epsilon\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]} | x_{N-2} \rangle$$
$$\vdots$$
$$\langle x_1 | e^{-i\epsilon\left\{\frac{\hat{p}^2}{2m} + V(\hat{x})\right\}} | x_0 \rangle$$

Now

$$\langle x_{j+1} | e^{-i\epsilon\left[\hat{p}^2/2m + V(\hat{x})\right]} | x_j \rangle = \int dp \, \langle x_{j+1} | e^{-i\epsilon\frac{\hat{p}^2}{2m}} | p \rangle \langle p | e^{-i\epsilon V(\hat{x})} | x_j \rangle$$

$$= \int dp \; e^{-i\epsilon\frac{p^2}{2m}} \, e^{-i\epsilon V(x)} \, e^{ip(x_{j+1} - x_j)}$$

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

$$\Rightarrow K(x_N, x_0, t)$$

$$= \lim_{\substack{N\to\infty \\ N\epsilon = t}} \left[\frac{m}{2\pi i\epsilon}\right]^{N/2} \int dx_1 \cdots dx_{N-1} \exp\left[i\epsilon \left(\sum_{j=0}^{N-1} \frac{m(x_{j+1}-x_j)}{2\epsilon^2} - V(x_j) \right)\right]$$

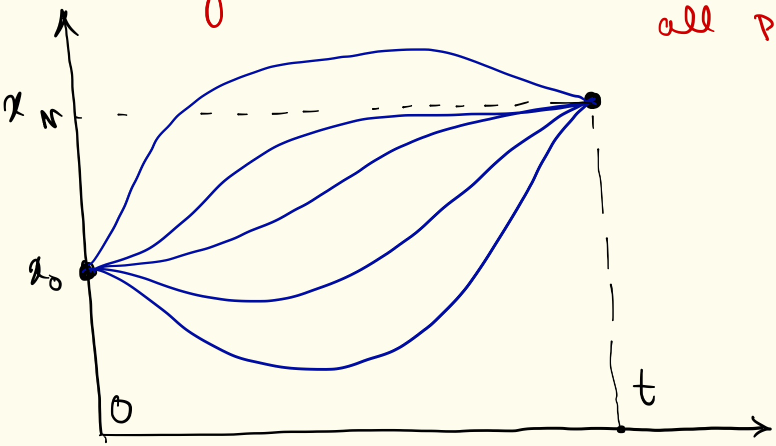
$$\sim \int Dx(t) \exp i\int_0^t dt \left[\frac{m\dot{x}^2}{2} - V(x)\right]$$

"Functional Integral"

$$= \int Dx(t) \exp\left[i \int L(x, \dot{x})\, dt \right]$$

with $x(t=0) = x_0$ and $x(t) = x_N$.

Pictorially: sum of exp(i action) over all paths.



Above, we didn't make any approximation. Now, lets consider the semiclassical limit and relate it to Gutzwiller's formula.

To derive the semiclassical propagator, we will make a stationary phase approximation. As a warm-up towards it, consider a 1-dimensional integral:

$$I = \int dx \quad e^{i\varphi(x)/a}$$ where 'a' is a positive number. As $a \to 0$ the integrand varies rapidly and the integral is dominated by those portions of a the integrand, i.e, where integrand varies the least

$$\left.\frac{d\varphi}{dx}\right|_{x_0} = 0 .$$

There may be many (including infinitely many) solutions to this eqn. and one has to add contributions from all of them.

Expanding the integrand around one such point

$$\int dx\, e^{i\varphi(x)/a} = \exp\left[\frac{i}{a}\left[\varphi(x_0) + \frac{(x-x_0)^2}{2}\varphi''(x_0) + \cdots\right]\right]$$

$$= \int d(x-x_0)\, \exp\left[\frac{i\varphi(x_0)}{a} + \frac{(x-x_0)^2}{2}\varphi''(x_0) + \cdots\right]$$

$$= \sqrt{\frac{2\pi i a}{\varphi''(x_0)}}\; e^{i\varphi(x_0)/a}$$

Let's write the prefactor to the exponential as

$$\sqrt{\frac{2\pi i a}{\varphi''(x_0)}} = \sqrt{\frac{2\pi i a\ \mathrm{sign}[\varphi''(x_0)]}{|\varphi''(x_0)|}}$$

$$= e^{i[\pi/4\ \mathrm{sign}\,\varphi''(x_0)]} \sqrt{\frac{2\pi a}{|\varphi''(x_0)|}}.$$

As mentioned above, there may be several saddle points. Denoting various such saddles by an index b.

$$I = \sum_b e^{i\nu_b \pi/4} \sqrt{\frac{2\pi a}{|\varphi''(x_b)|}}\, e^{\frac{i\varphi(x_b)}{a}}$$

where $\nu_b = \text{sign}(\varphi''(x_b))$.

To consider application to the path integral, we need to study the

Multi-dimensional version:

Let $x = (x_1 \ldots x_n)$

$$I_n = \int dx_1 \ldots dx_n \, e^{i\varphi(x)/a} \equiv \int d^n x \, e^{i\varphi(x)/a}$$

The stationary phase points are $\frac{\partial \varphi}{\partial x_i} = 0$ $\forall\ i = 1, 2, \ldots n$. Expanding φ to second order around such points,

$$\varphi(x) = \varphi(x_0) + \frac{1}{2}\sum_{ij}(x_i - x_{i0})(x_j - x_{j0}) \frac{\partial^2 \varphi}{\partial x_i \partial x_j}$$

Thus, the multi-dimensional integral is still Gaussian:

$$\int d^n x \, e^{i\varphi(x)/a} = e^{i\varphi(x_0)} \int d^n y \, \exp \left[\frac{i}{2a} y_i y_j \frac{\partial^2 \varphi}{\partial y_i \partial y_j}\Big|_{y_0}\right]$$

where $\vec{y} = \vec{x} - \vec{x}_0$.

$$= \int d^n y \quad \exp \quad \frac{i}{2a} \left[y^T M y \right]$$

where $\quad M_{ij} = \left.\frac{\partial^2 \varphi}{\partial y_i \, \partial y_j}\right|_{y_0}$.

Diagonalizing $\quad y^T M y = z^T D z$

where D is a diagonal matrix. The Jacobian is 1 because $y = Rz$ where R is orthogonal. Thus,

$$I_n = e^{i\varphi(x_0)/a} \int d^n z \; e^{\frac{i}{2a} \sum_k D_k z_k^2}$$

$$= e^{i\varphi(x_0)/a} \prod_k \left[\sqrt{\frac{2\pi a i}{D_k}} \right]$$

$$= e^{i\varphi(x_0)/a} \frac{(2\pi a)^{n/2}}{\prod_k \sqrt{|D_k|}} \prod_k \left[i^{\operatorname{sign}(D_k)} \right]^{1/2}$$

$$= e^{i\varphi(x_0)/a} \frac{(2\pi a)^{n/2}}{\sqrt{|\operatorname{Det}(M)|}} \; e^{i\nu\pi/4}$$

where ν = # of positive eigenvalues of M
— # of negative " " "

Finally, summing over all such saddle points,

$$I_a = \sum_b e^{i\nu_b \pi/4} (2\pi a)^{n/2} \left|\det\left(\frac{\partial^2 \phi}{\partial x_i \partial x_j}\right)\right|^{-1/2} e^{i\phi(x_b)/a}$$

Application to the Path Integral

$$S(x_0, x_1, \ldots x_N) = \epsilon \sum_{j=0}^{N-1} \left[\frac{m}{2} \left[\frac{x_{j+1} - x_j}{\epsilon}\right]^2 - V(x_j) \right]$$

$$\frac{\partial^2 S}{\partial x_k \partial x_l} = \frac{m}{\epsilon} \left[2\delta_{kl} - \delta_{k+1,l} - \delta_{k-1,l} - \frac{\epsilon^2}{m} V''(x_k)\delta_{kl} \right]$$

There is a very simple and interesting result:

$$\det\left(\frac{\partial^2 S}{\partial x_k \partial x_l}\right) = -\left[\frac{m}{\epsilon}\right]^N \left[\frac{\partial^2 S}{\partial x_0 \partial x_N}\right]^{-1}$$

Thus the determinant is just proportional to $\frac{\partial^2 S}{\partial x_0 \partial x_N}$! To determine the overall phase,

we need $\nu = \#$ of positive eigenvalues of $\frac{\partial^2 S}{\partial x_k \partial x_l}$ (ν_+) $-$ # of negative eigenvalues of $\frac{\partial^2 S}{\partial x_k \partial x_l}$ (ν_-)

Recall the expression for the pathintegral :

$$K(x_N, x_0, t)$$

$$= \lim_{\substack{N \to \infty \\ N\epsilon = t}} \left[\frac{m}{2\pi i \epsilon}\right]^{N/2} \int dx_1 \ldots dx_{N-1} \exp\left[i\epsilon\left(\sum_{j=0}^{N-1} \frac{m(x_{j+1}-x_j)}{2\epsilon^2} - V(x_j)\right)\right]$$

Thus, the overall phase is

$$e^{-\frac{i\pi}{4}N} \quad e^{i\nu\pi/4}$$

$$\nu_+ + \nu_- = N-1$$

$$\Rightarrow \nu = \nu_+ - \nu_- = N-1-2\nu_-$$

$$\Rightarrow \quad e^{-i\pi/4 N + i\nu\pi/4} = e^{-i\pi/4 N} \, e^{i\frac{\pi}{4}[N-1-2\nu_-]}$$

$$= e^{-i\pi/4} \; e^{-i\nu - \pi/2}.$$

Thus, we need only keep track of the number of negative eigenvalues of $\frac{\partial^2 S}{\partial x_k \partial x_l}$ along a classical trajectory.

This leads to the Van-Vleck formula:

$$K(x_N, x_0, t) = \sum_b \frac{e^{-i\nu_b - \frac{\pi}{2}}}{\sqrt{2\pi i}} \left| \frac{\partial^2 S_b}{\partial x_N \partial x_0} \right|^{1/2} e^{i S_b(x_N, x_0, t)}$$

where the sum is over all classical paths connecting x_b to x_a.

For a d-dimensional problem:

$$K = \sum_b \frac{e^{i\nu_b \pi/2}}{(2\pi i)^{d/2}} \left| \det \frac{\partial^2 S_b}{\partial \vec{x}_N \partial \vec{x}_0} \right| \exp(i S_b)$$

This formula is exact when

$$V(x) = a_0 + a_1 x + a_2 x^2 .$$

Intuition for Van Vleck's formula

$F(T)$ has a very important physical meaning: $|F|^2$ is the probability density to transition from x_0 to x_N in time t.

To determine this probability, consider the fan of classical trajectories from x_0 to x_N with ranging velocities at $t=0$. The variation in momenta is given by:

$$\delta p_a = m\, \delta \dot{x}_0 (t=0)$$

Since
$$m \frac{d^2 x}{dt^2} = -\frac{\partial V}{\partial x}$$

$$\Rightarrow \quad m \frac{d^2 \delta x}{dt^2} = -\left.\frac{\partial^2 V}{\partial x^2}\right|_{x_{cl}(t)} \delta x$$

The spread of initial momenta determine the spread of x_N at t, the more the spread, the lower the probability.

To determine δx_N, recall,

$$\frac{\partial S}{\partial x_0} = -P_0$$

$$\Rightarrow \frac{\partial^2 S}{\partial x_0 \partial x_N} = -\frac{\partial P_0}{\partial x_N}$$

$$\Rightarrow \delta P_0 = -\delta x_N \frac{\partial^2 S}{\partial x_0 \partial x_N}$$

$$\Rightarrow \delta x_N = -\delta p_0 \underbrace{\left[\frac{\partial^2 S}{\partial x_0 \partial x_N}\right]^{-1}}_{\text{inverse prob. of finding particle at } x_N \text{ after time } t \text{ starting at } x_0}$$

$$\Rightarrow |F(t)|^2 \sim \frac{\partial^2 S}{\partial x_0 \partial x_N}$$