☆ Derivation of the Path Integral

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

$$\langle x_1, t+\Delta t | x_0, t\rangle = \langle x_1 | \overset{\Downarrow\,\mathbb{1}}{|} e^{-\frac{iH\Delta t}{\hbar}} | x_0\rangle$$

$$= \int dp \underbrace{\langle x_1 | p\rangle}_{\frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx_1}{\hbar}}} \underbrace{\langle p | e^{-\frac{iH\Delta t}{\hbar}} | x_0\rangle}_{\langle p | \left(\mathbb{1} - \frac{i\Delta t}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(x)\right) + O(\Delta t^2)\right) | x_0\rangle}$$

$$\langle p | x_0\rangle \quad -\frac{i\Delta t\, p^2}{2m\hbar}\langle p | x_0\rangle \quad -\frac{i\Delta t}{\hbar} V(x_0) \langle p | x_0\rangle$$

$$\simeq \int dp \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx_1}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx_0}{\hbar}} e^{-\frac{i\Delta t}{\hbar}\left(\frac{p^2}{2m} + V(x_0)\right)}$$

$$= \frac{e^{-\frac{i\Delta t V(x_0)}{\hbar}}}{2\pi\hbar} \int_{-\infty}^{\infty} dp \; e^{\frac{i}{\hbar}\left(\underbrace{(x_1 - x_0)p - \frac{\Delta t}{2m} p^2}_{} \right)} \qquad \simeq -\frac{\Delta t}{2m}\left(p - \frac{m}{\Delta t}(x_1 - x_0)\right)^2 + \frac{m}{2\Delta t}(x_1 - x_0)^2$$

$$= \frac{1}{2\pi\hbar} e^{-\frac{i\Delta t}{\hbar} V(x_0)} e^{\frac{i}{\hbar}\frac{m}{2\Delta t}(x_1 - x_0)^2} \times \sqrt{\frac{2\pi m\hbar}{\hbar i \Delta t}} = \sqrt{\frac{m}{i 2\pi\hbar\Delta t}} \exp\left(\frac{i\Delta t}{\hbar} \underbrace{\left(\tfrac{1}{2} m v^2 - V(x_0)\right)}_{\shortparallel} \right)$$

$$\frac{m(x_1 - x_0)^2}{2\Delta t} = \Delta t \frac{m (x_1 - x_0)^2}{2\Delta t^2} = \frac{\Delta t}{2} m v^2 \qquad\qquad i\frac{\Delta t}{\hbar} L$$

Also, because $U(t_2, t_0) = U(t_2, t_1) U(t_1, t_0)$

$$\langle x_f, t_f | x_i, t_i\rangle = \langle x_f | U(t_N, t_{N-1}) \underset{\mathbb{1}}{\wedge} U(t_{N-1}, t_{N-2}) \underset{\mathbb{1}}{\wedge} \cdots \underset{\mathbb{1}}{\wedge} U(t_1, t_0) | x_i\rangle$$

$$= \int dx_{N-1}\, dx_{N-2} \cdots dx_1 \; \langle x_f | U(t_N, t_{N-1}) | x_{N-1}\rangle \langle x_{N-1} | U(t_{N-1}, t_{N-2}) | x_{N-2}\rangle \langle x_{N-2} | \cdots$$

$$| x_1\rangle\langle x_1 | U(t_1, t_0) | x_i\rangle$$

$$= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N-1}{2}} \int \prod_{i=1}^{N-1} dx_i \; \exp\left[i \sum_{i=0}^{N-1} \frac{L(t_i)\,\Delta t}{\hbar} \right] \qquad \text{let } N \to \infty$$

$$\Rightarrow \int D(x(t)) \exp \frac{i S[x(t)]}{\hbar} \qquad \Rightarrow \text{This is P.I.}$$

(The overall normalization is a headache ~)

(☆) matrix elements of operators can be written in terms of P.I.

eg. $\langle x_f, t_f | x(t_0) | x_i, t_i \rangle$ $\qquad t_f > t_0 > t_i$

$$= \int dx(t_0) \langle x_f, t_f | x(t_0), t_0 \rangle \, x_0(t_0) \langle x(t_0), t_0 | x_i, t_i \rangle$$

$$= \int dx(t_0) \int_{t_f > t > t_0} D(x(t)) \, e^{\frac{iS[x(t)]}{\hbar}} \, x(t_0) \int_{t_0 > t > t_i} D[x(t)] e^{\frac{iS[x(t)]}{\hbar}}$$

$$= \int_{t_f > t > t_i} D(x(t)) \, e^{\frac{iS[x(t)]}{\hbar}} \, x(t_0)$$

This is the expectation value of the position in the integral form.

moreover, we have similarly

$$\langle x_f, t_f | x(t_2) \, x(t_1) | x_i, t_i \rangle = \int_{t_f > t > t_i} D(x(t)) \, e^{i \frac{S(x(t))}{\hbar}} \, x(t_2) \, x(t_1)$$

We assumed $t_2 > t_1$ to be consistent with P.I.

⇒ Expectation values in the P.I corresponds to matrix elements of operators with correct ordering in time !!

☆ Such a product of operators is called "time-ordered", $T\, x(t_2) x(t_1)$ defined by

$$\begin{cases} x(t_2)\, x(t_1) & \text{if } t_2 > t_1 \\ x(t_1)\, x(t_2) & \text{if } t_1 > t_2 \end{cases}$$

(☆) Euler-Lagrangian Eq. (Is obtained by $x(t) \to x(t) + \delta x(t)$, $\delta x(t_i) = \delta x(t_f) = 0$)

Variable change doesn't modify the P.I.

$$\int D[x(t)] \, e^{\frac{i}{\hbar} S[x(t) + \delta x(t)]} = \int D[x(t)] \, e^{\frac{iS}{\hbar}[x(t)]}$$

Therefore.

$$0 = \int D[x(t)] \, e^{\frac{i}{\hbar} S[x(t) + \delta x(t)]} - \int D[x(t)] \, e^{\frac{i}{\hbar} S[x(t)]} \simeq \int D(x(t)) e^{\frac{i}{\hbar} S[x(t)]} \frac{i}{\hbar} \delta S$$

$$\delta S = S[x(t) + \delta x(t)] - S[x(t)] = \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t),$$

it holds for any $\delta x(t)$

$$\Rightarrow \int D[x(t)] \, e^{\frac{iS[x(t)]}{\hbar}} \frac{i}{\hbar} \int dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right) \delta x(t) = 0$$

Therefore $0 = \left\langle \frac{i}{\hbar} \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right) \right\rangle$ ⇒ Ehrenfest's theorem

Schrödinger Eq from PI

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t)\, e^{\frac{iS[x(t)]}{\hbar}}$$

$x(t) \to x(t) + \delta x(t)$
with $\delta x(t_i) = 0$ <u>only</u>.
but $\delta x(t_f) \neq 0$

$$\Rightarrow \langle x_f + \delta x(t_f), t_f | x_i, t_i \rangle - \langle x_f, t_f | x_i, t_i \rangle$$

$$\cong \frac{\partial}{\partial x_f} \langle x_f, t_f | x_i, t_i \rangle\, \delta x(t_f)$$

$$= \int \mathcal{D}[x(t)]\, e^{i\frac{S}{\hbar}[x(t)+\delta x(t)]} - \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]} = \int \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]} \frac{i}{\hbar} \delta S$$

Recall our previous discussion of CM.

$$\delta S = S[x(t) + \delta x(t)] - S[x(t)]$$

$$= \int_{t_i}^{t_f} dt\, \frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} = \int_{t_i}^{t_f} dt\, \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}} \delta x\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) \delta x + \frac{\partial L}{\partial x} \delta x$$

$$= \left(\frac{\partial L}{\partial \dot{x}}\right) \delta x \Big|_{t_i}^{t_f} + \int_{t_i}^{t_f} \underbrace{\left(\frac{\partial L}{\partial x} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right)\right)}_{\to 0} \delta x$$

$\to 0$ because < Euler-Lagrangian > $= 0$ E.O.M.

$$\Rightarrow \delta S = P(t_f)\, \delta x(t_f)$$

$$\Rightarrow \frac{\partial}{\partial x_f} \langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}[x(t)]\, e^{\frac{iS[x(t)]}{\hbar}} \frac{i}{\hbar} P(t_f) \quad \leftarrow \text{momentum}$$

By Hamilton-Jacobi eq. $\dfrac{\partial S}{\partial t_f} = -H(t_f)$

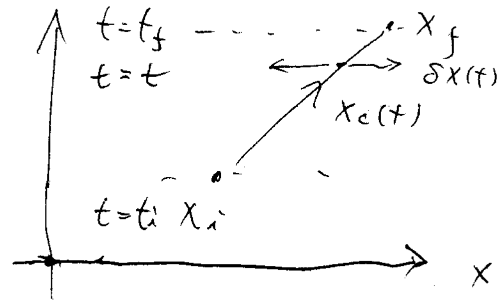
$$\Rightarrow \frac{\partial}{\partial t_f} \langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}[x(t)]\, e^{\frac{iS}{\hbar}[x(t)]} \left(-\frac{i}{\hbar} H(t_f)\right) \quad \leftarrow \text{energy}$$

So, if $H = \frac{p^2}{2m} + V(x)$

$$\Rightarrow i\hbar \frac{\partial}{\partial t_f} \langle x_f, t_f | x_i, t_i \rangle = \left(\frac{1}{2m}\left(-i\hbar \frac{\partial}{\partial x_f}\right)^2 + V(x_f)\right] \langle x_f, t_f | x_i, t_i \rangle$$

$\Rightarrow$ This is nothing but the Schrödinger Eq.

☆ Example : 1-D free particle & normalization



$$\langle x_f, t_f | x_i, t_i \rangle = \int D[x(t)]\, e^{\frac{i}{\hbar}\int dt \frac{m}{2}\dot{x}^2}$$

The classical path is

$$x_c(t) = x_i + \frac{x_f - x_i}{t_f - t_i}(t - t_i)$$

And write $x(t) = x_c(t) + \delta x(t)$. BC: $\delta x(t_i) = \delta x(t_f) = 0$

Because of the B.C.s we expand $\delta x(t)$ in Fourier series

$$\delta x(t) = \sum_{n=1}^{\infty} a_n \sin n\pi\left(\frac{t-t_i}{t_f-t_i}\right)$$

$$\int Dx(t) = c \int da_1 \cdot da_2 \cdots da_\infty$$

c ↑ some normalization factor

$$\dot{x} = \dot{x}_c + \delta\dot{x} = \frac{x_f - x_i}{t_f - t_i} + \sum_{n=1}^{\infty} \frac{a_n n\pi}{t_f - t_i} \cos\frac{n\pi(t-t_i)}{t_f-t_i}$$

$$S = \int_{t_i}^{t_f} dt\, \frac{1}{2} m \left[\left(\frac{x_f - x_i}{t_f - t_i}\right)^2 + \cancel{\sum_{n=1}^{\infty} 2\left(\frac{x_f-x_i}{t_f-t_i}\right)\frac{a_n \pi n}{(t_f-t_i)} \cos\frac{n\pi(t-t_i)}{t_f-t_i}} + \sum_{n=1}^{\infty} \frac{a_n^2 n^2 \pi^2}{(t_f-t_i)^2} \cos^2 \frac{n\pi(t-}{t_f-t} \right.$$

(∵ cosine functions are orthogonal to each other)

$$= \frac{1}{2} m \left[\frac{(x_f - x_i)^2}{t_f - t_i} + \sum_{n=1}^{\infty} \frac{1}{2} \frac{a_n^2 n^2 \pi^2}{t_f - t_i} \right]$$

$$\int da_n \exp \frac{-i}{\hbar} \frac{-m n^2 \pi^2}{4(t_f - t_i)} a_n^2 = \sqrt{\frac{4\pi\hbar(t_f - t_i)}{-i m n^2 \pi^2}}$$

$$\Rightarrow \langle x_f, t_f | x_i, t_i \rangle = \underbrace{c \prod_{n=1}^{\infty} \sqrt{\frac{4i\hbar(t_f - t_i)}{n^2 m \pi}}} \exp\left(\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2(t_f - t_i)}\right)$$

$\equiv C'(t_f - t_i)$ a const depends only on $(t_f - t_i)$

A hand waving way to determine the const is following

$$\langle x_f, t_f | x_i, t_i \rangle = \int dx \, \langle x_f, t_f | x, t \rangle \langle x, t | x_i, t_i \rangle$$

$$\Rightarrow \; c'(t_f - t_i) \exp\left[\frac{i}{\hbar} \frac{m}{2} \frac{(x_f - x_i)^2}{t_f - t_i} \right] = c'(t_f - t)\, c'(t - t_i) \int dx \, \exp\left(\frac{i}{\hbar} \frac{m (x_f - x)^2}{2(t_f - t)} + \frac{i}{\hbar} \frac{m (x - x_i)^2}{2(t - t_i)} \right)$$

$$\cancel{= c'(t_f - t)\, c'(t - t_i) \sqrt{\frac{2\hbar\pi(t_f - t)}{-im}} \sqrt{\frac{2\hbar\pi(t - t_i)}{im}}}$$

$$\frac{im}{2\hbar} \left(\frac{(x_f - x)^2}{t_f - t} + \frac{(x - x_i)^2}{t - t_i} \right) = \frac{im}{2\hbar} \frac{1}{(t_f - t)(t - t_i)} \Big[(t - t_i)(x_f^2 + x^2 - 2x x_f) + (t_f - t)(x_i^2 + x^2 - 2x x_i) \Big]$$

$$= \frac{im}{2\hbar} \frac{1}{(t_f - t)(t - t_i)} \Big[(t_f - t_i) x^2 - 2x \big(x_f (t - t_i) + x_i (t_f - t) \big) + x_f^2 (t - t_i) + x_i^2 (t_f - t) \Big]$$

$$= \frac{im}{2\hbar} \frac{1}{(t_f - t)(t - t_i)} \Big[(t_f - t_i) \Big(x - \frac{x_f (t - t_i) + x_i (t_f - t)}{t_f - t_i} \Big)^2 + x_f^2 (t - t_i) + x_i^2 (t_f - t) - \frac{[x_f (t - t_i) + x_i (t_f - t)]^2}{(t_f - t_i)} \Big]$$

$$\text{R.H.S.} = c'(t_f - t)\, c'(t - t_i) \exp\left(\frac{im}{2\hbar} \frac{(x_f - x_i)^2}{(t_f - t_i)} \right) \cancel{\exp\left[\frac{-im}{2\hbar} \frac{x_f^2 (t - t_i) + x_i^2 (t_f - t)}{(t_f - t_i)(t_f - t)(t - t_i)} \right]} \times \sqrt{\frac{2\hbar\pi(t_f - t)(t - t_i)}{-im(t_f - t_i)}}$$

$$\Rightarrow \; c'(t_f - t_i) = c'(t_f - t)\, c'(t - t_i) \sqrt{\frac{2\hbar\pi(t_f - t)(t - t_i)}{-im(t_f - t_i)}}$$

Therefore, we find

$$c'(t) = \sqrt{\frac{-im}{2\hbar\pi t}}$$

1D

$\Rightarrow$ For free particle

$$\langle x_f, t_f | x_i, t_i \rangle = \sqrt{\frac{m}{2i\hbar\pi(t_f - t_i)}} \exp\left(\frac{i}{\hbar} \frac{m (x_f - x_i)^2}{2(t_f - t_i)} \right)$$

And we recover the propagator we obtained by time-evolution operator.

Partition Function

$$Z = \sum_n e^{-\beta E_n} \qquad \left(\beta = \frac{1}{k_B T}\right)$$

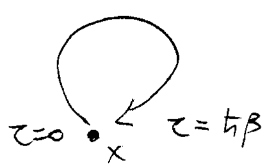
$$= \sum_n \langle n | \underset{\hat{\mathbb{1}}_x}{e^{-\beta H}} | n \rangle = \int dx \sum_n \langle n | x \rangle \langle x | e^{-\beta H} | n \rangle$$

$$= \int dx \sum_n \langle x | e^{-\beta H} | n \rangle \langle n | x \rangle = \int dx \langle x | e^{-\beta H} | x \rangle$$

compared with the propagator we are interested in in PI

$$\langle x_1, t_1 | x_0, t_0 \rangle = \langle x_1 | e^{-\frac{i}{\hbar} H \underbrace{(t_1 - t_0)}_{\Delta}} | x_0 \rangle \qquad x_0 = x_1 \quad \frac{i\Delta}{\hbar} = \beta$$

set $t_0 = 0$, $\Delta = t$, one gets Z from PI by the analytic continuation $t \Rightarrow -i\tau = -i\hbar\beta$, and PI now is the integral for all <u>closed</u> path!



$$L = \frac{1}{2} m \dot{x}^2 - V \Longrightarrow \boxed{-\frac{1}{2} m \left(\frac{\partial x}{\partial \tau}\right)^2 - V(x)}$$

(PI) $\qquad \frac{d}{dt} = i \frac{d}{d\tau}$

$$\frac{i}{\hbar} S = \frac{i}{\hbar} \int dt\, L \Rightarrow \frac{i}{\hbar} \int (-i\, d\tau) (L(\tau))$$

$$\Rightarrow \boxed{Z = \int_{x(0)=x(\hbar\beta)} D[x(\tau)] \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[\frac{m}{2} \left(\frac{\partial x}{\partial \tau}\right)^2 + V(x) \right] \right\}}$$

or simplily replace $\langle x_1, t | x_0, 0 \rangle \Rightarrow \int dx \langle x, -i\hbar\beta | x, 0 \rangle$

For example, for the free particle

P.I. (3-D) $\quad \langle x_1, t | x_0, 0 \rangle = \left(\sqrt{\frac{m}{2i\hbar\pi t}} \right)^3 \exp\left(\frac{i}{\hbar} \frac{m (\vec{x}_1 - \vec{x}_0)^2}{2t} \right)$

$$\Rightarrow Z = \int d^3x \langle \vec{x}, -i\hbar\beta | \vec{x}, 0 \rangle = \int_{-\infty}^{\infty} d^3x \left(\sqrt{\frac{m}{2\hbar^2 \pi \beta}} \right)^3 \exp(0) = \left(\frac{m k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} \underset{\text{Volume}}{\underline{\underline{V}}}$$

is exactly the same result obtained in Statistic Mechanics.

(H.W): You shall check the Z_{SHO} from its propagator.

$$= \sum_{n=0}^{\infty} e^{-\beta (n + \frac{1}{2}) \hbar \omega}$$