Lect 21 Path integral for quantum mechanics

§1 propagator of a point particle.

Consider $H = \frac{p^2}{2m} + V(x)$, and thus the time evolution operator is $\mathcal{U}(t_b, t_a) = e^{-i(t_b - t_a)H}$. Define the propagator

$$i\, G(x_b t_b; x_a t_a) \equiv \langle x_b | \mathcal{U}(t_b, t_a) | x_a \rangle,$$

the it satisfies the following Schrödinger Eq as

$$i\partial_t G(xt; x_a t_a) = \langle x | i\partial_t e^{-i(t-t_a)H} | x_a \rangle = \langle x | H\, \mathcal{U}(t, t_a) | x_a \rangle.$$

H in the coordinate Rep is a function of x and ∂_x, thus

$$\langle x | H\, \mathcal{U}(t, t_a) | x_a \rangle = \int dx'\, \delta(x - x')\, H(x', \partial_{x'})\, \mathcal{U}(t, t_a)\, \delta(x' - x_a)$$

$$= H(x, \partial_x) \int dx'\, \delta(x - x')\, \mathcal{U}(t, t_a)\, \delta(x' - x_a) = H(x, \partial_x) \langle x | \mathcal{U}(t, t_a) | x_a \rangle$$

$$\Rightarrow \boxed{i\partial_t G(xt, x_a t_a) = H(x, \partial_x)\, G(xt, x_a t_a)}$$

Ex: for 1D free space, with the initial condition $G(x t_a; x_a t_a) = -i\delta(x - x_a)$, we have $G(x_b t; x_a t_a) = (-i) \left(\frac{m}{2\pi i t}\right)^{1/2} \exp\left[\frac{i\, m (x_b - x_a)^2}{2t}\right]$.

Hint: Solve the differential Eq. $i\partial_t G(xt, x_a t_a) = \frac{-\hbar^2 \partial_x^2}{2m} G(xt, x_a t_a)$.

§2 Path integral representations of the propagator

$$\mathcal{U}(t_b, t_a) = \mathcal{U}(t_b\, t)\, \mathcal{U}(t, t_a) \Rightarrow i\, G(x_b t_b; x_a t_a) = \int dx\; i G(x_b t_b; x t)\, i G(x t; x_a t_a)$$

let us divide the time interval $[t_b, t_a]$ into N equal segments

$$iG(x_b t_b; x_a t_a) = \int dx_1 \cdots dx_{N-1}\, iG(x_b t_b; x_{N-1} t_{N-1}) \cdots iG(x_1 t_1; x_a t_a)$$

$$= A^N \int \prod_{i=1}^{N-1} dx_i \; \exp\left[i \sum \Delta t \, L\left(t_j, \frac{x_j + x_{j-1}}{2}, \frac{x_j - x_{j-1}}{\Delta t}\right) \right]$$

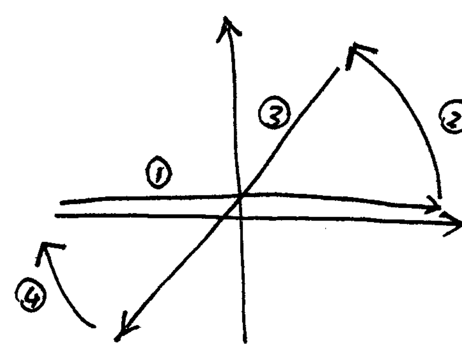
$$iG(x_i t_i, x_{i-1} t_{i-1}) = \langle x_i | \, e^{-i\frac{p^2}{2m}\Delta t} \, e^{-iV(x)\Delta t} \, | x_{i-1} \rangle$$

$$= \int dP_i \, \langle x_i | \, e^{-i\frac{p^2}{2m}\Delta t} \, | P_i \rangle \langle P_i | \, e^{-iV(x)\Delta t} \, | x_{i-1} \rangle$$

$$= \int_{-\infty}^{+\infty} \frac{dP_i}{2\pi} \; e^{-i\frac{P^2}{2m}\Delta t - iV(x)\Delta t} \; e^{+iP_i(x_i - x_{i-1})}$$

using Gauss integral $\displaystyle\int_{-\infty}^{+\infty} dx \, e^{-ax^2} = \sqrt{\frac{\pi}{a}}$

then what's the vaule of $\displaystyle\int_{-\infty}^{+\infty} dx \, e^{-iax^2} = ?$



For the contour $\underbrace{\oint}_{e^{-az^2}dz} = \int_1 + \int_2 + \int_3 + \int_4 = 0$, the contribution from ② and ④ $\longrightarrow 0$

$$\int_{-\infty}^{+\infty} dx \, e^{-ax^2} = \int_{-\infty e^{i\pi/4}}^{+\infty e^{i\pi/4}} dz \; e^{-az^2} = \int_{-\infty}^{+\infty} dy \; e^{-iay^2} \cdot e^{i\pi/4}$$

$$\Rightarrow \boxed{\int_{-\infty}^{+\infty} dy \, e^{-iay^2} = e^{-i\pi/4} \sqrt{\frac{\pi}{a}} = \sqrt{\frac{\pi}{ai}}}$$

$$\Rightarrow iG(x_i t_i, x_{i-1} t_{i-1}) = \left(\frac{m}{2\pi i \Delta t}\right)^{1/2} \exp\left[i \left(\frac{m}{2} \frac{(x_i - x_{i-1})^2}{(\Delta t)^2} - V\left(\frac{x_i + x_{i-1}}{2}\right) \right) \Delta t \right]$$

$$\Rightarrow \quad A = \left(\frac{m}{2\pi i \Delta t}\right)^{1/2} \quad \text{and} \quad \mathcal{L}(t, x, \dot{x}) = \frac{m}{2}\dot{x}^2 - V(x)$$

i.e.

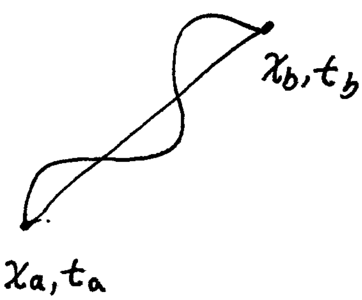
$$iG(x_b t_b, x_a t_a) = \left(\frac{m}{2\pi i \Delta t}\right)^{N/2} \int dx_1 \cdots dx_{N-1} \; e^{i\int_{t_a}^{t_b} dt \left[\frac{m}{2}\dot{x}^2 - V(x)\right]}$$

§ Evalution of the path integral:

We can first find the saddle point solution, which corresponds to the solution of the classic path, and then evaluate the fluctuation parts. Let us consider the free space propagator as an example.

The classic path

$$x_c(t) = x_a + \frac{x_b - x_a}{t_b - t_a}(t - t_a)$$



The action of this part $\int_{t_a}^{t_b} \mathcal{L}\, dt$

$$= \frac{m}{2}\dot{x}^2 (t_b - t_a) = \frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a}$$

The fluctuations $\delta x_j = x_j - x_c(t_j)$, $\left\{\begin{array}{l} x_0 = x_a \\ x_N = x_b \end{array}\right.$ $\quad \delta x_0 = \delta x_N = 0$

$$iG(x_b t_b; x_a t_a) = \left(\frac{m}{2\pi i \Delta t}\right)^{N/2} \int dx_1 \cdots dx_{N-1} \prod_{i=1}^{N} \exp\left[i \frac{m}{2} \frac{(x_i - x_{i-1})^2}{\Delta t}\right]$$

$$\frac{(x_i - x_{i-1})^2}{\Delta t} = \frac{(x_c(t_i) - x_c(t_{i-1}))^2}{\Delta t} + \frac{(\delta x_i - \delta x_{i-1})^2}{\Delta t} + 2(\delta x_i - \delta x_{i-1}) \frac{x_b - x_a}{t_b - t_a}$$

Add together, the linear term of δx_i vanishes,

$$\Rightarrow iG(x_b t_b ; x_a t_a) = \left(\frac{m}{2\pi i \Delta t}\right)^{N/2} e^{iS_c} \int dx_1 \cdots dx_{N-1} \underbrace{\prod_{i=2}^{N-1} e^{i\frac{m}{2}\frac{(\delta x_i - \delta x_{i-1})^2}{\Delta t}} \cdot e^{i\frac{m}{2}[(\delta x_1)^2 + (\delta x_{N-1})^2]}}$$

$$\exp\left[i \sum_{j,k} \delta x_j \, M_{jk} \, \delta x_k \right]$$

with $M_{jk} = \frac{m}{2\Delta t} \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & & \ddots & \\ & & -1 & 2 \end{bmatrix}$

$$\int dx_1 \cdots dx_{N-1} \exp\left[i \sum_{\substack{j,k \\ 1,\cdots N-1}} \delta x_j \, M_{jk} \, \delta x_k \right] = \frac{(\sqrt{\pi})^{N-1}}{\sqrt{\mathrm{Det}(-iM)}} \quad \text{(gaussian fluctation)}$$

tricks to calculate determinaint of $M_N = \begin{pmatrix} 2\cosh(u) & -1 & & \\ -1 & 2\cosh u & -1 & \\ & & \ddots & \\ & & -1 & 2\cosh u \end{pmatrix}$

$$\begin{cases} \mathrm{Det}\, M_N = 2\cosh u \,\mathrm{Det}\, M_{N-1} - \mathrm{Det}\, M_{N-2} \\ \mathrm{Det}\, M_1 = 2\cosh u \,, \quad \mathrm{Det}\, M_2 = 4\cosh^2 u - 1 \end{cases}$$

can be solved by the ansatz $\mathrm{Det}\, M_N = a e^{nu} + b e^{-nu}$

$$\Rightarrow \mathrm{Det}\, M_N = \frac{\sinh (N+1)u}{\sinh u} \longrightarrow N+1 \text{ as } u \to 0$$

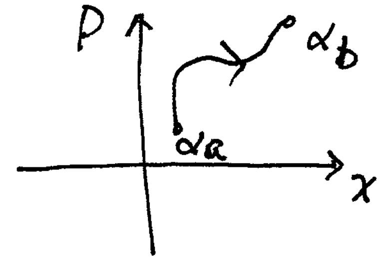
$$\Rightarrow \mathrm{Det}(-i M_{jk}) = \left(\frac{m}{2\Delta t i}\right)^{N-1} \times N$$

$$\Rightarrow iG(x_b t_b, x_a t_a) = \left(\frac{m}{2\pi i \Delta t}\right)^{N/2} \left(\frac{m}{2\pi i \Delta t}\right)^{-\frac{(N-1)}{2}} N^{-1/2} e^{iS_{cl}}$$

$$\boxed{iG(x_b t_b, x_a t_a) = \left(\frac{m}{2\pi i (t_b - t_a)}\right)^{1/2} e^{iS_{cl}}}$$

§ Coherent state path integral

Consider a harmonic oscilator $H = \omega a^{+} a$, and we define the coherent state $|\alpha\rangle$ satisfying $a|\alpha\rangle = \alpha|\alpha\rangle$. The propogator in the coherent state Rep is even simpler.



$$i G(\alpha_b t_b ; \alpha_a t_a) = \langle \alpha_b | \mathcal{U}(t_b t_a) | \alpha_a \rangle$$

Resolution identity

$$\boxed{\int \frac{d\,\mathrm{Re}\,\alpha \; d\,\mathrm{Im}\,\alpha}{\pi} \, |\alpha\rangle\langle\alpha| = 1}$$

Plug in
$$\boxed{\begin{aligned} |\alpha\rangle &= e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \\ &= N_\alpha \, e^{\alpha a^{+}} |0\rangle \end{aligned}}$$

Proof: $$\mathrm{LHS} = \int \frac{d\,\mathrm{Re}\,\alpha \; d\,\mathrm{Im}\,\alpha}{\pi} \, e^{-|\alpha|^2} \sum_{nn'} \frac{\alpha^n \alpha^{*n'}}{\sqrt{n!\,n'!}} |n\rangle\langle n'|$$

$$= \int \frac{d\theta}{\pi} |\alpha| \, d|\alpha| \, e^{-|\alpha|^2} \sum_n \frac{|\alpha|^{2n}}{n!} |n\rangle\langle n|$$

For those $n \neq n'$, they vanish after $\int d\theta$

$$= \sum_n \underbrace{\int_0^\infty d|\alpha|^2 \, \frac{e^{-|\alpha|^2} \, (|\alpha^2|)^n}{n!}}_{\Gamma\text{-function}} |n\rangle\langle n| = \sum_n |n\rangle\langle n| = 1$$

Inner product

$$\langle\alpha|\alpha'\rangle = e^{\frac{-|\alpha|^2}{2}} e^{-\frac{|\alpha'|^2}{2}} \langle 0 | e^{\alpha^* \hat{a}} e^{\alpha' \hat{a}^{+}} | 0 \rangle$$

$$e^{\alpha^* \hat{a}} e^{\alpha' \hat{a}^{+}} = e^{\alpha' \hat{a}^{+}} e^{\alpha^* \hat{a}} \, e^{\alpha^* \alpha' [\hat{a}, \hat{a}^{+}]}$$

$$\Rightarrow \boxed{\langle\alpha|\alpha'\rangle = e^{-\frac{1}{2}(|\alpha|^2 + |\alpha'|^2) + \alpha^* \alpha'}}$$

$$iG(\alpha_b t_b;\alpha_a t_a) = \int \frac{d^2a_1 \cdots d^2a_{N-1}}{\pi^{N-1}} \; iG(\alpha_b t_b, \alpha_{N-1} t_{N-1}) \cdots iG(\alpha_1 t_1; \alpha_a t_a)$$

$$iG(a_i t_i, a_{i-1} t_{i-1}) = \langle \alpha_i | \, e^{-i\Delta t\, \omega \hat{a}^\dagger a} \, | \alpha_{i-1} \rangle = e^{-i\Delta t\, \alpha_i^* \alpha_{i-1} \omega} \langle \alpha_i | \alpha_{i-1} \rangle$$

$$= e^{-i\Delta t\, \omega\, \alpha_i^* \alpha_{i-1} - \frac{1}{2}|\alpha_i|^2 - \frac{1}{2}|\alpha_{i-1}|^2 + \alpha_i^* \alpha_{i-1}}$$

$$= e^{-i\Delta t\, \omega\, \alpha_i^* \alpha_{i-1} - \frac{1}{2}\alpha_i^*(\alpha_i - \alpha_{i-1}) + \frac{1}{2}\alpha_{i-1}(-\alpha_{i-1}^* + \alpha_i^*)}$$

$$= e^{i\Delta t \left[-\omega\, \alpha_i^* \alpha_i + \frac{i}{2}(\alpha_i^* \dot{\alpha}_i - \alpha_i \dot{\alpha}_i^*) \right]}$$

$$\Rightarrow iG(\alpha_b t_b; \alpha_a t_a) = \int \frac{\prod_{i=1}^{N-1} d^2\alpha_i}{\pi^{N-1}} \; e^{i\int_{t_a}^{t_b} dt \left[\frac{i}{2}(\alpha^* \dot{\alpha} - \alpha \dot{\alpha}^*) - \omega \alpha^* \alpha \right]}$$

$$\longrightarrow \int D[\alpha(t)] \; e^{i\int_{t_a}^{t_b} dt\, \mathcal{L}}$$

where $\mathcal{L} = \frac{i}{2}(\alpha^* \dot{\alpha} - \alpha \dot{\alpha}^*) - \omega \alpha^* \alpha = p\dot{x} - H$.

§ Path integral Rep of partition function

$$Z(\beta) = \mathrm{tr}\, e^{-\beta H} = \int dx \; \mathcal{G}(x, x, \beta) \quad \text{where } \beta = \frac{1}{k_B T}$$

$$\mathcal{G}(x_b\, x_a; \beta) \equiv \langle x_b | \, e^{-\beta H} | x_a \rangle$$

$$= \left(\frac{m}{2\pi \Delta \tau}\right)^{N/2} \int D x(\tau) \; e^{-\int_0^\beta d\tau \; \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)}$$

$$\Rightarrow Z(\beta) = \int D x(\tau) \; e^{-\oint d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x) \right]} \quad \text{for closed path } x(0) = x(\beta).$$

$$\mathcal{G}(x_b, x_a, \tau)\Big|_{\tau = it} = i\, G(x_b, x_a; t)$$

imaginary time path integral