Review of path integrals for single particle QM: in one dimension

Consider particle with Hamiltonian $H = p^2/2m + V(x)$

and the amplitude $K(x' t', x t) = \langle x' | e^{-iH(t'-t)} | x \rangle$

to go from $(x\, t)$ to $(x'\, t')$.

$$\langle x' | e^{-iH(t'-t)} | x \rangle$$

$$= \prod_{i=1}^{N-1} \int dx_i \, \langle x' | e^{-i\epsilon H} | x_{N-1} \rangle \langle x_{N-1} | e^{-i\epsilon H} | x_{N-2} \rangle$$

$$\cdots \langle x_1 | e^{-i\epsilon H} | x \rangle .$$

with $N\epsilon = t' - t$.

$$\langle x_{j+1} | e^{-i\epsilon H} | x_j \rangle = \langle x_{j+1} | e^{-i\epsilon\left(p^2/2m + V(x)\right)} | x_j \rangle$$

If $N \to \infty$, $\epsilon \to 0$, $e^{-i\epsilon(T+V)} \approx \left(e^{-i\epsilon T}\right)\left(e^{-i\epsilon V}\right)$

with errors of $o(\epsilon^2)$.

$$\therefore \langle x_{j+1} | e^{-i\epsilon H} | x_j \rangle \xrightarrow{\epsilon \to 0} \langle x_{j+1} | e^{-i\epsilon p^2/2m} | x_j \rangle \, e^{-i\epsilon V(x_j)}$$

$$= \int_{-\infty}^{\infty} \frac{dp_j}{2\pi} \, e^{i p_j (x_{j+1} - x_j) - i\epsilon p_j^2/2m} \, e^{-i\epsilon V(x_j)} .$$

$$= \sqrt{\frac{2m\pi}{i\epsilon}} \, e^{+i \frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\epsilon} - i\epsilon V(x_j)}$$

$$\therefore K(x' t', x t) = \lim_{\substack{\epsilon \to 0 \\ N \to \infty \\ N\epsilon = t' - t}} \prod_{i=1}^{N-1} \left(\frac{2m\pi}{i\epsilon} \right)^{(N-1)} e^{+i \sum_{j=1}^{N-1} \left[\frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\epsilon} - \epsilon V(x_j) \right]}$$

$$= \int_{x(t)}^{x'(t')} [\mathcal{D} x(t)] \, e^{+i \int dt \left[\frac{m}{2} \left(\frac{dx}{dt} \right)^2 - V(x) \right]}$$

Can extract a lot of information about the quantum system by studying $K(x't', xt)$

In operator formulation

$$K(x't'\ xt) = \langle x' | e^{-iH(t'-t)} | x \rangle$$

$$= \sum_n \langle x' | n \rangle e^{-iE_n(t'-t)} \langle n | x \rangle$$

where $|n\rangle$ are energy eigenstates with eigenvalue E_n

Define $K(x't'\ xt) = 0$ if $t' < t$.

$$= \langle x' | e^{-iH(t'-t)} | x \rangle \quad \text{for } t' > t.$$

Then ~~K(x~~ Fourier transform

$$K(x'\ x\ \omega + i\epsilon) = \int_{-\infty}^{\infty} d(t'-t)\ e^{i\omega(t'-t)} K(x't'\ xt) e^{-\epsilon(t'-t)}$$

$(\epsilon > 0)$

$$= \sum_n \frac{\langle x' | n \rangle \langle n | x \rangle}{i(\omega - E_n + i0^+)}$$

Define $G(x't' \; xt) = i\, K(x't' \; xt)$

$$G(x' x, \omega) = i\, K(x' x\, \omega)$$

$$= \sum_n \frac{\langle x'|n\rangle\langle n|x\rangle}{\omega - E_n + i0^+}$$

G (or equivalently K) is known as the propagator.

The poles of the propagator (in frequency) are at the locations of the energy eigenvalues.

Example: Free particle $H = p^2/2m$

Directly $K(x't' \; xt) = \langle x'|\, e^{-i\, p^2/2m\, (t'-t)}\, |x\rangle$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \langle x'|p\rangle\langle p|x\rangle\, e^{-i\, p^2/2m\, (t'-t)}$$

$$= \int_{-\infty}^{\infty} dp/2\pi \; e^{ip(x'-x) - i\, p^2/2m\, (t'-t)}$$

$$= \sqrt{\frac{2m\pi}{i(t'-t)}}\; e^{i\, m/2\, \frac{(x'-x)^2}{t'-t}}$$

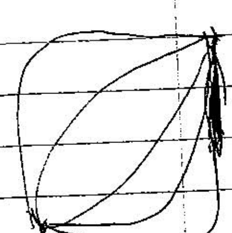
<u>Semiclassical limit</u> If we kept $\hbar$ in our derivation of the path integral, get

$$K(x't';xt) = \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}\int dt \left[\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x)\right]}$$

~~Tho~~ Note that the amplitude for a path is

$e^{iS/\hbar}$ where S is the classical action $= \int dt\, L$

evaluated along the path.



In the semiclassical limit $\hbar \to 0$, we may "evaluate" the integral by the stationary phase method, i.e focus on those trajectories where the action S is an extremum. These are the <u>classical</u> trajectories available for the particle* (as is presumably familiar from classical mechanics).

Thus as $\hbar \to 0$, sum over all possible paths reduces to sum over just the available classical trajectories of the particle.

Proof of *: Let $x = x_c(t)$ be an extremum path.

Vary about $x_c(t)$ i.e write $x = x_c(t) + \delta x(t)$

with $\delta x(t_{in}) = 0 = \delta x(t_{fin})$.

$$S[x(t)] = \int dt \, \frac{m}{2}\left(\frac{dx_{cl}}{dt} + \frac{d\delta x}{dt}\right)^2 - V(x_{cl} + \delta x)$$

$$= \underbrace{\int dt \left[\frac{m}{2}\left(\frac{dx_{cl}}{dt}\right)^2 - V(x_{cl})\right]}_{S[x_{cl}(t)]} + \int dt \left[m\frac{dx_{cl}}{dt}\frac{d\delta x}{dt} - V'(x_{cl})\,\delta x\right]$$

$$+ O(\delta x)^2$$

$$\equiv S_{cl} - \int dt \, \delta x(t) \left[m\frac{d^2x_{cl}}{dt^2} + V'(x_{cl})\right]$$

$$\frac{\delta S}{\delta(\delta x)} = 0 \Rightarrow m\frac{d^2x_{cl}}{dt^2} = -V'(x_{cl}) \Rightarrow$$ classical Newton eqns of motion.

Path integrals & statistical mechanics

The partition function of quantum stat. mech is $Z = tr(e^{-\beta H})$

The operator $e^{-\beta H}$ is formally e^{-itH} evaluated for $t = -i\beta$ (i.e for imaginary time).

Consider again a single particle with Hamiltonian

$$H = \vec{p}^{\,2}/2m + V(\vec{x})$$ at a finite temperature.

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right)$$

$$= \int d^d x \, \langle x | e^{-\beta H} | x \rangle$$

Follow same procedure as above to express this as a path-integral

$$Z = \int d^d x \, \langle x | \left(e^{-\epsilon H}\right)^N | x \rangle \quad \text{with } N\epsilon = \beta$$

$$Z = \int d^d x \prod_{j=1}^{N} dx_j \left\langle x \middle| e^{-\epsilon H} \middle| x_N \right\rangle \left\langle x_N \middle| e^{-\epsilon H} \middle| x_{N-1} \right\rangle$$

$$\cdots \left\langle x_{j+1} \middle| e^{-\epsilon H} \middle| x_j \right\rangle$$

$$\cdots \left\langle x_1 \middle| e^{-\epsilon H} \middle| x \right\rangle$$

$$\left\langle x_{j+1} \middle| e^{-\epsilon H} \middle| x_j \right\rangle = \left\langle x_{j+1} \middle| e^{-\epsilon \left(p^2/2m + V(x) \right)} \middle| x_j \right\rangle$$

$$\approx \left\langle x_{j+1} \middle| e^{-\epsilon p^2/2m} e^{-\epsilon V(x)} \middle| x_j \right\rangle$$

as $\epsilon \to 0$

$$= \left\langle x_{j+1} \middle| e^{-\epsilon p^2/2m} \middle| x_j \right\rangle e^{-\epsilon V(x_j)}$$

$$= \int \frac{d^d p_j}{(2\pi)^d} e^{i p_j (x_{j+1} - x_j)} e^{-\epsilon p_j^2/2m} e^{-\epsilon V(x_j)}$$

$$= \left(\frac{2m\pi}{\epsilon} \right)^{d/2} e^{-\frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\epsilon} - \epsilon V(x_j)}$$

$$Z = \lim_{\substack{N\to\infty \\ \epsilon\to 0 \\ N\epsilon=\beta}} \int \prod_{j=0}^{N} dx_j \left(\frac{2m\pi}{\epsilon}\right)^{\frac{Nd}{2}} e^{-\sum_{j=0}^{N}\left[\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\epsilon} + \epsilon V(x_j)\right]}$$

with $x_{N+1} = x_0$.

$$Z \equiv \int_{x(\beta)=x(0)} \left[\mathcal{D}x(\tau)\right] e^{-\int_0^\beta d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)\right]} .$$

Thus can express ~~path into~~ partition function as a path integral over trajectories in "imaginary-time" in a slab 0 to β with periodic boundary conditions.

Aside

Evaluation of imaginary time path integral for SHO

. Consider $Z = \mathrm{Tr}\, e^{-\beta H}$ with $H = p^2/2m + \frac{1}{2} m\omega^2 x^2$

$$= \int dx_0\, K(x_0, x_0; \beta)$$

$$K_\omega(x_0, x_0; \beta) = \int_{\substack{x(\beta) = x_0 \\ x(0) = x_0}} [\mathcal{D}x(\tau)]\; e^{-\int_0^\beta d\tau\, m/2 \left[\left(\frac{dx}{d\tau}\right)^2 + \omega^2 x^2\right]}.$$

First find "classical" path $x_{cl}(\tau)$ determined by minimizing the action:

$$\frac{d^2 x_{cl}}{d\tau^2} = \omega^2 x_{cl}$$

$$\Rightarrow \quad x_{cl}(\tau) = a \cosh \omega\tau + b \sinh \omega\tau$$

$$x_{cl}(0) = x_0, \quad x_{cl}(\beta) = x_0$$

$$\Rightarrow \quad a = x_0, \quad b = x_0 \tanh \frac{\beta\omega}{2}.$$

Now expand general $x(\tau) = x_{cl} + x'(\tau)$

$$x'(0) = x'(\beta) = 0$$

Expand x' in Fourier series with these boundary conditions:

$$x'(\tau) = \sum_n x_n \sin\left(\frac{n\pi\tau}{\beta}\right).$$

Then
$$K_\omega(x_0, x_0, \beta) = A\left(\int \prod_{n=1}^{\infty} dx_n\right)\left(e^{-S_{cl} - \sum_n \frac{m}{4}\left(\frac{n^2\pi^2}{\beta^2} + \omega^2\right)x_n^2}\right)$$

where A = proportionality const. independent of ω.

$$\therefore K_\omega(x_0\, x_0\, \beta) = A' e^{-S_{cl}}\left[\prod_{n=1}^{\infty} \frac{1}{\left(\frac{n\pi}{\beta}\right)^2 + \omega^2}\right]^{1/2}$$

The product is formally ∞ but then the proportionality const. A' is also ∞.

Precise meaning can only be given after

properly "regularizing" the short-time behaviour (in the actual derivation of the path integral this is done by discretizing time & defining carefully the limit as the time spacing goes to zero).

To get around the difficulties associated with the "high frequency" divergence, consider the ratio

$$\frac{K_\omega(x_0\, x_0\, \beta)}{K_0(x_0\, x_0\, \beta)} = \left(\frac{e^{-S_{cl,\omega}}}{e^{-S_{cl,\omega=0}}}\right)\left[\prod_{n=1}^{\infty}\frac{1}{1+\left(\frac{\beta\omega}{n\pi}\right)^2}\right]^{1/2}$$

where the A' cancels & what is left is finite.

Note that for $\omega = 0$ (ie free particle)

$$S_{cl,\omega=0} = 0$$

$$\therefore \text{RHS} = e^{-S_{cl,\omega}}\left(\frac{\beta\omega}{\sinh\beta\omega}\right)^{1/2}$$

$$\therefore\ K_\omega(x_0\, x_0\, \beta) = K_0(x_0\, x_0\, \beta)\, e^{-S_{cl,\omega}} \left(\frac{\beta\omega}{\sinh \beta\omega}\right)^{1/2}$$

$$K_0(x_0\, x_0\, \beta) = \langle x_0 |\, e^{-\beta p^2/2m} \,| x_0 \rangle$$

$$= \int \frac{dp}{2\pi}\, e^{-\beta p^2/2m} = \frac{1}{2\pi}\sqrt{\frac{2\pi m}{\beta}}$$

$$= \sqrt{\frac{m}{2\pi\beta}}$$

$$\therefore\ K_\omega(x_0\, x_0\, \beta) = \left(\sqrt{\frac{m}{2\pi\beta}}\right) e^{-S_{cl,\omega}} \sqrt{\frac{\beta\omega}{\sinh \beta\omega}}$$

$$= \left(\sqrt{\frac{m\omega}{2\pi \sinh(\beta\omega)}}\right) e^{-S_{cl,\omega}}$$

$$S_{cl,\omega} = \int_0^\beta d\tau\, \frac{m}{2}\left[\left(\frac{dx_{cl}}{d\tau}\right)^2 + \omega^2 x_{cl}^2\right]$$

$$= \int_0^\beta d\tau\, \frac{m}{2}\left[\frac{d}{d\tau}\left(x_{cl}\,\dot{x}_{cl}\right) + x_{cl}\cancel{\left(-\frac{d^2 x_{cl}}{d\tau^2} + \omega^2\right) x_{cl}}\right]$$

$$= \frac{m}{2} x_0 \left(\dot{x}_{cl}(\beta) - \dot{x}_{cl}(0) \right).$$

$$\dot{x}_{cl}(\tau) = x_0 \omega \left[Sh(\omega\tau) + \left(\tanh \frac{\beta\omega}{2}\right) \cosh \omega\tau \right]$$

$$\Rightarrow \dot{x}_{cl}(0) = \omega x_0 \tanh \frac{\beta\omega}{2}$$

$$\dot{x}_{cl}(\beta) = \omega x_0 \left[Sh\, \beta\omega + Th\left(\frac{\beta\omega}{2}\right) \cosh \beta\omega \right]$$

$$\dot{x}_{cl}(\beta) - \dot{x}_{cl}(0) = \omega x_0 \left[Sh\, \beta\omega + Th\left(\frac{\beta\omega}{2}\right) \left(\cosh \beta\omega - 1\right) \right]$$

$$= 2\omega x_0\, Sh \frac{\beta\omega}{2} \left[\cosh \frac{\beta\omega}{2} - \tanh\left(\frac{\beta\omega}{2}\right) \sinh \frac{\beta\omega}{2} \right]$$

$$= 2\omega x_0 \tanh\left(\frac{\beta\omega}{2}\right).$$

$$\therefore S_{cl,\omega} = m\omega x_0^2 \tanh\left(\frac{\beta\omega}{2}\right)$$

$$\therefore K_\omega(x_0, x_0, \beta) = \left(\sqrt{\frac{m\omega}{2\pi \sinh(\beta\omega)}} \right) e^{-m\omega x_0^2 \tanh\left(\frac{\beta\omega}{2}\right)}.$$

$$Z[\beta, \omega] = \int dx_0 \, K_\omega(x_0 \, x_0 \, \beta)$$

$$= \left(\sqrt{\frac{m\omega}{2\pi \sinh \beta\omega}} \right) \sqrt{\frac{\pi}{m\omega \tanh(\beta\omega/2)}}$$

$$= \sqrt{\frac{1}{4\left(\sinh \frac{\beta\omega}{2}\right)\left(\cosh \frac{\beta\omega}{2}\right) \cdot \frac{\sinh \beta\omega/2}{\cosh \beta\omega/2}}}$$

$$= \frac{1}{2 \sinh \frac{\beta\omega}{2}}$$

$$= \frac{1}{e^{\beta\omega/2} - e^{-\beta\omega/2}} = \frac{e^{-\beta\omega/2}}{1 - e^{-\beta\omega}}.$$

which is exactly the correct result for a SHO.