

§1. Many-particle quantum mechanics

* Single-particle QM : path integral formulation

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

Propagator :

$$U(x', t'; x, t) = \langle x' | e^{-\frac{i}{\hbar} \hat{H}(t'-t)} | x \rangle$$

$$= \int_{\substack{x(t)=x \\ x(t')=x'}} D x(t'') D p(t'')$$

$$\times e^{\frac{i}{\hbar} \int_t^{t'} dt'' [p(t'') \dot{x}(t'') - H(p(t''), x(t''))]}$$

↓
action S

Partition function :

$$Z = \text{Tr} e^{-\beta \hat{H}}$$

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

$$= \int_{x(0)=x(\beta)} D x(\tau) D p(\tau) e^{-\int_0^\beta d\tau [-i p(\tau) \dot{x}(\tau) + H(p(\tau), x(\tau))]}$$

$$0 \quad \Delta\tau = \frac{\beta}{N} \quad \beta = \frac{1}{T}$$

- Gaussian integration

Set $\hbar = 1$

$$Z = \int dx_0 \langle x_0 | e^{-\beta \hat{H}} | x_0 \rangle$$

$$= \int dx_0 dx_1 \dots dx_{N-1} \langle x_0 | e^{-\Delta\tau \hat{H}} | x_{N-1} \rangle \dots \langle x_1 | e^{-\Delta\tau \hat{H}} | x_0 \rangle$$

$$\langle x_1 | e^{-\Delta\tau \hat{H}} | x_0 \rangle = \int dp_1 \langle x_1 | p_1 \rangle \langle p_1 | (1 - \Delta\tau \hat{H}) | x_0 \rangle$$

$$\downarrow$$

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

$$= \int dp_1 \langle x_1 | p_1 \rangle \langle p_1 | x_0 \rangle [1 - \Delta\tau H(p_1, x_0)]$$

$$= \int dp_1 \frac{1}{\sqrt{2\pi}} e^{ip_1 x_1} \frac{1}{\sqrt{2\pi}} e^{-ip_1 x_0} e^{-\Delta\tau H(p_1, x_0)}$$

$$= \int \frac{dp_1}{2\pi} e^{-\frac{\Delta\tau}{2m} p_1^2 + i p_1 (x_1 - x_0)} e^{-\Delta\tau V(x_0)}$$

Gaussian integral: $\int_{-\infty}^{\infty} dp e^{-a(p+b)^2} = \sqrt{\frac{\pi}{a}}$

Complete square:

$$\int dp_1 e^{-\frac{\Delta\tau}{2m} p_1^2 + i p_1 (x_1 - x_0)} = \int_{-\infty}^{\infty} dp_1 e^{-\frac{\Delta\tau}{2m} [p_1 - i \frac{m}{\Delta\tau} (x_1 - x_0)]^2} \times e^{-\frac{m}{2\Delta\tau} (x_1 - x_0)^2}$$

$$= \sqrt{\frac{2\pi m}{\Delta\tau}} e^{-\frac{m}{2\Delta\tau} (x_1 - x_0)^2}$$

$$\Rightarrow \langle x_1 | e^{-\Delta\tau \hat{H}} | x_0 \rangle = \sqrt{\frac{2\pi m}{\Delta\tau}} e^{-\frac{m}{2\Delta\tau} (x_1 - x_0)^2 - \Delta\tau V(x_0)}$$

→ other matrix elements are similar

$$Z = \int dx_0 dx_1 \dots dx_{N-1} \langle x_0 | e^{-\Delta\tau \hat{H}} | x_{N-1} \rangle \dots \langle x_1 | e^{-\Delta\tau \hat{H}} | x_0 \rangle$$

$$= \int \prod_{j=0}^{N-1} dx_j \left(\frac{2\pi m}{\Delta\tau} \right)^{N/2} e^{-\frac{m}{2\Delta\tau} \sum_{k=0}^{N-1} (x_{k+1} - x_k)^2 - \Delta\tau \sum_{k=0}^{N-1} V(x_k)}$$

\downarrow
 $x_N = x_0$

Exercise: Calculate the partition function for the harmonic oscillator with $V(\hat{x}) = \frac{1}{2} m \omega^2 \hat{x}^2$.

(hint: Gaussian integrals over x_k , $k=0, \dots, N-1$)

$$N \rightarrow \infty \quad \Delta\tau \rightarrow 0 : \quad x_{k+1} - x_k \rightarrow \dot{x} \Delta\tau$$

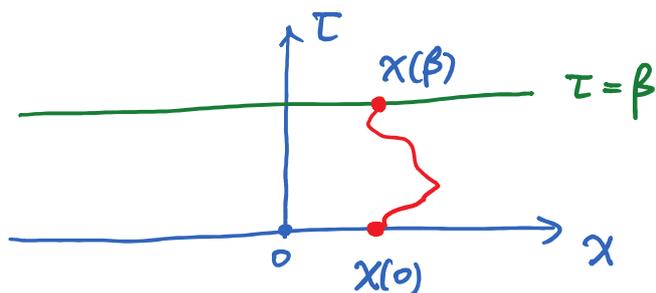
$$\int \prod_{k=0}^{N-1} dx_k \rightarrow \int \mathcal{D}x(\tau)$$

$$\Rightarrow Z = \int_{x(0)=x(\beta)} \mathcal{D}x(\tau) e^{-\int_0^\beta d\tau \left[\underbrace{\frac{1}{2} m \dot{x}(\tau)^2}_{\text{kinetic energy}} + \underbrace{V(x(\tau))}_{\text{potential energy}} \right]}$$

\uparrow
 Boltzmann weight

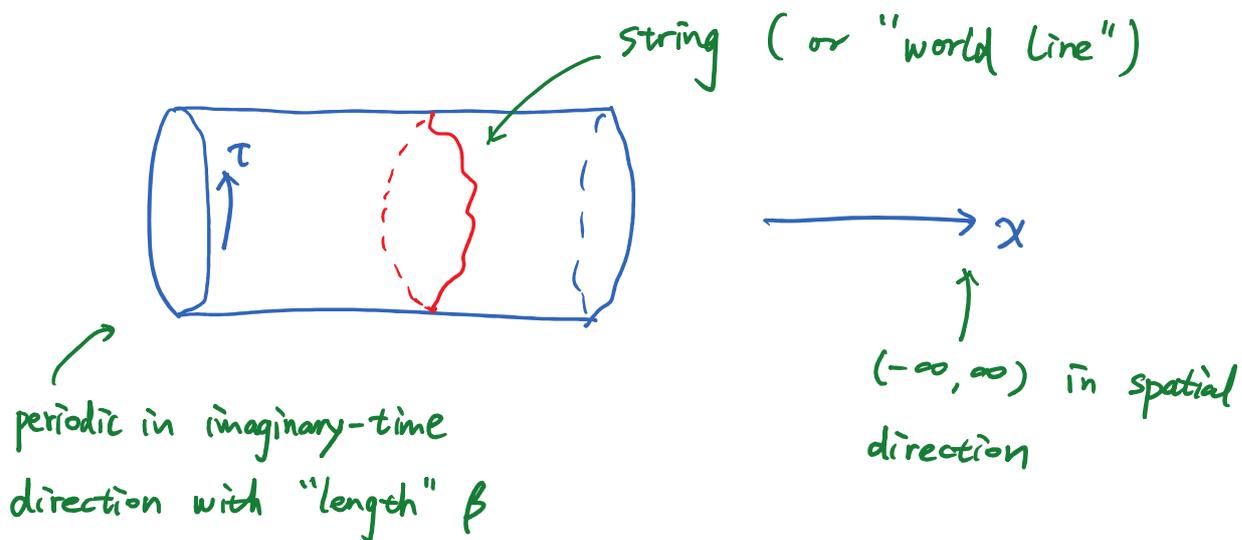
Classical partition function of a string!

string picture :



string, described by $x(\tau)$, has a Boltzmann weight

$$e^{-\int_0^\beta d\tau [\underbrace{T(x(\tau))}_{\frac{1}{2}m\dot{x}(\tau)^2} + V(x(\tau))]}$$



Gaussian integration for functional integrals:

$$Z = \int_{x(0)=x(\beta)} Dx(\tau) Dp(\tau) e^{-\int_0^\beta d\tau [-i p(\tau) \dot{x}(\tau) + \underbrace{H(p(\tau), x(\tau))}_{\frac{p^2}{2m} + V(x)}]}$$

$$= \int_{x(0)=x(\beta)} Dx(\tau) Dp(\tau) e^{-\int_0^\beta d\tau \left[\underbrace{\frac{1}{2m} (p(\tau) - im\dot{x}(\tau))^2}_{\text{complete square}} + \frac{1}{2} m \dot{x}(\tau)^2 + V(x(\tau)) \right]}$$

functional integral

over $p(\tau)$ is Gaussian

$$= \text{const.} \times \int_{x(0)=x(\beta)} Dx(\tau) e^{-\int_0^\beta d\tau \left[\frac{1}{2} m \dot{x}(\tau)^2 + V(x(\tau)) \right]}$$

same result recovered by "functional" Gaussian integration!

This form is convenient for semiclassical analysis.

↑
approximation scheme

Why approximation?



We only know how to exactly calculate Gaussian integrals ...

*) Second quantization: bosons

— Algebra

$$\hat{a}, \hat{a}^+ \quad [\hat{a}, \hat{a}^+] = 1$$

Hilbert space: $|0\rangle$ ($\hat{a}|0\rangle = 0$)

$$\hat{a}^+|0\rangle$$

$$(\hat{a}^+)^2|0\rangle$$

⋮

$$\hat{a}(\hat{a}^+)^2|0\rangle = [\hat{a}, (\hat{a}^+)^2]|0\rangle + (\hat{a}^+)^2 \hat{a}|0\rangle$$

use identity

$$[A, BC] = B[A, C] + [A, B]C$$

$$= (\hat{a}^+ \underbrace{[\hat{a}, \hat{a}^+]}_{=1} + \underbrace{[\hat{a}, \hat{a}^+]}_{=1} \hat{a}^+) |0\rangle$$

$$= 2\hat{a}^+|0\rangle \Rightarrow \text{proportional to } \hat{a}^+|0\rangle$$

Similarly, other states with \hat{a} inserted are not independent from the states of the form $(\hat{a}^+)^n|0\rangle$.

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle, \quad n=0, 1, \dots, \infty$$

$$\begin{cases} \langle n | n' \rangle = \delta_{nn'} \\ \sum_{n=0}^{\infty} |n\rangle \langle n| = \hat{1} \end{cases}$$

orthonormal & complete basis!

boson-number operator:

$$\hat{n} = \hat{a}^\dagger \hat{a}$$

$$\hat{n} |n\rangle = n |n\rangle \quad (\text{Proof: use commutator})$$

Example: 1D harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \quad [\hat{x}, \hat{p}] = i\hbar$$

bosonic representation:
$$\begin{cases} \hat{x} = \frac{1}{\sqrt{2}} \sqrt{\frac{\hbar}{m\omega}} (\hat{a} + \hat{a}^\dagger) \\ \hat{p} = -\frac{i}{\sqrt{2}} \hbar \sqrt{\frac{m\omega}{\hbar}} (\hat{a} - \hat{a}^\dagger) \end{cases}$$
 Hermitian!

$$\begin{aligned} [\hat{x}, \hat{p}] &= -\frac{i}{2} \hbar [\hat{a} + \hat{a}^\dagger, \hat{a} - \hat{a}^\dagger] \\ &= -\frac{i}{2} \hbar (-[\hat{a}, \hat{a}^\dagger] + [\hat{a}^\dagger, \hat{a}]) \end{aligned}$$

$$= i\hbar \Rightarrow \text{commutator correctly reproduced}$$

$$\Rightarrow \hat{H} = \hbar\omega \left(\underbrace{\hat{a}^\dagger \hat{a}}_{\hat{n}} + \frac{1}{2} \right)$$

Eigenstates: $|n\rangle$

$$\hat{H} |n\rangle = \underbrace{(n + \frac{1}{2}) \hbar\omega}_{E_n} |n\rangle$$

E_n : energies

$\psi_n(x) = \langle x | n \rangle$: Hermite polynomials

($n=0$: Gaussian wave packet)

partition function:

$$\begin{aligned}
 Z &= \text{Tr} e^{-\beta \hat{H}} \\
 &= \sum_{n=0}^{\infty} \langle n | e^{-\beta \hat{H}} | n \rangle \quad \leftarrow \hat{H} |n\rangle = (n + \frac{1}{2}) \hbar \omega |n\rangle \\
 &= \sum_{n=0}^{\infty} e^{-(n + \frac{1}{2}) \beta \hbar \omega} \quad \leftarrow \text{geometric series} \\
 &= \left(\sum_{n=0}^{\infty} e^{-n \beta \hbar \omega} \right) e^{-\frac{1}{2} \beta \hbar \omega} \\
 &= \frac{1}{1 - e^{-\beta \hbar \omega}} e^{-\frac{1}{2} \beta \hbar \omega} \\
 &= \frac{1}{e^{\frac{1}{2} \beta \hbar \omega} - e^{-\frac{1}{2} \beta \hbar \omega}} \Rightarrow \text{Check your path-integral result!}
 \end{aligned}$$

- Many bosons

$$\hat{a}_j, \hat{a}_j^+ \quad j=1, \dots, N$$

$$\begin{cases} [\hat{a}_j, \hat{a}_l] = [\hat{a}_j^+, \hat{a}_l^+] = 0 \\ [\hat{a}_j, \hat{a}_l^+] = \delta_{jl} \end{cases}$$

e.g. bosons on a 1D chain:



$$|n_1, n_2, \dots, n_N\rangle = \frac{1}{\sqrt{n_1! \dots n_N!}} (\hat{a}_1^\dagger)^{n_1} \dots (\hat{a}_N^\dagger)^{n_N} |0\rangle$$

orthonormal & complete basis!

— Quadratic Hamiltonians of bosons

(Note: pairing not considered here)

$$\hat{H} = \sum_{j,l=1}^N t_{jl} \hat{a}_j^\dagger \hat{a}_l$$

$$t_{jl} = t_{lj}^* \\ \text{(required by } \hat{H}^\dagger = \hat{H}\text{)}$$

Eigenstates & energies?

Unitary transformation on bosonic modes:

$$\hat{b}_p = \sum_{j=1}^N U_{pj} \hat{a}_j$$

$$\hat{b}_p^\dagger = \sum_{j=1}^N \hat{a}_j^\dagger (U^\dagger)_{jp}$$

$$\hat{b} = U \hat{a}$$

$$\hat{b}^\dagger = \hat{a}^\dagger U^\dagger$$

$$\begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \\ \vdots \\ \hat{b}_N \end{pmatrix} = U \begin{pmatrix} \hat{a}_1 \\ \hat{a}_2 \\ \vdots \\ \hat{a}_N \end{pmatrix}$$

$$(\hat{b}_1^\dagger, \hat{b}_2^\dagger, \dots, \hat{b}_N^\dagger) = (\hat{a}_1^\dagger, \hat{a}_2^\dagger, \dots, \hat{a}_N^\dagger) U^\dagger$$

U : $N \times N$ unitary matrix

$$\begin{aligned}
\Rightarrow \left\{ \begin{aligned} [\hat{b}_p, \hat{b}_q] &= [\hat{b}_p^+, \hat{b}_q^+] = 0 && \text{(easy to prove)} \\ [\hat{b}_p, \hat{b}_q^+] &= \left[\sum_{j=1}^N U_{pj} \hat{a}_j, \sum_{l=1}^N \hat{a}_l^+ (U^+)_{lq} \right] \\ &= \sum_{j,l=1}^N U_{pj} (U^+)_{lq} \underbrace{[\hat{a}_j, \hat{a}_l^+]}_{\delta_{jl}} \\ &= \sum_{j=1}^N U_{pj} (U^+)_{jq} \\ &= (U U^+)_{pq} \\ &\quad \underbrace{\quad}_{\parallel} \quad \underbrace{\quad}_{\parallel} \\ &\quad \quad \quad I_{N \times N} \text{ (since } U \text{ is } N \times N \text{ unitary)} \\ &= \delta_{pq} \end{aligned} \right.
\end{aligned}$$

\Rightarrow Unitary transformation preserves bosonic commutation relations.

$$\hat{H} = \sum_{j,l=1}^N t_{jl} \hat{a}_j^+ \hat{a}_l$$

$$= \hat{a}^+ T \hat{a}$$

$$T_{jl} = t_{jl}, \quad T \text{ Hermitian}$$

$$= \underbrace{\hat{a}^+}_{\parallel \hat{b}^+} U^+ \underbrace{U T U^+}_{\parallel} \underbrace{\hat{a}}_{\parallel \hat{b}}$$

$$\text{since } t_{jl} = t_{lj}^*$$

Choose U such that $U T U^+ = \begin{pmatrix} \epsilon_1 & & \\ & \epsilon_2 & \\ & & \ddots \\ & & & \epsilon_N \end{pmatrix}$

$$\Rightarrow \hat{H} = \hat{b}^\dagger \begin{pmatrix} \epsilon_1 & & & \\ & \epsilon_2 & & \\ & & \ddots & \\ & & & \epsilon_N \end{pmatrix} \hat{b}$$

$$= \sum_{p=1}^N \epsilon_p \hat{b}_p^\dagger \hat{b}_p$$

$$\hat{n}_p = \hat{b}_p^\dagger \hat{b}_p, \quad [\hat{n}_p, \hat{n}_q] = 0$$

$$\text{Eigenstates: } |n_1, n_2, \dots, n_N\rangle_b = \frac{1}{\sqrt{n_1! \dots n_N!}} (b_1^\dagger)^{n_1} \dots (b_N^\dagger)^{n_N} |0\rangle_b$$

In this case the vacuum of b-boson and the vacuum of a-boson are identical,

$$|0\rangle_b = |0\rangle_a$$

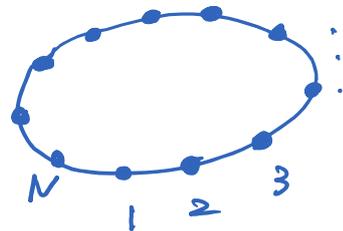
$$\hat{H} |n_1, \dots, n_N\rangle_b = \left(\sum_{p=1}^N \epsilon_p n_p \right) |n_1, \dots, n_N\rangle_b$$

↓
energy

$$\text{Example: } t_{jl} = -t(\delta_{j,l+1} + \delta_{j,l-1})$$

periodic boundary condition (PBC):

$$\hat{a}_{N+1} = \hat{a}_1$$



$$\Rightarrow \hat{b}_k = \frac{1}{\sqrt{N}} \sum_{j=1}^N \hat{a}_j e^{-ikj} \quad \left(k = 0, \pm \frac{2\pi}{N}, \pm \frac{4\pi}{N}, \dots, \pm \frac{2\pi}{N} \left(\frac{N}{2} - 1 \right), \pi \right)$$

↙ Fourier transformation

$$\hat{H} = \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \hat{b}_{\mathbf{k}'}^\dagger \hat{b}_{\mathbf{k}}$$

$$\hookrightarrow \epsilon_{\mathbf{k}} = -2t \cos k$$

↑ defines
"first Brillouin zone"
 $k \in (-\pi, \pi]$