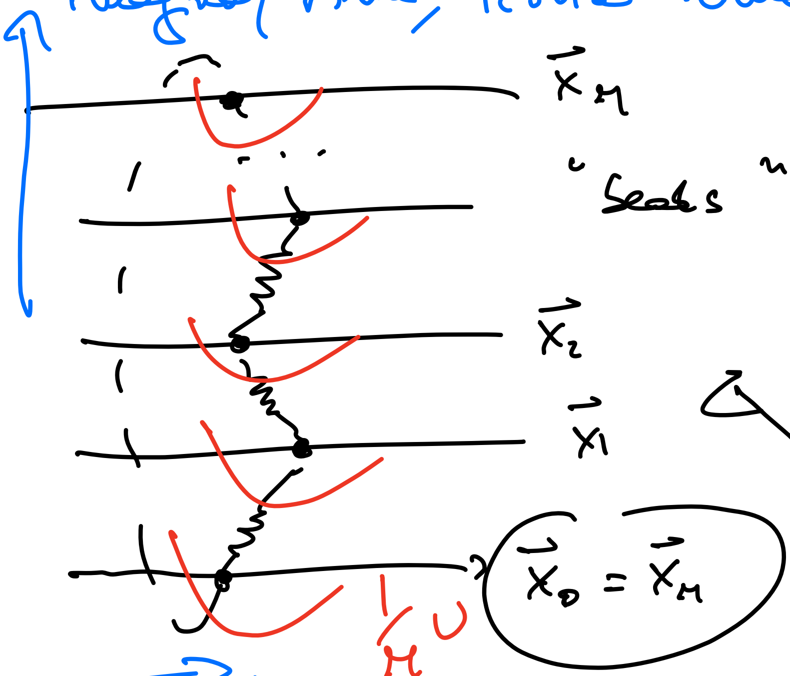
Path-integral MC (PIMC)

For a single quantum particle

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

$$Z(\beta) = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right)$$

$$= \lim_{M \to \infty} \left(\frac{M^{1/2}}{\Lambda}\right)^{Md} \int \left(\prod_{n=1}^{M} d\vec{x}_n\right) e^{-S[\{\vec{x}_n\}]}$$



"elastic ring polymer"

d-dimensional quantum system

≅

(d+1)-dimensional classical system

$$S[\{\vec{x}_n\}] = \beta H_{\mathrm{eff}}[\{\vec{x}_n\}]$$

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

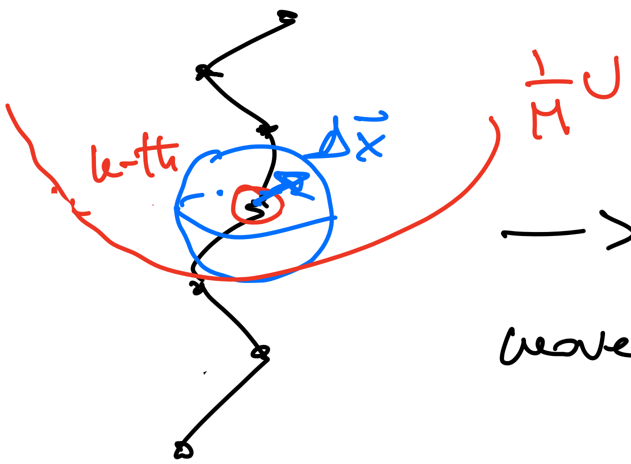
$$K = \frac{2\pi M}{\beta \Lambda^2} \to \begin{cases} \infty & \beta \to 0 \quad T \to \infty \\ 0 & \beta \to \infty \quad T \to 0 \end{cases}$$

$$= \frac{(2\pi)^2 M (k_B T)^2\, m}{h} \begin{cases} \nearrow \infty & m \to \infty \\ \searrow 0 & m \to 0 \end{cases}$$

$$\begin{cases} \nearrow \infty & h \to 0 \\ \searrow 0 & h \to \infty \end{cases}$$

MC simulation to sample the configurations of the classical ring polymer

pick a bead (k) at random → choose a displ. $\Delta\vec{x}$



⟶ move

$$\Delta S = S[\{\vec{x}_k^{(0)} + \Delta\vec{x}\}] - S[\{\vec{x}_k^{(0)}\}]$$

$\{x_k^{(0)}\}$

$$A(\vec{x} \to \vec{y})$$

$$\boxed{p_{move} = \min\left(1,\ e^{-\Delta S}\right)}$$

$M < \infty$: Trotter approximation

u error

$$\left[e^{-\frac{\beta}{M}\left(\frac{\hat{p}^2}{2m}+\hat{U}\right)}\right]^M \simeq \left[e^{-\frac{\beta}{M}\frac{\hat{p}^2}{2m}}\, e^{-\frac{\beta}{M}\hat{U}} + O\left(\frac{\beta^2}{M^2}\right)\right]^M$$

Trotter decomposition

I

$$= \left[e^{(\;)}\, e^{(\;)}\right]^M + \cancel{M}\, O\left(\frac{\beta^2}{M^{\cancel{2}}}\right)$$

more elaborate Trotter decompositions

$$\left[e^{-\frac{\beta}{M}\left(\frac{\hat{p}^2}{2m}+\hat{U}\right)}\right]^M \simeq \left[e^{-\frac{\beta}{2M}\hat{U}}\, e^{-\frac{\beta}{M}\frac{\hat{p}^2}{2m}}\, e^{-\frac{\beta}{2M}\hat{U}} + O\left(\frac{\beta^3}{M^3}\right)\right]^M$$

II

$$= \left(e^{-\frac{\beta}{2M}\hat{U}}\, e^{-\frac{\beta}{M}\frac{\hat{p}^2}{2m}}\, e^{-\frac{\beta}{2M}\hat{U}}\right)^M + O\left(\frac{\beta^3}{M^2}\right)$$

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

If we had exact decomposition (a)

$$S = \beta \mathcal{H}_{eff} = \beta \Big[\tfrac{1}{2} \mathrm{Tr}(\qquad)$$

$$\vec{x}_M = \vec{x}_0 \qquad + \underbrace{\frac{1}{2M} \sum_{k=0}^{M-1} \left(U(\vec{x}_k) + U(\vec{x}_{k+1}) \right)}_{= \frac{1}{M} \sum_k U(\vec{x}_k)} \Big]$$

$\Rightarrow$ Trotter error

$$Z_M = Z_{ex} + O\left(\frac{\beta^3}{M^2} \right)$$

Observables :

$$\langle \hat{A} \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta \hat{\mathcal{H}}} \hat{A} \right)$$

$$\mathrm{Tr}\left(e^{-\beta \hat{\mathcal{H}}} \right) \xrightarrow[\text{classical mapping}]{\text{quantum-to}} \text{"} \sum_{\{\vec{x}_k\}} \text{"} e^{-S[\{\vec{x}_k\}]}$$

Estimator

$$\langle \hat{A} \rangle = \langle A[\{\vec{x}_u\}] \rangle_S$$

$$= \frac{1}{Z} \left(\frac{M^{1/2}}{\Lambda} \right)^{dM} \int \left(\Pi_u \, d^d x_u \right) e^{-S} \, \underline{\underline{A[\{\vec{x}_u\}]}}$$

Energy : $\langle \hat{H} \rangle$

$$\langle \hat{H} \rangle = E = \frac{\partial (\beta F)}{\partial \beta} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta}$$

T

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

$$\langle \hat{H} \rangle = \langle E[\{\vec{x}_u\}] \rangle_S$$

energy estimator

$$E[\{\vec{x}_u\}] = \boxed{k_B T\left(\frac{Md}{2} - \sum_{u=0}^{M-1} \frac{\pi M}{\Lambda^2}(\vec{x}_u - \vec{x}_{u+1})^2\right)} + \frac{1}{M}\sum_{u=1}^{M} U(\vec{x}_u)$$

alternative estimator for $\langle E \rangle$:

<u>virial estimator</u>

$$\left\langle \sum_{u=0}^{M-1} \frac{\pi M}{\Lambda^2}(\vec{x}_u - \vec{x}_{u+1})^2 \right\rangle$$

$$= \left(\quad \right)^{Md} \int \Pi(\quad)\, e^{-S} \sum_u \frac{\pi M}{\Lambda^2}(\vec{x}_u - \vec{x}_{u+1})^2$$

$$\vec{x}_u = (x_u^{(1)}, x_u^{(2)}, \dots, x_u^{(d)})$$

quadratic polynomial in $\{\vec{x}_u\}$

$$\alpha(\{\vec{x}_u\}) = \frac{1}{2}\sum_{u=1}^{M}\sum_{i=1}^{d} x_u^{(i)} \frac{\partial}{\partial x_u^{(i)}} \alpha(\{\vec{x}_u\})$$

$$x^2 = \frac{1}{2} x \frac{d}{dx}(x^2)$$

$$\int dx\, \dot{f} g = (\text{boundary terms}) - \int dx\, f \dot{g}$$

Integration by parts

kinetic energy

$$\left\langle k_B T \left[\frac{Md}{2} - \sum_{a=0}^{M-1} \frac{\pi M}{\Lambda^2} (\vec{x}_a - \vec{x}_{a+1})^2 \right] \right\rangle_S$$

$$= \left\langle \frac{1}{2M} \sum_{i,a} x_a^{(i)} \frac{\partial U}{\partial x_a^{(i)}} \right\rangle_S$$

$=$

fundamental assumption : U is a confining potential

$$E_{\mathrm{virial}}[\{\vec{x}_u\}] = \frac{1}{2M}\sum_{i,u} x_u^{(i)} \frac{\partial U}{\partial x_u^{i}} + \frac{1}{M}\sum_u U(\vec{x}_u)$$

Estimators of "diagonal" observables

$$\hat{A}\,|\vec{x}\rangle = A(\vec{x})\,|\vec{x}\rangle$$

$\downarrow$

$$U(\hat{\vec{x}})$$

$$\langle \hat{A} \rangle = \langle A(\vec{x}_0) \rangle_S$$

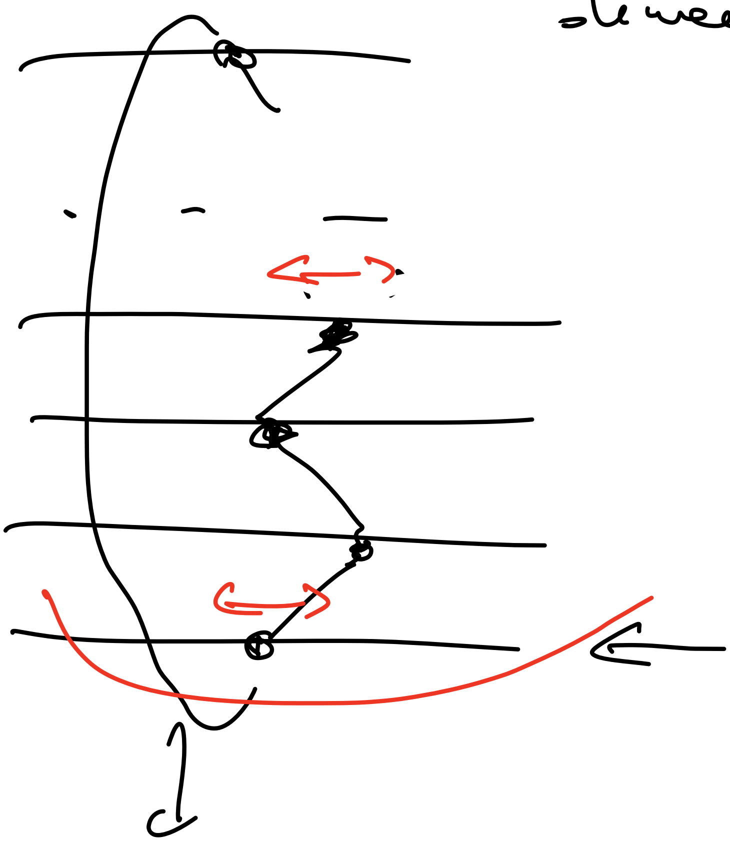
$$= \frac{1}{Z}\,\mathrm{Tr}\left(\hat{A}\, e^{-\beta H}\right)$$

$$= \frac{1}{Z}\int d^d x\, \langle \vec{x}|\hat{A}\, e^{-\beta H}|\vec{x}\rangle$$

$\downarrow \vec{x}_0$

$$= \frac{1}{Z}\int d^d x\, A(\vec{x})\, \langle \vec{x}|e^{-\beta H}|\vec{x}\rangle$$

Ring polymer: on average it is translationally invariant along the imaginary time dimension



periodic b.c. along the imaginary time dimension

$$\langle \hat{A} \rangle = \frac{1}{M} \sum_{k=1}^{M} \langle A(\vec{x}_k) \rangle_S$$

One particle $\to$ many particles

Many-body PIMC

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

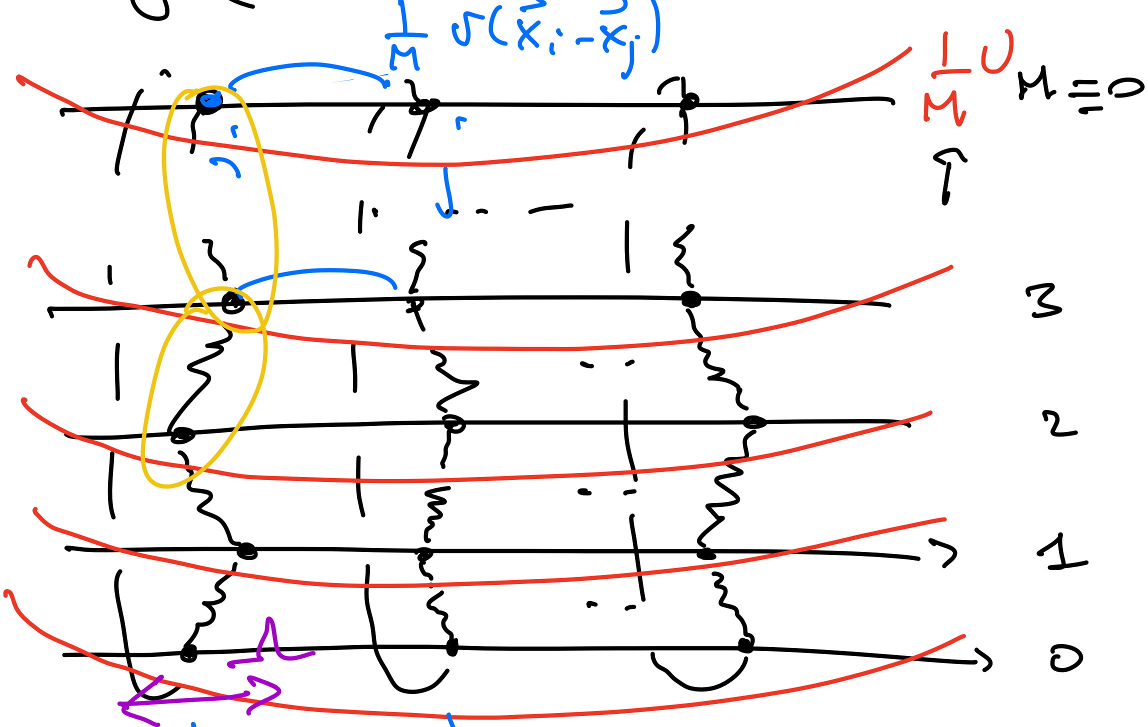
$\Uparrow$

physically legitimate if particles are DISTINGUISHABLE

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

position eigenbasis $\quad |\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N\rangle$

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



$n^{1/d}$

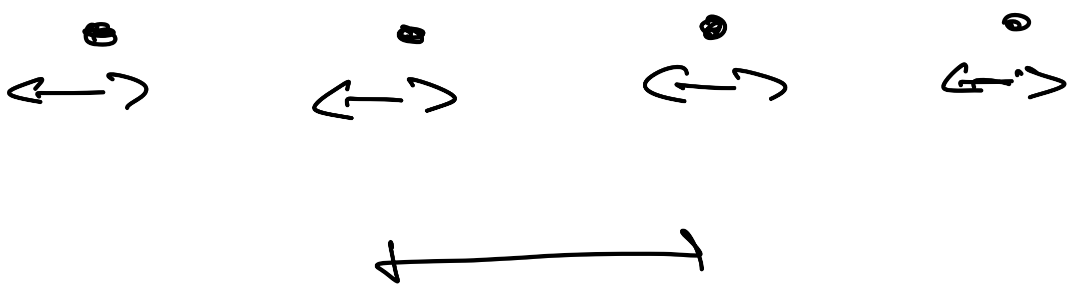
$$S[\{\vec{X}_{i,k}\}] = \frac{1}{2} T K \sum_{i=1}^{N} \sum_{k=0}^{n-1} (\vec{X}_k - \vec{X}_{k+1})^2$$

$$+ \frac{1}{M} \sum_{i,k} U(\vec{X}_{i,k})$$

$$+ \frac{1}{M} \sum_{i<j} \sum_{k} v(\vec{X}_{i,k} - \vec{X}_{j,k})$$

Ex. of distinguishable particles

solid



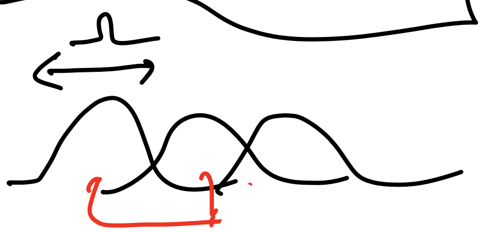
Indistinguishable / overlapping quantum particles

$\Longrightarrow$ <u>quantum degeneracy</u>

@ finite T $\rightarrow$ $\Lambda = \dfrac{h}{\sqrt{2\pi m k_B T}}$

quantum degeneracy

$$\boxed{\Lambda \sim \frac{1}{n^{1/d}}}$$



$a = n^{1/d}$

$$k_B T \sim \frac{h^2}{2\pi m} n^{2/d}$$

$\rightarrow$ Fermi temperature (fermions)

$\rightarrow$ BEC temperature (for bosons)

with identical indistinguishable particles

$$|\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N\rangle \rightarrow |\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N\rangle_\eta$$

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

sign of the permutation

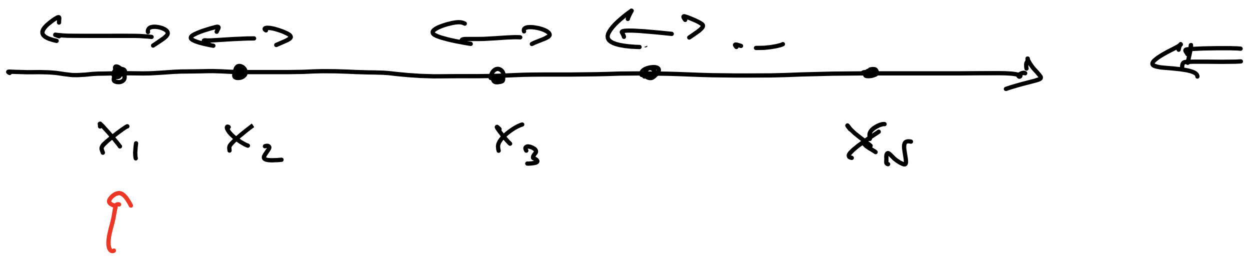
$$\eta = \begin{cases} +1 & \text{BOSONS} \\ -1 & \text{FERMIONS} \end{cases}$$

$Z_N =$

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

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

$d = 1$



2 particles

$$Z_2 = \frac{1}{2!} \cancel{\frac{1}{2!}} \int d^d x_1 \, d^d x_2 \Big[\langle \vec{x}_1 \, \vec{x}_2 | e^{-\beta H} | \vec{x}_1, \vec{x}_2 \rangle$$

$$+ \eta \langle \vec{x}_1 \, \vec{x}_2 | e^{-\beta H} | \vec{x}_2 \, \vec{x}_1 \rangle$$

$=$

$$+ \eta \langle \vec{x}_2 \, \vec{x}_1 | e^{-\beta H} | \vec{x}_1, \vec{x}_2 \rangle$$

$=$

$$+ \langle \vec{x}_2 \, \vec{x}_1 | e^{-\beta H} | \vec{x}_2 \, \vec{x}_1 \rangle \Big]$$

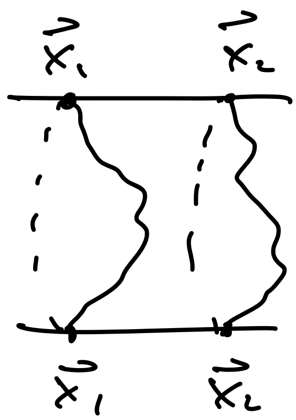
$$\int_{-\infty}^{+\infty} dx_1 \int_{x_1}^{\infty} dx_2 \dots \int_{x_{N-1}}^{\infty} dx_N (\dots) = \frac{1}{N!} \int_{-\infty}^{+\infty} \left(\prod_{i=1}^{N} dx_i \right) (\dots)$$

$$Z_N = \frac{1}{N!}\sum_{P} \eta^{P} \int \left(\prod_{i=1}^{N} d^d x_i\right) \langle \vec{x}_1\, \vec{x}_2 \dots \vec{x}_N | e^{-\beta \mathcal{H}} | \vec{x}_{P(1)} \dots \vec{x}_{P(N)} \rangle$$

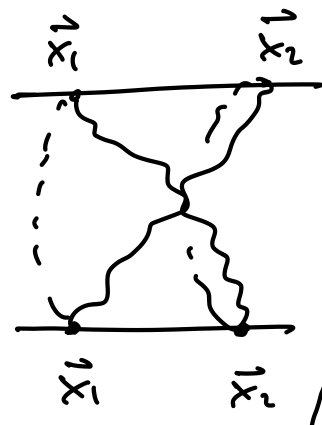
$$Z_2 = \frac{1}{2}\int d^d x_1\, d^d x_2 \left[\langle \vec{x}_1\, \vec{x}_2 | e^{-\beta \mathcal{H}} | \vec{x}_1\, \vec{x}_2 \rangle + \eta \langle \vec{x}_1\, \vec{x}_2 | e^{-\beta \mathcal{H}} | \vec{x}_2\, \vec{x}_1 \rangle \right]$$

I assume that particles are distinguishable

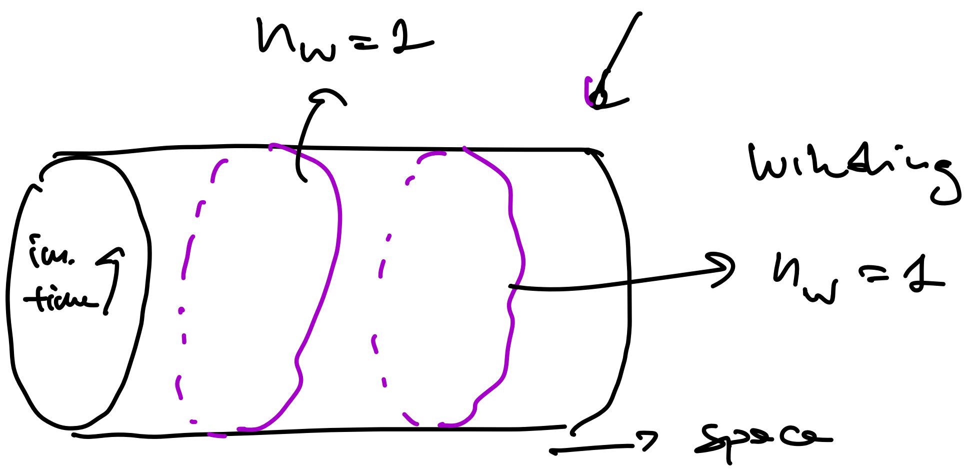
$$= \frac{1}{2}\int d^d x_1\, d^d x_2 \Bigg($$



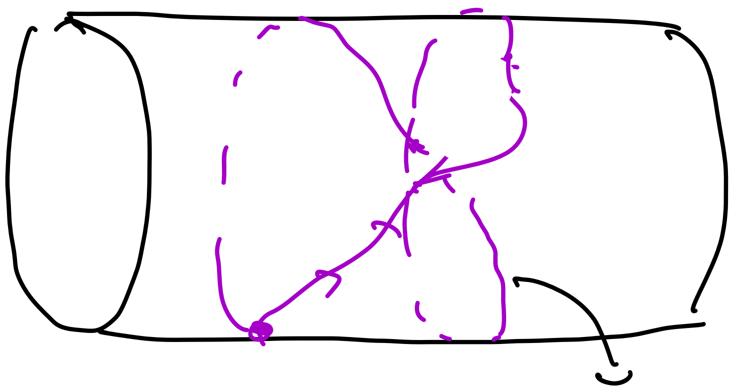
$+\eta$



$\Bigg)$



winding number



"permutation cycle of 2" $n_w = 2$

"topological invariant"

Quantum degeneracy ⇒ sample over different "topologies" of ring polymers

Fermion sign problem $\eta = -1$

$$Z_F = \frac{1}{N!}\Big[\sum_{P\ \text{even}} \int \Big(\prod_i d^d x_i\Big) \underbrace{\langle \vec{x}_1 \dots \vec{x}_N | e^{-\beta H} | \vec{x}_{P(1)} \dots \vec{x}_{P(N)} \rangle} - \sum_{P\ \text{odd}} \int \Big(\prod_i d^d x_i\Big) (\dots) \Big]$$

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

$$Z_B = (\quad) + (\quad)$$

$$Z_F = Z_B \underbrace{\frac{1}{Z_B} \frac{1}{N!} \sum_P \int (\mu_i\, d^d x)\, \eta^P \langle 1 | 1 \rangle}_{\langle \text{sign}(P) \rangle_B}$$

$$\eta^P$$

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

$$\leq 1$$

$$\langle \text{sign}(P) \rangle_B = \frac{Z_F}{Z_B} = e^{-\beta \overbrace{(f_F - f_B)}^{>0} N}$$

$$\Delta f > 0$$

$$Z_F = e^{-\beta f_F N} \qquad Z_B = e^{-\beta f_B N}$$

$$\langle \text{sign}(P) \rangle_B = e^{-\beta \Delta f N} \sim O(\exp(-\beta N))$$