Path-integral Monte Carlo (PIMC)

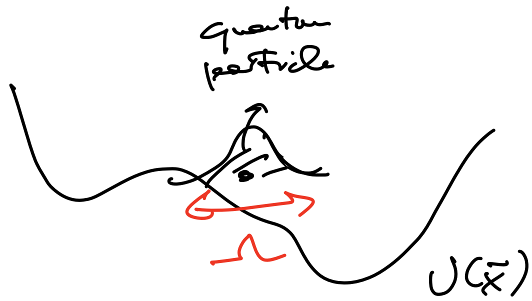
$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} + U(\hat{\vec{x}}) \qquad \beta = \frac{1}{k_B T}$$

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] = \lim_{M \to \infty} Z_M$$

$$Z_M(\beta) = \left(\frac{M^{1/2}}{\lambda}\right)^{Md} \int \left(\prod_{k=0}^{M-1} d^d x_k\right) e^{-S[\{\vec{x}_n\}]} \qquad S[\{\vec{x}_n\}] = \beta H_{eff}[\{\vec{x}_n\}]$$

$$\vec{x}_0 = \vec{x}_M$$

$$H_{eff}[\{\vec{x}_n\}] = \sum_{k=0}^{M-1} \frac{1}{2}\kappa \left(\vec{x}_n - \vec{x}_{n+1}\right)^2 + \frac{1}{M} \sum_{k=0}^{M-1} U(\vec{x}_n)$$



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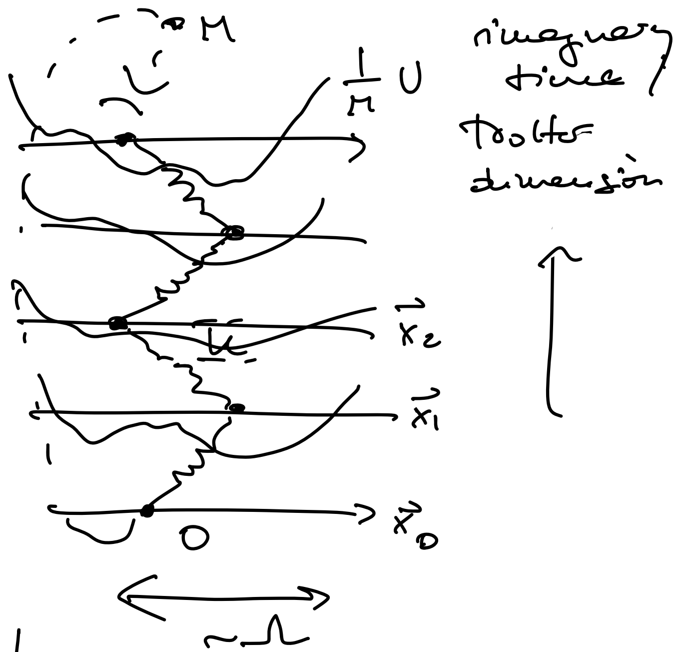


$$\kappa = \frac{2\pi M}{\beta \lambda^2} \qquad \lambda = \frac{h}{\sqrt{2\pi m k_B T}}$$

$$\langle U(\hat{\vec{x}}) \rangle \underset{M \gg 1}{\simeq} \langle U(\vec{x}_0) \rangle_S$$

$$= \frac{1}{Z_M} \int \left(\frac{M^{1/2}}{\lambda}\right)^{Md} \left(\prod_{n=0}^{M-1} d^d x_n\right) U(\vec{x}_0)\, e^{-S}$$

$$= \frac{1}{M} \sum_{k=0}^{M-1} \langle U(\vec{x}_k) \rangle_S$$ diagonal observable

$\hat{H}$: off-diagonal in $|\vec{x}\rangle$

$$\langle \hat{H} \rangle = \langle E(\{\vec{x}_k\}) \rangle_S \neq \langle H_{eff} \rangle$$

estimator

$$\langle \hat{H} \rangle = \frac{\partial(\beta F)}{\partial \beta} = -\frac{\partial(\log Z)}{\partial \beta}$$

$$= -\frac{1}{Z}\frac{\partial Z}{\partial \beta},$$

$$F = -k_B T \log Z$$

$$Z = \sum_\alpha e^{-\beta E_\alpha}$$

$$\langle \hat{H} \rangle \simeq \langle E_M \rangle_S$$

$$E_M(\{\vec{x}_k\}) \quad (\neq \quad H_{eff}(\{\vec{x}_k\}) \quad)$$

$$= k_B T \left(\frac{Md}{2} - \sum_{k=0}^{M-1} \frac{\pi M}{\Lambda^2} (\vec{x}_k - \vec{x}_{k+1})^2 \right)$$

$$+\frac{1}{M}\sum_{k=0}^{M-1} U(\vec{x}_k)$$

Alternative estimator

$$\sum_k (\vec{x}_k - \vec{x}_{k+1})^2 = \alpha(\{\vec{x}_k\})$$

$$= 2\sum_k \vec{x}_k \cdot \vec{\nabla}_{\vec{x}_k} \alpha$$

$$\left(\frac{M^{1/2}}{\Lambda}\right)^{Md}\left(\prod_{k=0}^{M-1} d^d x_k\right)$$

$$\left\langle \sum_k (\vec{x}_k - \vec{x}_{k+1})^2 \right\rangle = \frac{1}{Z}\int \mathcal{D}[\{\vec{x}_k\}] \times \sum_k (\vec{x}_k - \vec{x}_{k+1})^2 e^{-S}$$

$$\left\langle k_B T\left[\frac{Md}{2} - \frac{\pi M}{\Lambda^2}\sum_k (\vec{x}_k - \vec{x}_{k+1})^2\right]\right\rangle_S$$

kinetic energy

$$= \left\langle \frac{1}{2M}\sum_k \vec{x}_k \cdot \vec{\nabla}_{\vec{x}_k} U \right\rangle_S$$

Virial estimator

$$\langle \hat{\mathcal{H}} \rangle = \left\langle \frac{1}{M} \left[\sum_{n=0}^{M-1} U(\vec{x}_n) + \frac{1}{2} \sum_n \vec{x}_n \cdot \vec{\nabla}_{\vec{x}_n} U \right] \right\rangle_S$$

PIMC : from one particle to <u>N particles</u>

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} U(\vec{x}_i) + \frac{1}{2} \sum_{i \neq j} v(\vec{x}_i - \vec{x}_j)$$

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{\mathcal{H}}} \right]$$

$$|\vec{x}\rangle \longrightarrow |\vec{x}_1 \vec{x}_2 \ldots \vec{x}_N\rangle$$

<u>distinguishable</u>

$$\rho(\vec{x}_1 \vec{x}_2 \ldots \vec{x}_N | \vec{x}_1' \vec{x}_2' \ldots \vec{x}_N' ; \beta)$$

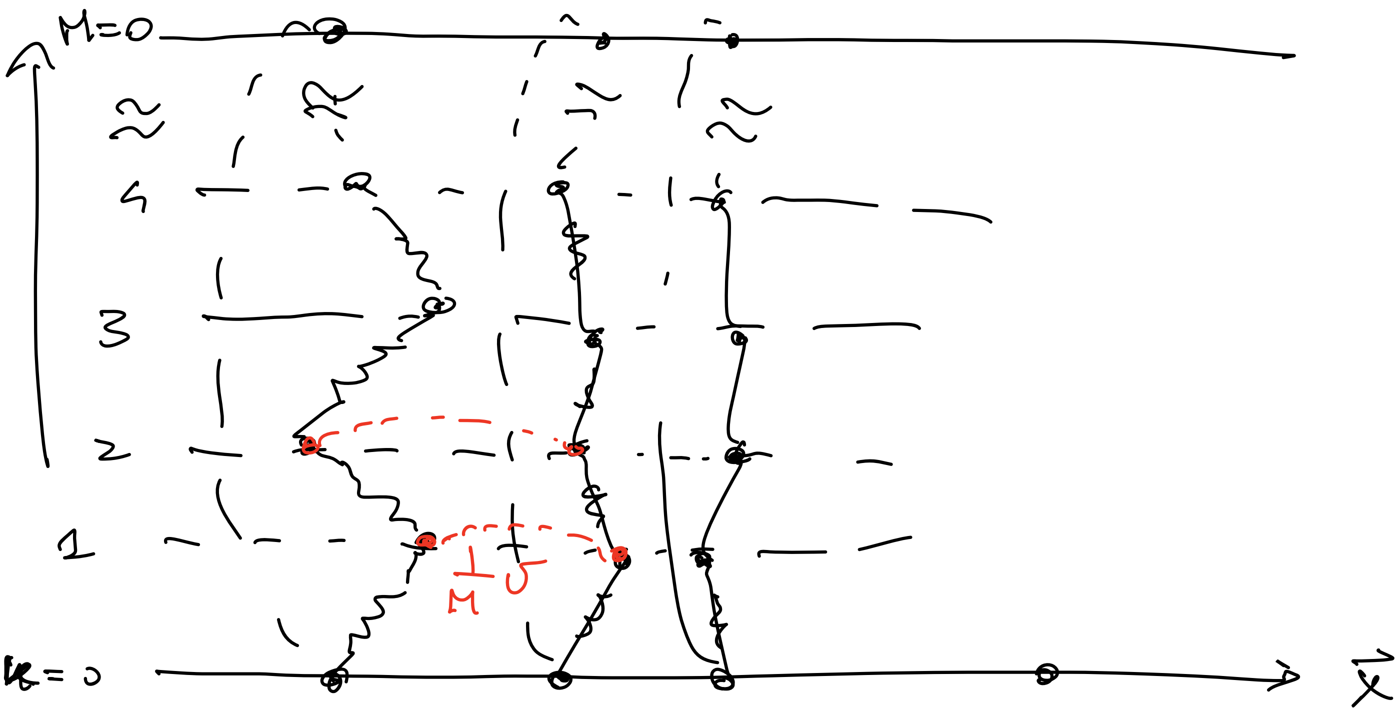
$$= \langle \vec{x}_1 \vec{x}_2 \ldots \vec{x}_N | e^{-\beta \hat{\mathcal{H}}} | \vec{x}_1' \vec{x}_2' \ldots \vec{x}_N' \rangle$$

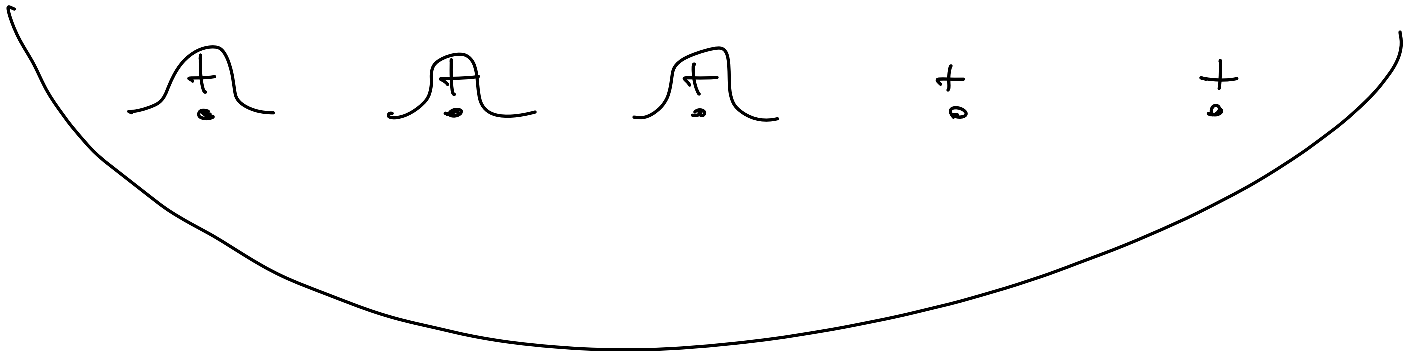
$$Z = \int \left(\prod_{i=1}^{N} d^d x_i \right) \rho(\vec{x}_1 \ldots \vec{x}_N | \vec{x}_1 \ldots \vec{x}_N ; \beta)$$

$$= \lim_{M\to\infty} \underbrace{\int \left(\frac{M}{\lambda}\right)^{\frac{1}{2}MdN} \left(\prod_{i=1}^{N} \prod_{k=0}^{M-1} d^d x_{i,k}\right)}_{\mathcal{D}[\{\vec{x}_{i,k}\}]} e^{-S'[\{\vec{x}_{i,k}\}]}$$

$$S'[\{\vec{x}_{i,k}\}] = \beta\, \mathcal{H}_{eff}[\{\vec{x}_{i,k}\}]$$

$$\mathcal{H}_{eff}[\{\vec{x}_{i,k}\}] = \sum_{i=1}^{N} \left[\sum_{k=0}^{M-1} \frac{1}{2} \underline{k} \left(\vec{x}_{i,k} - \vec{x}_{i,k+1}\right)^2 + \frac{1}{M} \sum_{k=0}^{M-1} U(\vec{x}_k) \right] + \frac{1}{2M} \sum_{i\neq j} \sum_{k=0}^{M-1} v(\vec{x}_{i,k} - \vec{x}_{j,k})$$



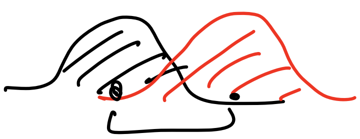


Wigner crystal

Indistinguishable quantum particles

quantum degeneracy

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}} \sim n^{-1/d} = a \qquad \text{average density}$$



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$$T \sim \frac{h^2}{2\pi m} n^{2/d} \nearrow \sim T_{BEC} \qquad \underline{\text{bosons}}$$

$$\searrow \sim T_F \qquad \underline{\text{fermions}}$$

$$|\vec{x}_1 \, \vec{x}_2 \ldots \vec{x}_N \rangle$$

$$\to |\vec{x}_1 \, \vec{x}_2 \ldots \vec{x}_N\rangle_\eta$$

$$= \frac{1}{\sqrt{N!}} \sum_P \eta^P \, \underbrace{|\vec{x}_{P(1)} \, \vec{x}_{P(2)} \cdots \vec{x}_{P(N)}\rangle}$$

η^P = sign of the permutation

$$\eta = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases}$$

$$\rho_\eta(\vec{x}_1 \, \vec{x}_2 \ldots \vec{x}_N | \vec{x}_1 \, \vec{x}_2 \ldots \vec{x}_N) \quad \longleftarrow$$

$$= \cancel{\frac{1}{N!}} \sum_{P \cancel{P'}} \eta^{P + \cancel{P'}} \langle \vec{x}_{P'(1)} \, \vec{x}_{P'(2)} \ldots \vec{x}_{P'(N)} | e^{-\beta \hat{\mathcal{H}}} | \vec{x}_{P(1)} \ldots \vec{x}_{P(N)}\rangle$$

$$Z_\eta = \int \underbrace{\left(\prod_{i=1}^N d^d x_i\right)} \cancel{\frac{1}{N!}} \sum_{P \cancel{P'}} \eta^{P + \cancel{P'}} \langle \vec{x}_{P'(1)} \, \vec{x}_{P'(2)} \ldots \vec{x}_{P'(N)} | e^{-\beta \hat{\mathcal{H}}} | \vec{x}_{P(1)} \, \vec{x}_{P(2)} \ldots \vec{x}_{P(N)}\rangle$$

$$\underline{\prod_{i=1}^N d^d x_{\underline{\underline{P'(i)}}}} \to \vec{y}_i$$

$$= \sum_P \eta^P \int \left(\prod_{i=1}^N d^d x_i\right) \langle \vec{x}_1 \, \vec{x}_2 \ldots \vec{x}_N | e^{-\beta \hat{\mathcal{H}}} | \vec{x}_{P(1)} \, \vec{x}_{P(2)} \ldots \vec{x}_{P(N)}\rangle$$

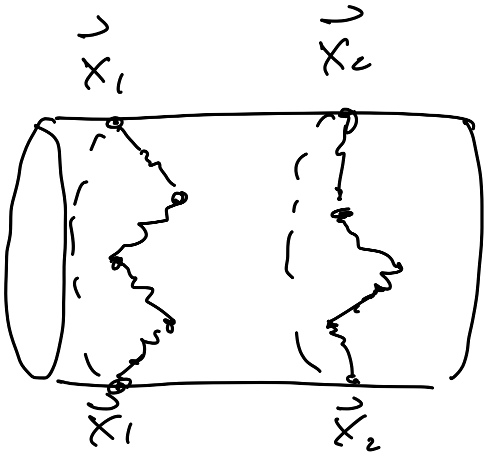
Example: 2 particles

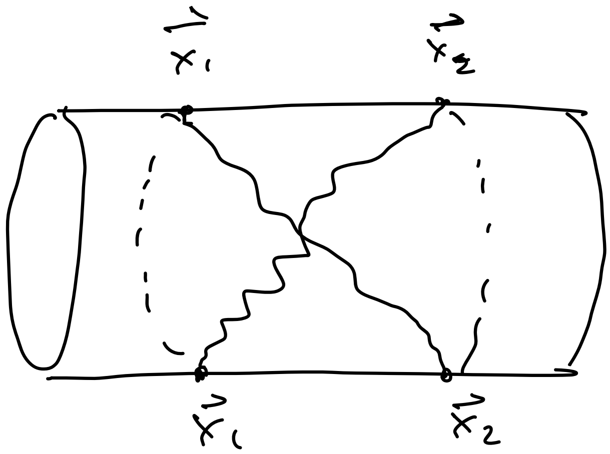
$$|\vec{x}_1\, \vec{x}_2\rangle_\eta = \frac{1}{\sqrt{2}}\left(|\vec{x}_1\, \vec{x}_2\rangle + \eta\, |\vec{x}_2\, \vec{x}_1\rangle \right)$$

$$Z = \frac{1}{2}\frac{1}{2}\int d^d x_1\, d^d x_2 \left(\langle \vec{x}_1\, \vec{x}_2| + \eta \langle \vec{x}_2\, \vec{x}_1| \right) e^{-\beta \hat{\mathcal{H}}} \left(|\vec{x}_1\, \vec{x}_2\rangle + \eta\, |\vec{x}_2\, \vec{x}_1\rangle \right)$$

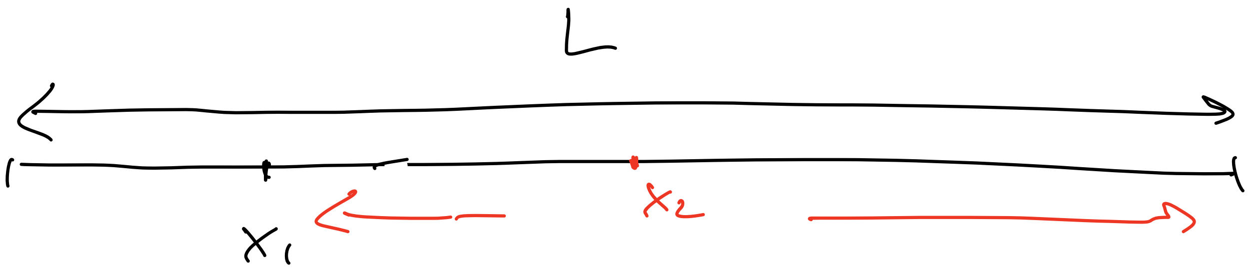
$$= \frac{1}{2}\cancel{\frac{1}{2}} \int d^d x_1\, d^d x_2 \Big[\langle \vec{x}_1\, \vec{x}_2 | e^{-\beta \hat{\mathcal{H}}} | \vec{x}_1\, \vec{x}_2\rangle + \cancel{\langle \vec{x}_2\, \vec{x}_1 | e^{-\beta \mathcal{H}}} |\vec{x}_2\, \vec{x}_1\rangle$$
$$\eta \left(\langle \vec{x}_1\, \vec{x}_2 | e^{-\beta \mathcal{H}} | \vec{x}_2\, \vec{x}_1\rangle + \cancel{\langle \vec{x}_2\, \vec{x}_1 | e^{-\beta \mathcal{H}}} |\vec{x}_1\, \vec{x}_2\rangle \right) \Big]$$

$$= \frac{1}{2}\int d^d x_1\, d^d x_2 \Big[\langle \vec{x}_1\, \vec{x}_2 | e^{-\beta \mathcal{H}} | \vec{x}_1\, \vec{x}_2\rangle + \eta \langle \vec{x}_1\, \vec{x}_2 | e^{-\beta \mathcal{H}} | \vec{x}_2\, \vec{x}_1\rangle \Big]$$





$$Z = \int d^d x_1 \int d^d x_2 \quad (\qquad)$$

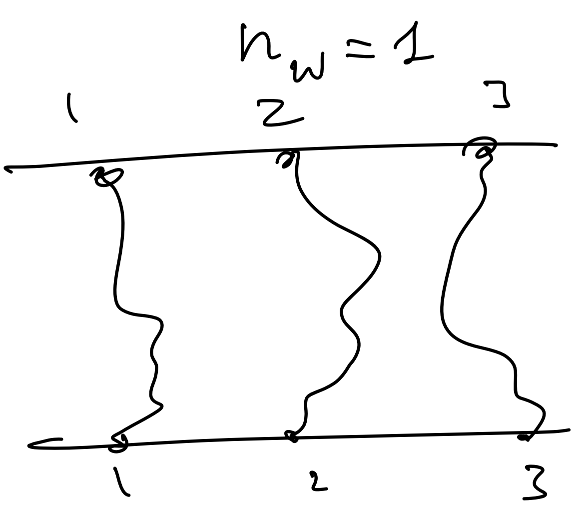


$$\int_0^L dx_1 \int_{x_1}^L dx_2 (\ldots) = \frac{1}{2} \int dx_1 \int dx_2$$

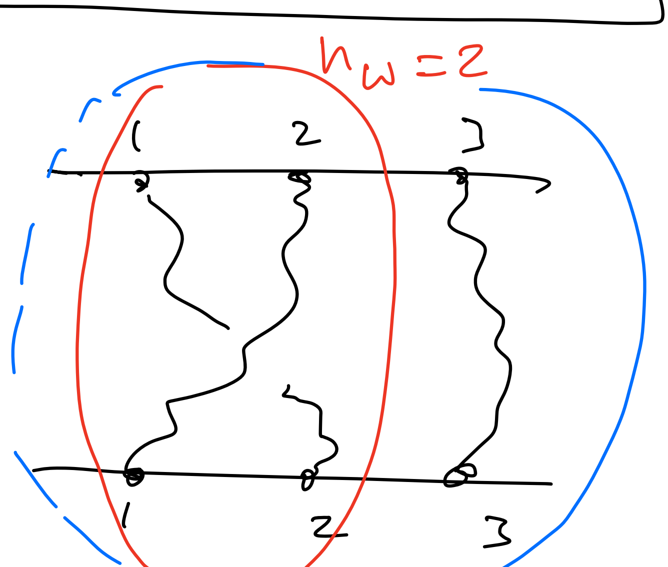
$$\int dx_1 \int_{x_1}^{L} dx_2 \int_{x_{N-1}}^{L} dx_N = \frac{1}{N!} \int dx_1 \, dx_2 \ldots dx_N$$

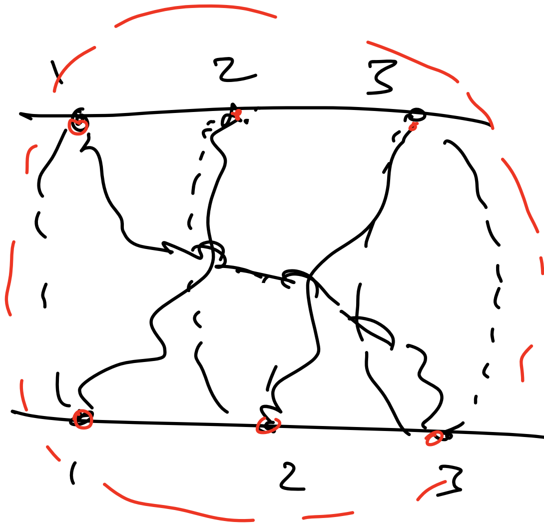
$$Z_\eta = \frac{1}{N!} \underline{\sum_P} \eta^P \int \left(\prod_{i=1}^{N} d^d x_i \right)$$

$$\underbrace{\langle \vec{x}_1 \vec{x}_2 \ldots \vec{x}_N | e^{-\beta H} | \vec{x}_{P(1)} \vec{x}_{P(2)} \ldots \vec{x}_{P(N)} \rangle}$$



$+\ \eta$

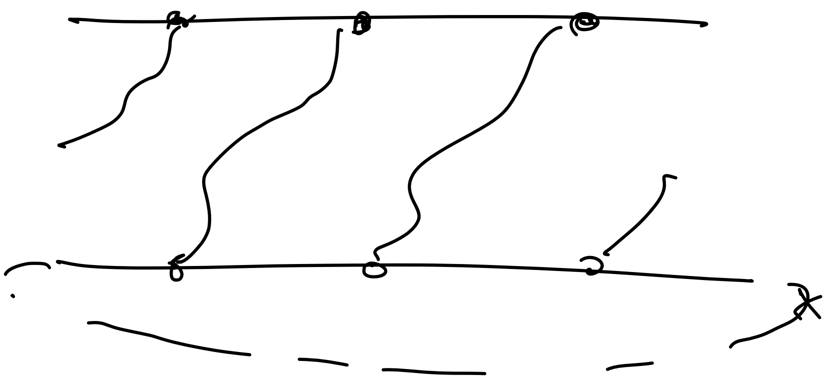


$+ \eta^2$ 

winding number

$n_w = 3$

"permutation cycles"

(or 

with periodic boundary conditions in real space)

<u>BEC</u> : macroscopic permutation cycles

$O(N)$ particles involved in the same ring polymer

<u>challenge</u> for PIMC of N identical quantum particles

→ sample over { → positions of the beads of each polymer
→ permutation cycles }

(Exchange n_w)

The SIGN PROBLEM for fermions

$$Z_F = \sum_{P \text{ even}} \int_{\{\vec{x}_{i,0}\} \to \{\vec{x}_{P(i),M}\}} \mathcal{D}[\{\vec{x}_{i,n}\}]\, e^{-S}$$

$$- \sum_{P \text{ odd}} \int_{\{\vec{x}_{i,0}\} \to \{\vec{x}_{P(i),M}\}} \mathcal{D}[\{\vec{x}_{i,n}\}]\, e^{-S}$$

$$= \underbrace{Z_{\text{even}} - Z_{\text{odd}}}$$

$$\left[\begin{array}{l} Z_B = \sum_P \int_{\{\vec{x}_{i,0}\} \to \{\vec{x}_{P(i),M}\}} \mathcal{D}[\{\vec{x}_{i,n}\}] \\ (\eta = 1) \end{array} \right]$$

$$= Z_B \underbrace{\frac{1}{Z_B} \left(\sum_P \int \mathcal{D}[\ ]\, e^{-S}\, \eta^P \right)}$$

$$\langle \text{sign}(P) \rangle_B$$

$$\langle \hat{O} \rangle = \frac{1}{Z_F} \mathrm{Tr}\left[\hat{O}\, e^{-\beta \hat{\mathcal{H}}} \right]$$

$$= \frac{1}{\cancel{Z_B} \langle \mathrm{sign}(P) \rangle_B} \cancel{Z_B} \frac{1}{Z_B}$$

$$\sum_P \int \mathcal{D}[\{\vec{x}_{i,n}\}]\, O(\{\vec{x}_n\})\, \eta^P e^{-S}$$

$$\langle O \;\; \mathrm{sign}(P) \rangle_B$$

$$= \frac{\langle O\, \mathrm{sign}(P) \rangle_B}{\langle \mathrm{sign}(P) \rangle_B}$$

1) $\langle \mathrm{sign}(P) \rangle_B = \dfrac{Z_F}{Z_B} \geq 0$

$$Z_F = \exp(-\beta F_F)$$

$$Z_B = \exp(-\beta F_B) \qquad \Delta F = F_F - F_B$$

$$\langle \mathrm{sign}(P) \rangle_B = \exp(-\beta \Delta F) < 1$$

$$\Delta F > 0$$

$$\Delta F \sim O(N) \qquad \Delta F = N \, \Delta f$$

$$\langle \text{sign}(P) \rangle_\beta = \underbrace{\exp(-\Delta f \, N\beta)}$$

$$1 \; 1 \; -1 \; -1 \; 1 \; 1 \; 1 \; -1 \; -1$$

$$\frac{1}{N_{MC}} \underbrace{\sum_{j=1}^{N_{MC}} \text{sign}_j}_{O(1)} \simeq$$

$\sim O(\exp(-N\beta))$

to correctly estimate $\langle \text{sign} \rangle$ I need exponentially large statistics in N and β.

<u>Phase problem</u> : bosons or fermions in a gauge field

<u>ex.</u> : $$\mathcal{H} = \frac{(\vec{p} - q\vec{A})^2}{2m}$$

$$\vec{A} = (0, Bx, 0) \qquad \vec{B} = B \, \vec{e}_z$$

$$\rho_{\vec{A}}(\vec{x}, \vec{x}'; \beta) \equiv \langle \vec{x} | e^{-\beta \mathcal{H}} | \vec{x}' \rangle$$

$$= \sum_n e^{-\beta E_n} \psi_n(\vec{x}) \psi_n^*(\vec{x}') \in \mathbb{C}$$

$$\vec{A} = 0 \qquad \rho = (\quad) e^{-\frac{(\vec{x}-\vec{x}')^2}{\pi \lambda^2}} \in \mathbb{R}^+$$

harmonic oscillator

$$\psi_n(\vec{x}) = e^{i(k_y y + k_z z)} \varphi_{n'}\left(x - \frac{\hbar k_y}{m\omega_L}\right)$$

$$n = (k_x, k_y, n') \qquad \omega_L = \frac{qB}{m}$$

$$Z = \int d^d x \langle \vec{x} | e^{-\beta \mathcal{H}} | \vec{x} \rangle$$

$$= \int \left(\frac{m^{1/2}}{\lambda}\right)^{Md} \left(\prod_n d^d x_n\right) e^{-S}$$

$$\in \mathbb{C}$$

$$|e^{-S}| e^{i\phi}$$

$$= \langle e^{i\phi} \rangle_{|e^{-S}|} Z_{|e^{-S}|}$$

$$\langle e^{i\phi} \rangle_{|e^{-S}|} \sim O(\exp(-\beta N))$$

in an N-particle system

PIMC works for

- systems of many bosons without gauge fields

- systems of "distinguishable" particles ("Boltzmannons")