§1. Path Integral Formulation in Quantum Mechanics

§1.1 Bosonic Quantum Mechanical Systems

Derivation

~~Consider a quantum mechanical system~~

H : Hamiltonian

~~(q, p) canonical conjugate pair~~

initial state $\boxed{\cancel{\psi_0(q_{in}, t_{in})} \text{ @ } t = t_{in}}$

Time evolution ~~of the wave function~~

$$\psi(q, t; \psi_0) = e^{-i\int_{t_{in}}^{t} dt' H(t')} \psi_0(q_{in}, t_{in})$$

(~~time-ordered~~ exp. to be more precise)

(already $\hbar = 1$ convention.)

This time-evolution can be rewritten as follows:

$$\psi(q, t; \psi_0) = \langle q, t | e^{-iHT} | \psi_0 \rangle = \int dq_{in} \langle q, t | e^{-iHT} | q_{in}, t_{in} \rangle \psi_0(q_{in}, t_{in})$$

~~$H(t)$ for simplicity~~ $\quad T := (t - t_{in})$

$$\boxed{\langle q, t | e^{-iHT} | q_{in}, t_{in} \rangle}$$

$$= \int dq_{N-1} \cdots \int dq_1 \langle q, t | e^{-iH\Delta t} | q_{N-1}, t_{N-1} \rangle \cdots \langle q_2, t_2 | e^{-iH\Delta t} | q_1, t_1 \rangle \langle q_1, t_1 | e^{-iH\Delta t} | q_{in}, t_{in} \rangle$$

~~inserted a complete system of states. at a time slice t_i~~

$$(t = t_N) > t_{N-1} > \cdots > t_2 > t_1 > (t_{in} = t_0) \quad \text{interval } \Delta t = \frac{T}{N}.$$

In cases with $H = \frac{p^2}{2m} + V(q)$ —— (**)

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

use $e^{-iH\Delta t} = e^{-i\frac{p^2}{2m}\Delta t} e^{(O((\Delta t)^2) \cdot p \,\&\, q)} e^{-iV(q)\Delta t}$

$$= \int \frac{dp_k}{2\pi} e^{ip_k q_k} e^{-i\frac{p^2}{2m}\Delta t} e^{-i O((\Delta t)^2)} e^{-ip_k q_{k-1}} e^{-iV(q_{k-1})\Delta t}$$

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

~~Therefore~~

$$\boxed{\begin{aligned} \langle q, t | e^{-iHT} | q_{in}, t_{in} \rangle &= \underbrace{\int}_{\lim_{N\to\infty}} \frac{dp_N}{2\pi} \prod_{k=1}^{N-1} \left(\int dq_k \frac{dp_k}{2\pi} \right) e^{i\Delta t \sum_{k=1}^{N} \left\{ p_k \left(\frac{q_k - q_{k-1}}{\Delta t} \right) - H(q_{k-1}) \right\}} \\ &\overset{\text{denoted}}{\underset{\text{by}}{=:}} \int_{\substack{q = q_{in} @ \tau = t_{in} \\ q = q @ \tau = t}} \mathcal{D}q(t') \mathcal{D}p(t') \, e^{i\int dt' (p\dot{q} - H)} \end{aligned}}$$

(drop $(\Delta t)^2$ in the exp. $(N \to \infty)$)

As long as (**) holds : do 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~~

$$\boxed{\langle q, t_f | e^{-iHT} | q_i, t_i \rangle \propto \int_{\substack{q(t_i) = q_i \\ q(t_f) = q_f}} \mathcal{D}q(t') \, e^{i\int dt' L}}$$

(the Gaussian integral factors " $\sqrt{\frac{mN}{2\pi i T}}$ " is indep. of q_i or q_f)

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

$$\left[\begin{array}{l} q = q_{in} \ @\ t = t_{in} \\ q = q_f \ @\ t = t_{fin} \end{array}\right] \ (*) \qquad \text{take } t_i = 0, \quad T := (t_{fin} - t_{in})$$

$$\boxed{\langle q_f, t_f | e^{-iHT} | q_{in}, t_i \rangle = \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \int_{(*)\,\text{bdry cond}} (\mathcal{D}q(t') = dq_1 dq_2 \cdots dq_{N-1})\, e^{i\int_0^T dt' \frac{m}{2}(\dot{q})^2}}$$

$$q_k = q(t' = (t_{in}=0) + (\Delta t)\cdot k) = \underbrace{\left(q_{in} + \frac{(\Delta t)\cdot k}{T}(q_f - q_{in})\right)}_{\hookrightarrow q_{cl}(t')} + \delta q_k$$

$\Big\{$ bdry cond $(*)$ satisfied
split into (classical solution q_{cl}) and (fluctuat'n around it)

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

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

So

$$\langle q_f, t_f | e^{-iHT} | q_{in}, t_i \rangle = \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} e^{i\left(\frac{m}{2}\frac{(q_f - q_{in})^2}{T} = S_{cl}\right)} \int d(\delta q_1)\cdots d(\delta q_{N-1})\, e^{iS_{fl}}$$

$$iS_{fl} = i\frac{m}{2}\sum_{k=1}^{N}\left(\frac{\delta q_k - \delta q_{k-1}}{(\Delta t)}\right)^2 (\Delta t) \simeq i\frac{mN}{2T}(\delta q_{N-1}, \cdots, \delta q_1)\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}\begin{pmatrix} \delta q_{N-1} \\ \vdots \\ \vdots \\ \delta q_1 \end{pmatrix}$$

$$\boxed{= \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} e^{i\frac{(q_f - q_{in})^2}{T}\frac{m}{2}} \times \left(\frac{2\pi T}{-imN}\right)^{\frac{N-1}{2}} \frac{1}{\sqrt{\det\begin{bmatrix} 2 & -1 & \\ -1 & \ddots & -1 \\ & -1 & 2 \end{bmatrix}}} = \sqrt{\frac{m}{2\pi i T}}\, e^{i\frac{m}{2}\frac{(q_f - q_{in})^2}{T}}}$$

$$\left(\det\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}_{(N-1)\times(N-1)} = N \qquad \det[2] = 2, \quad \det\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} = 3 \quad \text{use recursion relat'n} \right)$$

[X.G. Wen's textbook p.24 ~ 25]

We have reproduced $\displaystyle\int \frac{dp}{2\pi} \langle q_f, T| e^{-i\frac{p^2}{2m}T} | q_{in}, 0\rangle = \int \frac{dp}{2\pi} e^{ip(q_f - q_{in})} e^{-i\frac{p^2}{2m}T} = \sqrt{\frac{m}{2\pi i T}}\, e^{i\frac{m}{2}\frac{(q_f - q_{in})^2}{T}}$ PLUS

An early version of this lecture note had a little more naive evaluation, which shows the subtlety in talking about the path integral measure.

It went as follows.

Expand $q(t') = \left(q_{cl} = q_{in} + (q_{fin} - q_{in})\frac{k}{N}\right) + \sum_{n=1}^{N-1} X_n \sin\left(\frac{t'}{T}\pi n\right)$, $\quad \frac{t'}{T}\pi n = \left(\frac{k}{N}\pi n\right)$

$t' = t_{in} + \frac{T}{N}k \qquad k = 1, 2, \cdots$

and convert the integration measure from

$$\prod_{k=1}^{N-1}\left[d(\delta q_k)\right] \quad \text{to} \quad \prod_{k=1}^{N-1}\left[d(\delta q_k)\right] = \prod_{n=1}^{N-1}\left[dX_n\right] \left|\det\left[\underbrace{\left(\frac{\partial q_k}{\partial X_n}\right)_{k,n}}_{(N-1)\times(N-1)\ \text{matrix}}\right]\right|$$

So,

$$\langle q_f, t_f | e^{-iHT} | q_{in}, t_{in} \rangle = \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} e^{iS_{cl}} \int \prod_{n=1}^{N-1}\left[dX_n\right] \mathrm{Jac} \cdot e^{iS_{fl}}$$

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

cross terms vanish after integration

so the Gaussian integrand is diagonalized when X_n's are used instead of (δq_k)'s.

$$= e^{iS_{cl}} \cdot \left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \left(\prod_{n=1}^{N-1}\sqrt{\frac{4\pi}{-imT\left(\frac{\pi}{T}n\right)^2}}\right) \times \left(\mathrm{Jac} = \det\left[\sin\left(\frac{\pi}{N}kn\right)\right]\right)$$

$$= e^{iS_{cl}}\sqrt{\frac{m}{2\pi i T}} \times \left[\mathrm{Jac} \times \left(\frac{2}{\pi^2}\right)^{\frac{N-1}{2}} \frac{N^{\frac{N}{2}}}{(N-1)!}\right].$$

Does the factor $[\cdots]$ go to 1 in $N \to \infty$? $\Rightarrow$ No, actually.

for $N = 10, 11, \cdots, 18$ used Mathematica to see that

$\ln[\cdots] \sim 3.34 - 1.96\ln(N)$ linear fit.

$[\cdots] \sim 28/N^{1.96}$ not $\simeq 1$.

although the N-dependence has almost cancelled in

$$\ln[\quad] \simeq \frac{N}{2}\ln(N) - (N-1)\ln(N-1) + \frac{N-1}{2}\ln(2/\pi^2) + \ln(\mathrm{Jac}).$$

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

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

Expand. (parametrize)

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

$$q_i = A\cos(\delta)$$
$$q_f = A\cos(\omega T + \delta) = A\left[\cos(\omega T)\cos(\delta) - \sin(\omega T)\sin(\delta)\right]$$
$$\Rightarrow \tan(\delta) = \frac{\cos(\omega T) - (q_f/q_i)}{\sin(\omega T)}$$

$$S_{cl} = \int_0^T dt\, \frac{m}{2}A^2\omega^2\left\{\sin^2(\omega t+\delta) - \cos^2(\omega t+\delta)\right\}$$
$$= -\frac{m}{2}A^2\omega^2\int_0^T dt\, \cos\left(2(\omega t+\delta)\right)$$
$$= \frac{m\omega}{2}\frac{A^2}{2}\left\{\sin(2\delta) - \sin(2\omega T + 2\delta)\right\}$$
$$= \frac{m\omega}{2}\frac{A^2}{2}\left[\sin(2\delta)\left\{1 - \cos(2\omega T)\right\} - \cos(2\delta)\sin(2\omega T)\right]$$
$$= \frac{m\omega}{2}A^2\sin(\omega T)\left[\sin(2\delta)\sin(\omega T) - \cos(2\delta)\cos(\omega T)\right]$$

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

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

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

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

Gaussian integral over the fluctuations:

$$\left|\det\left(\frac{\partial q_k}{\partial X_n}\right)\right| \prod_{n=1}^{N-1} \int dX_n \, e^{i\frac{mT}{4}\left\{\left(\frac{\pi n}{T}\right)^2 - \omega^2\right\}(X_n)^2} = \left|\det\left(\frac{\partial q_k}{\partial X_n}\right)\right| \cdot \prod_{n=1}^{N-1} \sqrt{\frac{4\pi}{-imT\left\{\left(\frac{\pi}{T}n\right)^2 - \omega^2\right\}}} \quad . \quad (***)$$

The $(\omega = 0)$ case is the free particle case.

$$(***)_\omega = (***)_{\omega=0} \times \frac{1}{\sqrt{\prod_{n=1}^{N-1}\left\{1 - \left(\frac{\omega T}{\pi n}\right)^2\right\}}} \xrightarrow[N\to\infty]{\lim} (***)_{\omega=0} \times \sqrt{\frac{\omega T}{\sin(\omega T)}} \; .$$

So,

$$\langle q_f @ T | e^{-iHT} | q_i @ 0 \rangle = e^{iS_{cl}} \cdot \underbrace{\left(\frac{mN}{2\pi i T}\right)^{\frac{N}{2}} \times (***)_{\omega=0}}_{\text{(free particle)}} \times \sqrt{\frac{\omega T}{\sin(\omega T)}}$$

$$= e^{iS_{cl}} \sqrt{\frac{m}{2\pi i T}} \times \sqrt{\frac{\omega T}{\sin(\omega T)}} \qquad \text{(use the result in p.3)}$$

$$= e^{iS_{cl}} \sqrt{\frac{m\omega}{2\pi i \sin(\omega T)}}$$

S_{cl}: worked out in p.5

Quantum states from path integral

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

$\mathrm{fn}(q_f, q_i ; t_f-t_i)$

$$\boxed{= \int \frac{d\omega}{2\pi}\, e^{-i\omega(t_f-t_i)}\ \psi_\omega(q_f)\,[\psi_\omega(q_i)]^*}$$

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

Time-ordered product expectation value

Consider

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

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

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

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.

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

is reproduced from the path integral formulation.