Path-integral Monte Carlo for indistinguishable particles

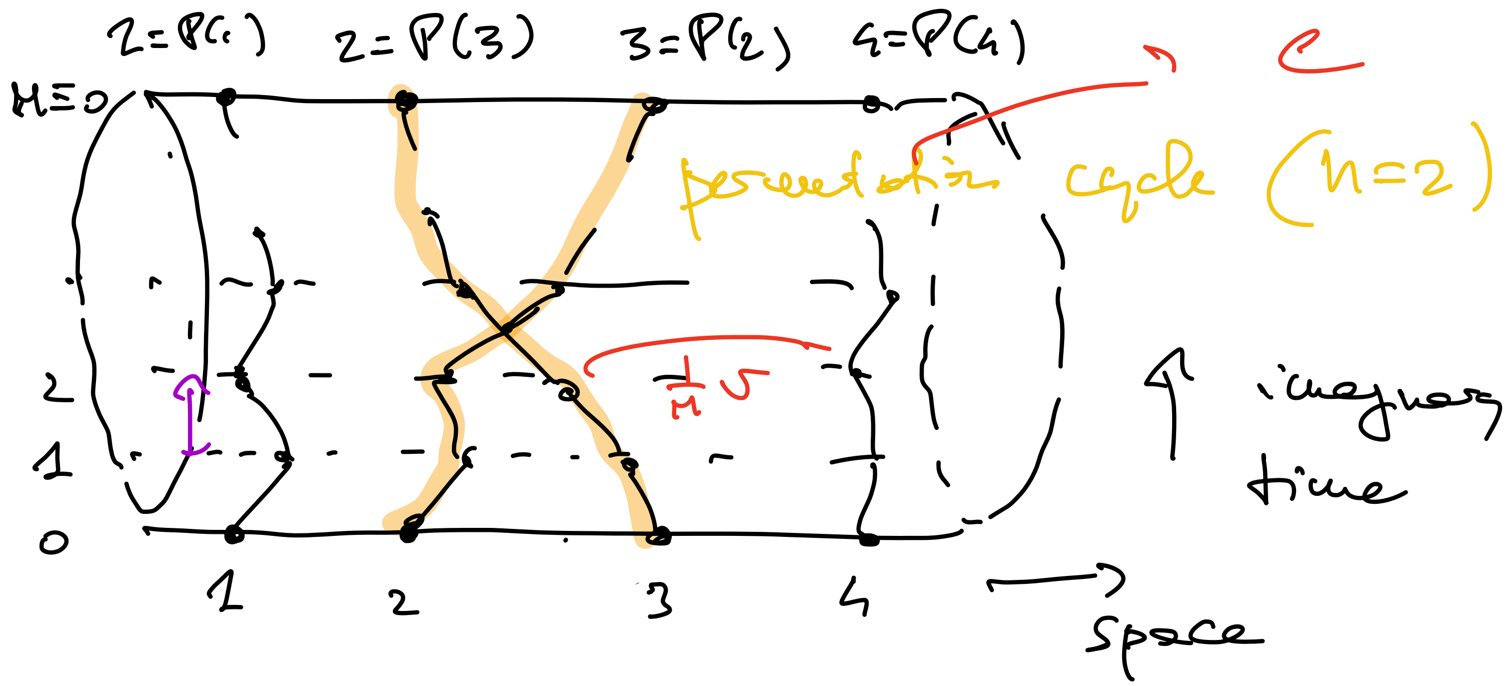
$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) \qquad H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} U(\vec{x}_i) + \sum_{i<j} v(|\vec{x}_i - \vec{x}_j|)$$

$$= \lim_{M\to\infty} \sum_{P} \eta^{P} \left(\frac{M^{1/2}}{\lambda}\right)^{MdN} \int \left(\prod_{i=1}^{N}\prod_{k=1}^{M} d^d x_{i,k}\right) e^{-S[\{\vec{x}_{i,k}\}]}$$

$$\{x_{i,0} = x_{P(i),M}\}$$

$$S[\{\vec{x}_{i,k}\}] = \frac{1}{2}\kappa \sum_{i=1}^{N}\sum_{k=1}^{M} \left(\vec{x}_{i,k} - \vec{x}_{i,k+1}\right)^2 + \frac{1}{M}\sum_{i=1}^{N}\sum_{k} U(\vec{x}_{i,k}) + \frac{1}{M}\sum_{i<j}\sum_{k} v(|\vec{x}_{i,k} - \vec{x}_{j,k}|)$$

$$\eta = \begin{cases} +1 & B \\ -1 & F \end{cases}$$



$Z \doteq$ sum over configurations + topologies ($\equiv$ permutation cycles) of ring polymers.

Fermions: sign problem

$$Z_F = \sum_{\text{even } P} \boxed{\quad\quad} \; \ominus \; \sum_{\text{odd } P} \boxed{\quad\quad}$$

$$= \underset{\eta = 1}{\underset{\downarrow}{Z_B}} \left\langle \underset{(-1)^P}{\underset{\downarrow}{\operatorname{sign}(P)}} \right\rangle_B$$

$$\langle \operatorname{sign}(P) \rangle_B = \frac{Z_F}{Z_B} = e^{-\beta N \Delta f}$$

$$\Rightarrow \Delta f = \frac{F_F - F_B}{N} \sim O(1)$$

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

$$\langle \hat{A} \rangle_F = \frac{\langle \operatorname{sign}(P) A \rangle_B}{\langle \operatorname{sign}(P) \rangle_B}$$

$$\boxed{c = \{\vec{x}_{i,n}\}}$$

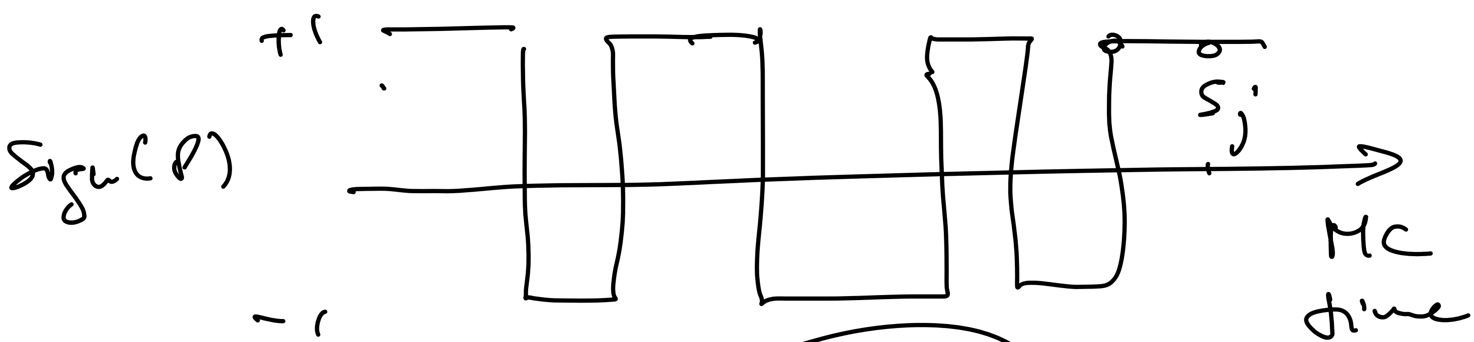
$$\langle \hat{A} \rangle_F = \langle A(\{\vec{x}_{i,n}\}) \rangle_F$$

$$= \frac{\sum_c e^{-S_c}\left(\eta^{P_c} A_c\right)}{\sum_c e^{-S_c}\,\eta^{P_c}}$$

$$= \frac{\sum_c e^{-S_c}\left(\eta^{P_c} A_c\right)}{\sum_c e^{-S_c}} \times \frac{\sum_c e^{-S_c}}{\sum_c e^{-S_c}\,\eta^{P_c}}$$

$$\langle \mathrm{sign}(P)\, A \rangle_B \qquad \frac{1}{\langle \mathrm{sign}(P) \rangle_B}$$

$$\longleftarrow \quad t \quad \longrightarrow$$



$$\langle \mathrm{sign}(P) \rangle \simeq \frac{1}{L} \sum_{j=1}^{L} s_j \sim O(1)$$

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

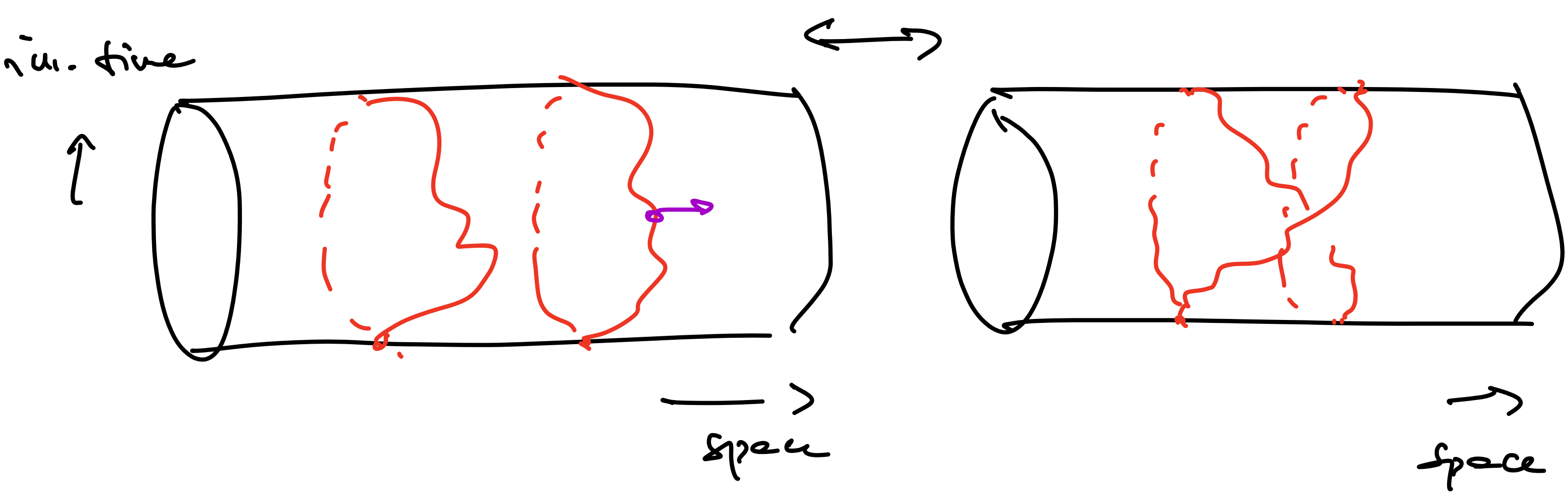
$$L \sim \exp(\beta N)$$

you need exponential statistics

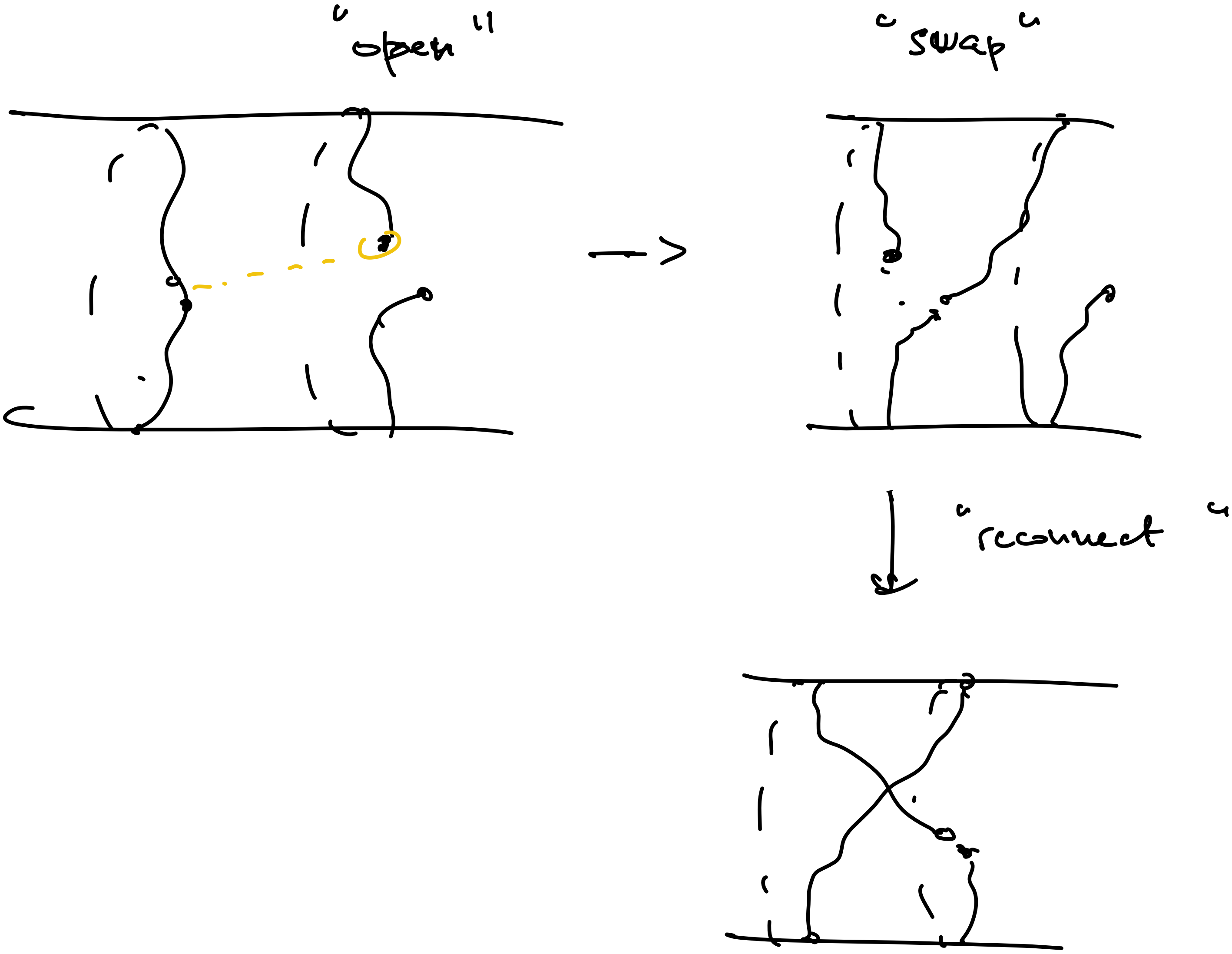
SIGN PROBLEM

major obstacle in:
→ quantum chemistry
→ strongly correlated electrons
→ high-energy physics
→ ...

Problem (solved): sampling over "topologies" of ring polymers



"worm algorithm" Boninsegni & Prokof'ev 2006



Problem (open): "phase problem"

particles immersed in a gauge field

magnetic field $\vec{B} \to \vec{A} = (0, Bx, 0)$

$\vec{B} = \vec{\nabla} \times \vec{A}$

$$\mathcal{H} = \frac{(\vec{p} - q\vec{A})^2}{2m}$$

$$\langle \vec{x} | e^{-\frac{\beta}{M}\mathcal{H}} | \vec{x}' \rangle \underset{\vec{A}=0}{=} \text{real, positive \#}$$

$$\underset{\vec{A}\neq 0}{=} \underline{\text{complex}} \text{ number}$$

$$Z \neq \sum_c e^{-\vec{S}_c} \in \mathbb{C}$$

$$= \sum_c e^{i\phi_c} |e^{-S_c}|$$

$$= Z_{|e^{-S_c}|} \langle e^{i\phi_c} \rangle_{|e^{-S_c}|}$$

$$\langle e^{i\phi_c} \rangle \sim \exp(-\beta N)$$

exponentially large statistics is needed to reconstruct $\langle e^{i\phi_c} \rangle$.

$\Rightarrow$ PIMC works for $\underline{\underline{\text{bosons}}}$ (or distinguishable particles) in the absence of gauge fields.

("Boltzmannons")

Ground-state properties : variational Monte Carlo

find $|\Psi\rangle$ which approximates $|\Phi_0\rangle$: $\mathcal{H}|\Phi_0\rangle = E_0|\Phi_0\rangle$

$$\min_{|\Psi\rangle} \underbrace{\frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}}_{E(|\Psi\rangle)} = E_0 \quad \text{ground-state energy}$$

$$|\Psi\rangle = \sum_x \Psi_x |x\rangle$$

$|x\rangle$ basis of Hilbert space with D dimensions

$$\min_{\{\Psi_x\}} E(|\Psi\rangle) \to \frac{\partial E(|\Psi\rangle)}{\partial \Psi_x} = 0 \quad \text{D equations}$$

same as imposing that

$$\mathcal{H}|\Psi\rangle = E_\Psi |\Psi\rangle$$

eigenstate

$D \sim \exp(N)$

<u>Variational approach</u> : $\boxed{\underline{\underline{\Psi}}_x =: f(x; \vec{\alpha})}$ postulating / guessing

parameters $\vec{\alpha} = (\alpha_1, \ldots, \alpha_M)$

1) $M \sim \mathrm{poly}(N)$

2) $f(\underline{\underline{x}}; \underline{\underline{\vec{\alpha}}})$ efficiently computable (in a time $\sim \mathrm{poly}(N)$)

$$|\underline{\underline{\Psi}}(\vec{\alpha})\rangle = \sum_x f(x; \vec{\alpha}) |x\rangle$$

$$\min_{\vec{\alpha}} E(\vec{\alpha}) = \min_{\vec{\alpha}} \frac{\langle \Psi(\vec{\alpha}) | \mathcal{H} | \Psi(\vec{\alpha}) \rangle}{\langle \Psi(\vec{\alpha}) | \Psi(\vec{\alpha}) \rangle}$$

$$\underline{\underline{E(\vec{\alpha})}} = \frac{\sum_{xx'} f^*(x, \vec{\alpha}) f(x', \vec{\alpha}) \langle x | \mathcal{H} | x' \rangle}{\sum_x |f(x, \vec{\alpha})|^2}$$

$$= \frac{\sum_x |f(x,\vec\alpha)|^2 \underbrace{\left(\sum_{x'} \frac{f(x',\vec\alpha)}{f(x,\vec\alpha)} \langle x | H | x' \rangle \right)}_{E_L(x)}}{\sum_x |f(x,\vec\alpha)|^2}$$

MC sample $|f|^2$

$E_L(x)$ "local energy"

$$= \langle E_L(x) \rangle_{|f|^2}$$

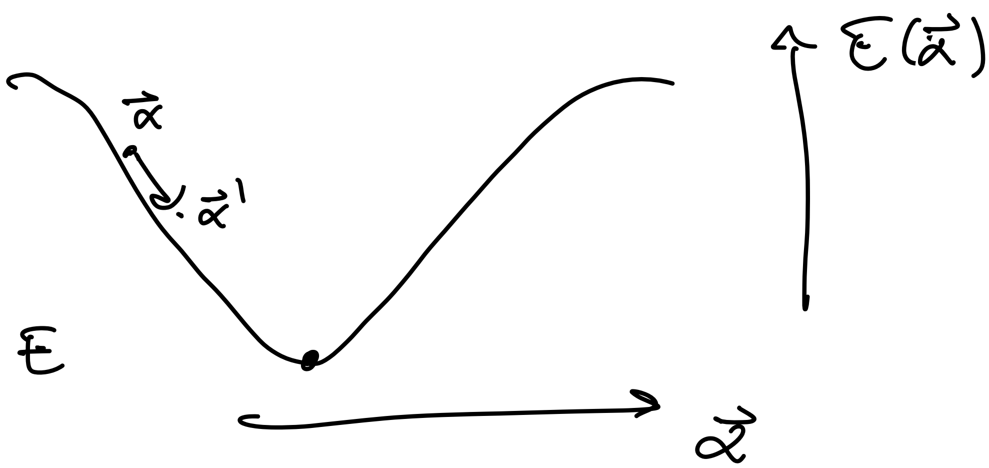
$\langle x | H | x' \rangle$ is a sparse matrix:

given x there are only $\sim \mathrm{poly}(N)$ terms

$$\langle x | H | x' \rangle \neq 0$$

To find $\min_{\vec\alpha} E(\vec\alpha)$: gradient descent

$\nabla_{\vec\alpha} E(\vec\alpha)$



$$\vec\alpha \to \vec\alpha' = \vec\alpha - \epsilon \vec\nabla_{\vec\alpha} E$$

$$\frac{\partial}{\partial \alpha_k} E(\vec{\alpha}) = \frac{\partial}{\partial \alpha_k}\left[\frac{\sum_x |f(x,\vec{\alpha})|^2 \sum_{x'} \frac{f(x',\vec{\alpha})}{f(x,\vec{\alpha})} \langle x|H|x'\rangle}{\sum_x |f(x,\vec{\alpha})|^2}\right]$$

$$O_k(x) = \frac{\partial_{\alpha_k} f(x;\vec{\alpha})}{f(x,\vec{\alpha})} = \frac{\partial}{\partial \alpha_k} \log f(x,\vec{\alpha})$$

$$= \dots = \langle O_k^*(x) E_L(x)\rangle + \langle O_k(x) E_L^*(x)\rangle$$

$$- \langle O_k^*(x)\rangle\langle E_L(x)\rangle - \langle O_k(x)\rangle\langle E_L^{(*)}(x)\rangle$$

correlation between O_k and E_L

Examples of variational states = Ansätze

$$f(x,\vec{\alpha}) \to \Psi(\vec{x}_1,\vec{x}_2,\dots,\vec{x}_N;\vec{\alpha})$$

1) Bosons : pair-product state, Jastrow state ..

$$\Psi(\vec{x}_1,\vec{x}_2,\dots,\vec{x}_N;\vec{\alpha}) =$$

$$= \frac{1}{N}\prod_{i<j} w(|\vec{x}_i-\vec{x}_j|)$$

symmetric under particle permutations

$$= \frac{1}{N} \quad e^{\sum_{i<j} u(|\vec{x}_i - \vec{x}_j|) + \sum_{i<j<k} v(|\vec{x}_i - \vec{x}_j|, |\vec{x}_j - \vec{x}_k|) + \cdots}$$

2) <u>Fermions</u> : anti-symmetric state

$$\phi_\alpha(\vec{x}) \, \chi_\alpha(\sigma) \qquad \sigma = \uparrow, \downarrow$$

space

$\to$ spin

$$D(\vec{x}_1, \sigma_1; \vec{x}_2, \sigma_2; \cdots; \vec{x}_N, \sigma_N)$$

$$= \det \left[\phi_i(x_j) \, \chi_i(\sigma_j) \right]$$

$$\Psi(\vec{x}_1, \sigma_1, \cdots; \vec{x}_N, \sigma_N) = D(\quad) \, e^{\sum_{i<j} u(|\vec{x}_i - \vec{x}_j|)}$$

$\downarrow$

Jastrow factor

$\vec{a}$ parameters ?

$\underline{\underline{\text{ex:}}}$ $u(|\vec{x}_i - \vec{x}_j|) = \alpha_0 + \alpha_1 |\vec{x}_i - \vec{x}_j| + \alpha_2 |\vec{x}_i - \vec{x}_j|^2$

$+ \cdots$