Path Integral Formulation

§1. Quantum Mechanics in Path Integral Formulation

Derivation

Consider a quantum mechanical system

H : Hamiltonian

(q, p) : canonical conjugate pair.

Time evolution of the wave function

$$\psi(q, t ; q_*, t_*) = e^{-i\int^t H(t')dt'} \psi(q_*, t_*)$$

$$\longrightarrow e^{-iH(t-t')} \psi(q_*, t_*)$$

This time evolution is rewritten as follows.

$$\langle q ; t | e^{-iH(\Delta t)} | q_{N-1} ; t_{N-1}\rangle \cdots \langle q_2 ; t_2 | e^{-iH\Delta t} | q_1 ; t_1 \rangle \langle q_1 ; t_1 | e^{-iH\Delta t} | q_* ; t_* \rangle$$

$$\left(\begin{array}{l} (t - t_*) = N \cdot (\Delta t) \\ \quad (t = t_N) > t_{N-1} > \cdots > t_2 > t_1 > (t_* = t_0) \qquad \Delta t \text{ interval.} \end{array} \right)$$

integrated over $(q_{N-1}, q_{N-2}, \cdots, q_2, q_1) \in \mathbb{R}^{N-1}$.

In the limit that $N \to +\infty$, $\Delta t \to +0$.

$$\cancel{\langle q_k ; t_k | e^{iH\Delta t} | q_{k-1} ; t_{k-1}\rangle \simeq \delta(q_k - q_{k-1}) + (-i\Delta t) \langle q_k ; t_k | H | q_{k-1} ; t_{k-1}\rangle}.$$

In an example $H = \frac{1}{2m} p^2 + V(q) = \frac{-1}{2m} \partial_q^2 + V(q)$,

$$\langle q_k ; t_k | e^{-iH\Delta t} | q_{k-1} ; t_{k-1}\rangle \cong \int \frac{dp_k}{2\pi} \langle q_k ; t_k | p_k ; t_k \rangle \langle p_k ; t_k | e^{-iH\Delta t} | q_{k-1} ; t_{k-1}\rangle$$

$$= \int \frac{dp_k}{2\pi} e^{i q_k p_k} e^{-i p_k q_{k-1}} e^{-iH\Delta t}$$

$$= \int \frac{dp_k}{2\pi} e^{i\Delta t \left\{ p_k \left(\frac{q_k - q_{k-1}}{\Delta t} \right) - H \right\}}$$

Therefore.

$$\boxed{\begin{aligned}\langle q; t_f | e^{-iH\Delta t} | q_*; t_* \rangle &\cong \prod_{k=1}^{N-1} \int dq_k \int \frac{dp_k}{2\pi} \int \frac{dp_N}{2\pi}\, e^{i(\Delta t) \sum_{k=1}^{N} \left\{ p_k \left(\frac{q_k - q_{k-1}}{\Delta t} \right) - H(p_k, q_{k-1}) \right\}} \\ &\overset{\text{denoted by}}{=\!=}: \int_{\substack{q=q_* \\ \text{at } t=t_* \\ q=q \\ \text{at } t=t_f}} \mathcal{D}q(t)\, \mathcal{D}p(t)\; e^{i\int dt' (p\dot{q} - H)}\end{aligned}}$$

In systems where $H(q,p)$ is *quadratic* in p.

(as in the example).

we can do the Gaussian integral:

$$\int \frac{dp_k}{2\pi}\, e^{-i\Delta t \frac{p_k^2}{2m} + i\Delta t\, p_k \dot{q}_k} = \int \frac{dp_k}{2\pi}\, e^{-i\frac{\Delta t}{2m}(p_k - m\dot{q}_k)^2 + i(\Delta t)\frac{m}{2}(\dot{q}_k)^2}$$

$$= \sqrt{\frac{m}{2\pi i(\Delta t)}}\; e^{i(\Delta t)\frac{m}{2}(\dot{q}_k)^2}.$$

So, there is an alternative expression

$$\boxed{\langle q; t_f | e^{-iH\Delta t} | q_*; t_* \rangle \propto \int_{\substack{q(t_*)=q_* \\ q(t_f)=q}} \mathcal{D}q(t)\; e^{i\int dt\, \mathcal{L}}}$$

Example 1 free particle $(V(q)=0)$

$$\left[\begin{array}{l} q = q_i \ @\ t=t_i \\ q = q_f \ @\ t=t_f \end{array}\right] — ⊛ \qquad \text{Take } t_i=0. \quad T := (t_f - t_i)$$

$$\boxed{\psi(q_f, T; q_i, 0) = \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \int_{N\text{ step}} \mathcal{D}q(t)\ e^{i\int_0^T dt' \frac{m}{2}(\dot{q})^2}}$$

⊛ bdry cond.

Expand

$$q(t') = \left(q_i + \frac{(q_f - q_i)}{T} t'\right) + \sum_{n=1}^{\infty} X_n \sin\left(\frac{t'}{T}\pi n\right) =: q_{cl}(t') + q_{fl}(t')$$

⊛ bdry condition is satisfied.

classical solution + fluctuation around it.

$\prod_{k=1}^{N-1} dq\left(\frac{T}{N}\cdot k\right)$ It is also OK to use $(X_1, \cdots, X_{N-1}) \in \mathbb{R}^{N-1}$ to parametrize the space of path.

$$S = \int_0^T dt' \frac{m}{2}(\dot{q}_{cl} + \dot{q}_{fl})^2 = \frac{m}{2}\int_0^T dt' \left\{(\dot{q}_{cl})^2 + (\dot{q}_{fl})^2\right\}$$

$$m\int_0^T dt'\ \dot{q}_{cl}\dot{q}_{fl} = m\int_0^T dt' \frac{d}{dt'}(\dot{q}_{cl} q_{fl}) = m\left[\dot{q}_{cl} q_{fl}\right]_0^T$$
$$= 0.$$

$$\psi(q_f, T; q_i, 0) = \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \cdot e^{iS_{cl}} \cdot \text{Jac} \cdot \int \prod_{k=1}^{N-1} dX_k\ e^{iS_{fl}}$$

$$S_{cl} = \frac{m}{2}\frac{(q_f - q_i)^2}{T}$$

$$S_{fl} = \frac{m}{2}\sum_{n=1}^{N-1} X_n^2 \left(\frac{\pi}{T}n\right)^2 \int_0^T dt' \cos^2\left(\frac{t'}{T}\pi n\right) = \sum_{n=1}^{N-1} \frac{mT}{4}\left(\frac{\pi}{T}n\right)^2 X_n^2.$$

$$= e^{i\frac{m}{2}\frac{(q_f-q_i)^2}{T}} \times \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \cdot \text{Jac} \prod_{n=1}^{N-1}\left[\frac{4\pi}{-imT}\frac{1}{\left(\frac{\pi}{T}n\right)^2}\right]^{1/2}$$

$$\text{Jac} = \left|\frac{\partial q(\frac{T}{N}k)}{\partial X_n}\right| = \left|\sin\left(\frac{\pi}{N}k \cdot n\right)\right| \quad : \text{indep. of } (m, T, q_i, q_f).$$

We know the right answer....

$$\langle q_f @ T \,|\, e^{-iHT} \,|\, q_i @ 0\rangle = \int \langle q_f @ T \,|\, e^{-i\frac{p^2}{2m}T} \,|\, p @ 0\rangle \frac{dp}{2\pi}\, e^{-ipq_i}$$

$$= \int \frac{dp}{2\pi}\, e^{-i\frac{p^2}{2m}T}\, e^{ip(q_f - q_i)} = \sqrt{\frac{m}{2\pi i T}}\; e^{i\frac{m}{2T}(q_f - q_i)^2}.$$

So, probably

$$\sqrt{\frac{m}{2\pi i T}} = \sqrt{\frac{mN}{2\pi i T}}^{\,N} \times \mathrm{Jac} \times \sqrt{\frac{4\pi}{-imT}\left(\frac{T}{\pi}\right)^2}^{\,N-1} \frac{1}{(N-1)!}$$

$$= \sqrt{\frac{m}{2\pi i T}} \times \underbrace{\left[\mathrm{Jac} \times \left(\frac{2}{\pi^2}\right)^{\frac{N-1}{2}} \frac{N^{N/2}}{(N-1)!}\right]}_{\to\, 1?}$$

Example 2 harmonic oscillator $H = \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 q^2$

$$\left.\begin{array}{l} q = q_i \ @\ t = \tau_i = 0. \\ q = q_f \ @\ t = \tau_f = T \end{array}\right\} \text{ bdry condition} \text{ --- } (*)$$

Expand. (parametrize.)

$$q(t) = q_{cl}(t) + q_{fl}(t)$$

$$= A\cos(\omega t + \delta) + \sum_{n=1}^{N-1} X_n \sin\left(\frac{t}{T}\pi n\right)$$

$$q_i = A\cos(\delta)$$

$$q_f = A\cos(\omega T + \delta) = A\left[\cos(\omega T)\cos(\delta) - \sin(\omega T)\sin(\delta)\right]$$

$$\Longrightarrow \tan(\delta) = \frac{\cos(\omega T) - (q_f/q_i)}{\sin(\omega T)}$$

$$S_{cl} = \int_0^T dt\, \frac{m}{2} A^2 \omega^2 \left\{\sin^2(\omega t + \delta) - \cos^2(\omega t + \delta)\right\}$$

$$= -\frac{m}{2} A^2 \omega^2 \int_0^T dt\, \cos(2(\omega t + \delta))$$

$$= \frac{m\omega}{2}\frac{A^2}{2}\left\{\sin(2\delta) - \sin(2\omega T + 2\delta)\right\}$$

$$= \frac{m\omega}{2}\frac{A^2}{2}\left[\sin(2\delta)\left\{1 - \cos(2\omega T)\right\} - \cos(2\delta)\sin(2\omega T)\right]$$

$$= \frac{m\omega}{2} A^2 \sin(\omega T)\left[\sin(2\delta)\sin(\omega T) - \cos(2\delta)\cos(\omega T)\right]$$

use $\sin(2\theta) = \frac{2\tan(\theta)}{1+\tan^2\theta}$ $\quad \cos(2\theta) = \frac{1-\tan^2\theta}{1+\tan^2\theta}$.

$$= \frac{m\omega}{2}\sin(\omega T)(q_i)^2\left[2\left(\cos(\omega T) - \frac{q_f}{q_i}\right) - \frac{\left\{\sin^2(\omega T) - \left(\cos(\omega T) - q_f/q_i\right)^2\right\}\cos(\omega T)}{\sin^2(\omega T)}\right]$$

$$= \frac{m\omega}{2}\frac{(q_i)^2}{\sin(\omega T)}\left[\left(\frac{q_f}{q_i}\right)^2\cos(\omega T) + \cos(\omega T) - 2\frac{q_f}{q_i}\right]$$

$$= \frac{m\omega}{2}\frac{1}{\sin(\omega T)}\left[\cos(\omega T)(q_i^2 + q_f^2) - 2q_i q_f\right]$$

$$S_{fl.} = \frac{m}{2}\sum_n (X_n)^2 \int_0^T dt \left\{ \left(\frac{\pi}{T}n\right)^2 \cos^2\left(\frac{t}{T}\pi n\right) - \omega^2 \sin^2\left(\frac{t}{T}\pi n\right) \right\}$$

$$= \sum_n \frac{mT}{4} \left\{ \left(\frac{\pi}{T}n\right)^2 - \omega^2 \right\} (X_n)^2 .$$

Gaussian integral over the fluctuations.

$$\prod_{n=1}^{N-1} \int dX_n \, e^{i\frac{mT}{4}\left\{\left(\frac{\pi}{T}n\right)^2-\omega^2\right\}(X_n)^2} = \prod_{n=1}^{N-1} \sqrt{\frac{4\pi}{-imT} \frac{1}{\left\{\left(\frac{\pi}{T}n\right)^2-\omega^2\right\}}}$$

So

$$\langle q_f @ T | e^{-iHT} | q_i @ 0 \rangle = e^{iS_{cl}} \cdot \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \times \mathrm{Jac} \times \prod_{n=1}^{N-1} \sqrt{\frac{4\pi}{-imT} \frac{1}{\left\{\left(\frac{\pi}{T}n\right)^2-\omega^2\right\}}}$$

$$= e^{iS_{cl.}} \sqrt{\frac{m}{2\pi i T}} \times \frac{1}{\prod_{n=1}^{N-1}\sqrt{1-\left(\frac{\omega T}{\pi n}\right)^2}} . = e^{iS_{cl.}} \sqrt{\frac{m\omega}{2\pi i \sin(\omega T)}}$$

Now. use

$$\left(\prod_{n=1}^{\infty} \left(1 - \frac{z}{n}\right) = \frac{1}{\Gamma(1-z)} \right)$$

$$\prod_{n=1}^{\infty} \left(1 - \left(\frac{z}{n}\right)^2\right) = \frac{1}{\Gamma(1-z)\,\Gamma(1+z)} = \frac{\sin(\pi z)}{(\pi z)}$$

Quantum states from path integral

If $\langle q_f \text{ at } t_f | e^{-iH(t_f-t_i)} | q_i @ t_i \rangle = f_{in}(q_f, q_i, t_f-t_i)$ is given.

$$\boxed{\begin{aligned} & f_{in}(q_f, q_i; t_f-t_i) \\ & = \int \frac{d\omega}{2\pi} e^{-i\omega(t_f-t_i)} \psi_\omega(q_f) [\psi_\omega(q_i)]^* . \end{aligned}}$$

So, the spectrum and wavefunctions can be extracted from $f_{in}(q_f, q_i; t_f-t_i)$ by Fourier transformation.

Time-ordered product expectation value

Consider

$$\int_{\substack{q_f @ t_f \\ q_i @ t_i}} \frac{dp_N}{2\pi} dq_{N-1} \frac{dp_{N-1}}{2\pi} \cdots \quad dq_1 \frac{dp_1}{2\pi} \; e^{i(\Delta t) \sum_{k=1}^{N} \left\{ p_k \dot{q}_k - H(p_k, q_{k-1}) \right\}}$$

$$\times \left(f_{i_1}(q_{i_1}) \, f_{i_2}(q_{i_2}) \cdots \quad \tilde{f}_{j_1}(p_{j_1}) \, \tilde{f}_{j_2}(p_{j_2}) \cdots \right)$$

$$= \langle q_f \text{ at } t_f | \, T\left\{ \prod_i \left(f_i(q_i)\right) \prod_j \left(\tilde{f}_j(p_j)\right) e^{-i\int dt' H(t')} \right\} | q_i \text{ at } t_i \rangle$$

instead of $\langle q_f \text{ at } t_f | \, e^{-iHT} \, | q_i \text{ at } t_i \rangle$.

The commutation relation $[q, p] = i$ (equal time)

$$0 = \int \prod_{k=1}^{N} \left[dq_k \frac{dp_k}{2\pi} \right] \frac{\partial}{\partial p_i} \left(p_j \, e^{i\Delta t \sum_{k=1}^{N} \{ p_k \dot{q}_k - H(p_k, q_{k-1}) \}} \right)$$

$$= \int \prod_{k=1}^{N} \left[dq_k \frac{dp_k}{2\pi} \right] \left(\delta_{ij} + i p_j (q_i - q_{i-1}) - i(\Delta t) \frac{\partial H(p_i, q_{i-1})}{\partial p_i} \cdot p_j \right) e^{i\Delta t \sum_{k=1}^{N} \left\{ \begin{matrix} p_k \dot{q}_k \\ -H \end{matrix} \right\}}.$$

In the $N \to \infty$, $\Delta t \to 0$ limit.

$$\langle q_i p_i - p_i q_{i-1} \rangle = i$$ (equal time commutator $[q, p] = i$)

is reproduced from the path integral formulation.