PIMC for quantum spin models

PIMC for transverse-field Ising model

$$\mathcal{H} = \underbrace{\sum_{\langle ij\rangle} J_{ij}\, \sigma_i^z \sigma_j^z}_{\sigma^z \to -\sigma^z} - \underbrace{\sum_i g_i\, \sigma_i^x}_{\mathbb{Z}_2 \text{ symmetry}}$$

on a lattice

for XXZ model

$$\mathcal{H} = -J \sum_{\langle ij\rangle} \Big[\underbrace{S_i^x S_j^x + S_i^y S_j^y}_{x \quad x} + \Delta \underbrace{S_i^z S_j^z}_{z} \Big]$$

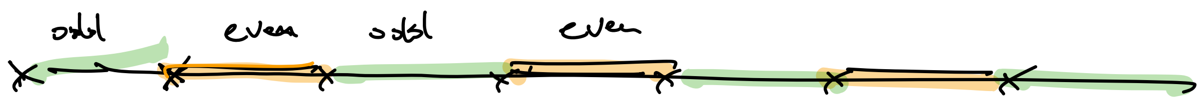
nearest neighbors on a lattice

$\Delta = 1$ $SU(2)$

$\Delta \neq 1$ $U(1) \times \mathbb{Z}_2$

$$= \sum_{\langle ij\rangle} \left(\mathcal{H}_{ij}^{xy} + \mathcal{H}_{ij}^{zz} \right)$$

$$= \underbrace{\sum_{\langle ij\rangle_{\text{even}}} \mathcal{H}_{ij}}_{\mathcal{H}_{\text{even}}} + \underbrace{\sum_{\langle ij\rangle_{\text{odd}}} \mathcal{H}_{ij}}_{\mathcal{H}_{\text{odd}}}$$



$$= \sum_{\langle ij\rangle_{\text{even}}} \left(\mathcal{H}_{ij}^{xy} + \mathcal{H}_{ij}^{zz} \right) + \sum_{\langle ij\rangle_{\text{odd}}} \left(\mathcal{H}_{ij}^{xy} + \mathcal{H}_{ij}^{zz} \right)$$

$$|\vec{\sigma}\rangle = |\sigma_1 \cdots \sigma_N\rangle \qquad S_i^z |\sigma_i\rangle = \frac{\sigma_i}{2} |\sigma_i\rangle, \quad \sigma_i = \pm 1$$

$$\mathrm{Tr}\left[e^{-\beta \mathcal{H}}\right] = Z \qquad \mathcal{H} \to \mathcal{H}_{even} + \mathcal{H}_{odd}$$

$$\prod_{\langle ij\rangle_{odd}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}} \simeq \prod_{\langle ij\rangle_{odd}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{xy}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{zz}}$$

$$= \lim_{M\to\infty} \mathrm{Tr}\left[\left(\underbrace{e^{-\frac{\beta}{M}\mathcal{H}_{odd}}} e^{-\frac{\beta}{M}\mathcal{H}_{even}}\right)^M\right]$$

$$= \lim_{M\to\infty} \mathrm{Tr}\left[\left(\prod_{\langle ij\rangle_{odd}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{zz}} \; e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{xy}} \prod_{\langle ij\rangle_{even}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{zz}} \; e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{xy}}\right)^M\right]$$

$$\sum_{\vec\sigma} |\vec\sigma\rangle\langle\vec\sigma|$$

$$= \lim_{M\to\infty} \sum_{\{\vec\sigma^{(k)}\}} \underbrace{\langle\vec\sigma^{(0)}| \prod_{\langle ij\rangle_{odd}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{xy}} |\vec\sigma^{(1)}\rangle} \langle\vec\sigma^{(1)}| \prod_{\langle ij\rangle_{even}} e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{xy}} |\vec\sigma^{(2)}\rangle$$

$k = 0, \ldots, 2M-1$

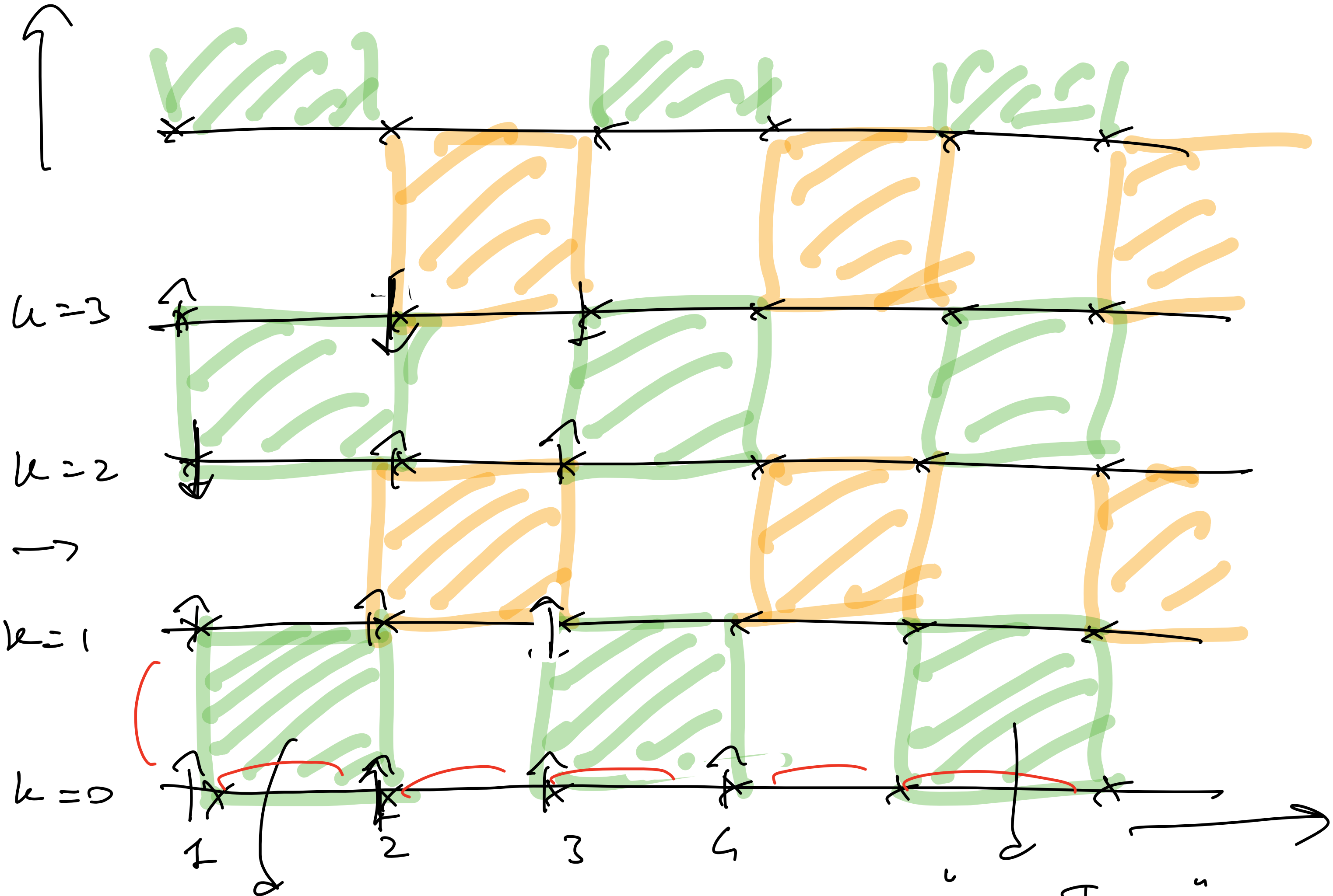
$$\cdots \langle\vec\sigma^{(2M-2)}| \prod_{\langle ij\rangle_{odd}} (\quad) |\vec\sigma^{(2M-1)}\rangle$$

$$\langle\vec\sigma^{(2M-1)}| \prod_{\langle ij\rangle_{even}} (\quad) |\vec\sigma^{(0)}\rangle$$

$$e^{+\frac{\beta J}{8M}\Delta \sum_{k=0}^{2M-1} \sum_{\langle ij\rangle} \sigma_i^{(k)} \sigma_j^{(k)}} \qquad \sigma_i^{(k)} = \pm 1$$

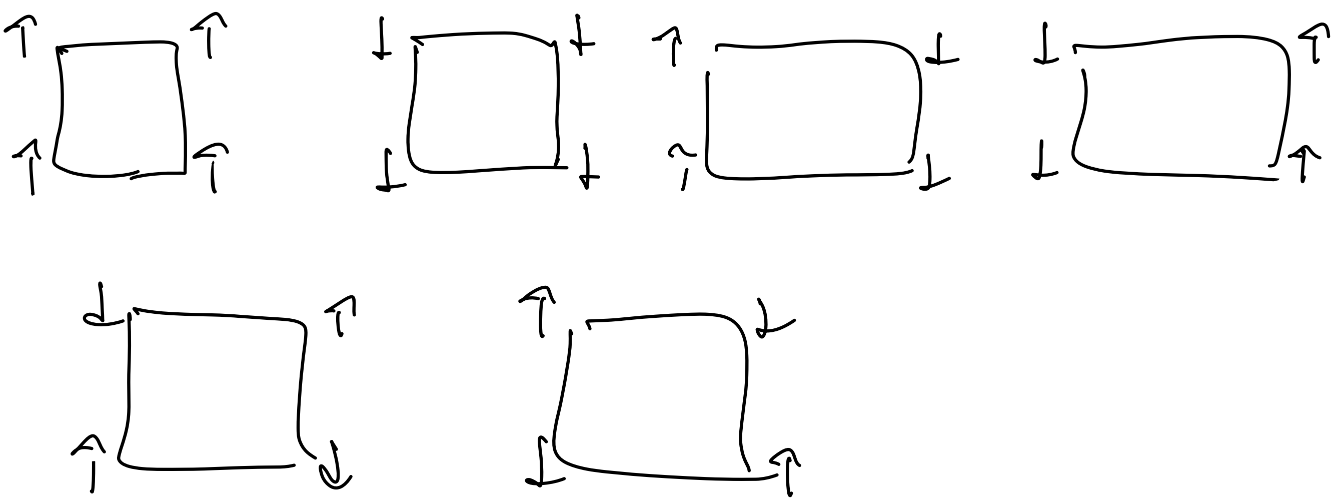
$$\prod_{\langle ij\rangle_{odd}} \underbrace{\langle \sigma_i^{(k)} \sigma_j^{(k)} | e^{-\frac{\beta}{M}\mathcal{H}_{ij}^{xy}} | \sigma_i^{(k+1)} \sigma_j^{(k+1)}\rangle}$$

$$W(\sigma_i^{(k)} \sigma_j^{(k)} ; \sigma_i^{(k+1)} \sigma_j^{(k+1)})$$



"vertices"

$W(\sigma_1^{(0)}\,\sigma_2^{(0)}\,;\,\sigma_1^{(1)}\,\sigma_2^{(1)})$ for "plaquettes"

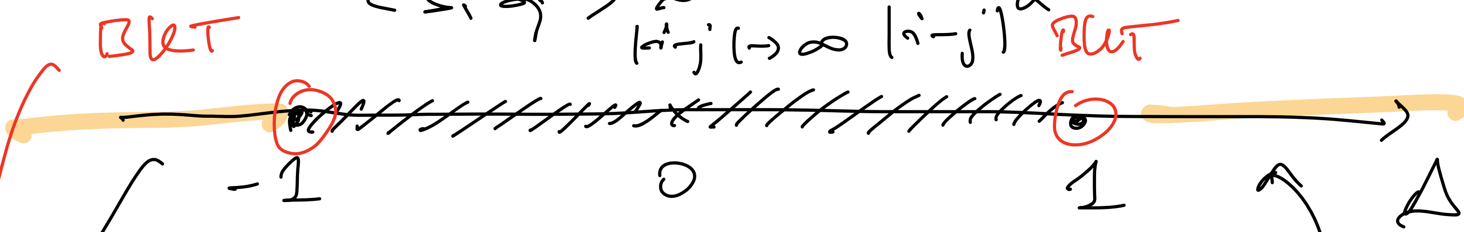


6-vertex model

$$
\begin{array}{c|cccc}
 & \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \\
\hline
\uparrow\uparrow & 1 & 0 & 0 & 0 \\
\uparrow\downarrow & 0 & \cosh\left(\frac{\beta J}{2M}\right) & \sinh\left(\frac{\beta J}{2M}\right) & 0 \\
\downarrow\uparrow & 0 & \sinh\left(\frac{\beta J}{2M}\right) & \cosh\left(\frac{\beta J}{2M}\right) & 0 \\
\downarrow\downarrow & 0 & 0 & 0 & 1
\end{array}
$$

$\beta \to \infty$ $\boxed{J > 0}$

$$\langle S_i^x S_j^x \rangle \underset{|i-j| \to \infty}{\sim} \frac{1}{|i-j|^\alpha}$$



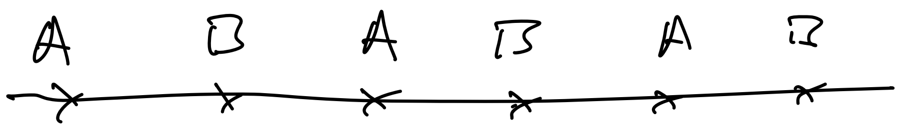
SU(2) AF SU(2) FM

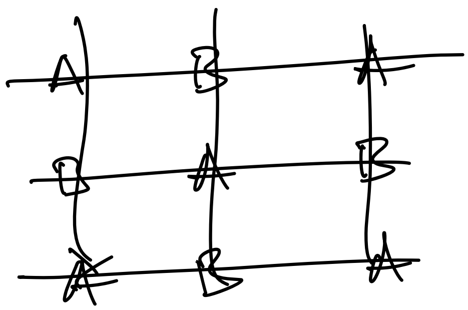
$$\langle S_i^x S_j^x \rangle \underset{|i-j| \to \infty}{\sim} e^{-\left(|i-j|/\xi\right)}$$

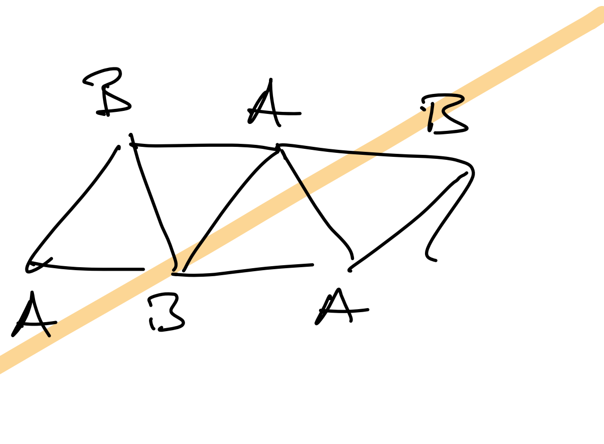
Berezhinskii - Kosterlitz - Thouless transition

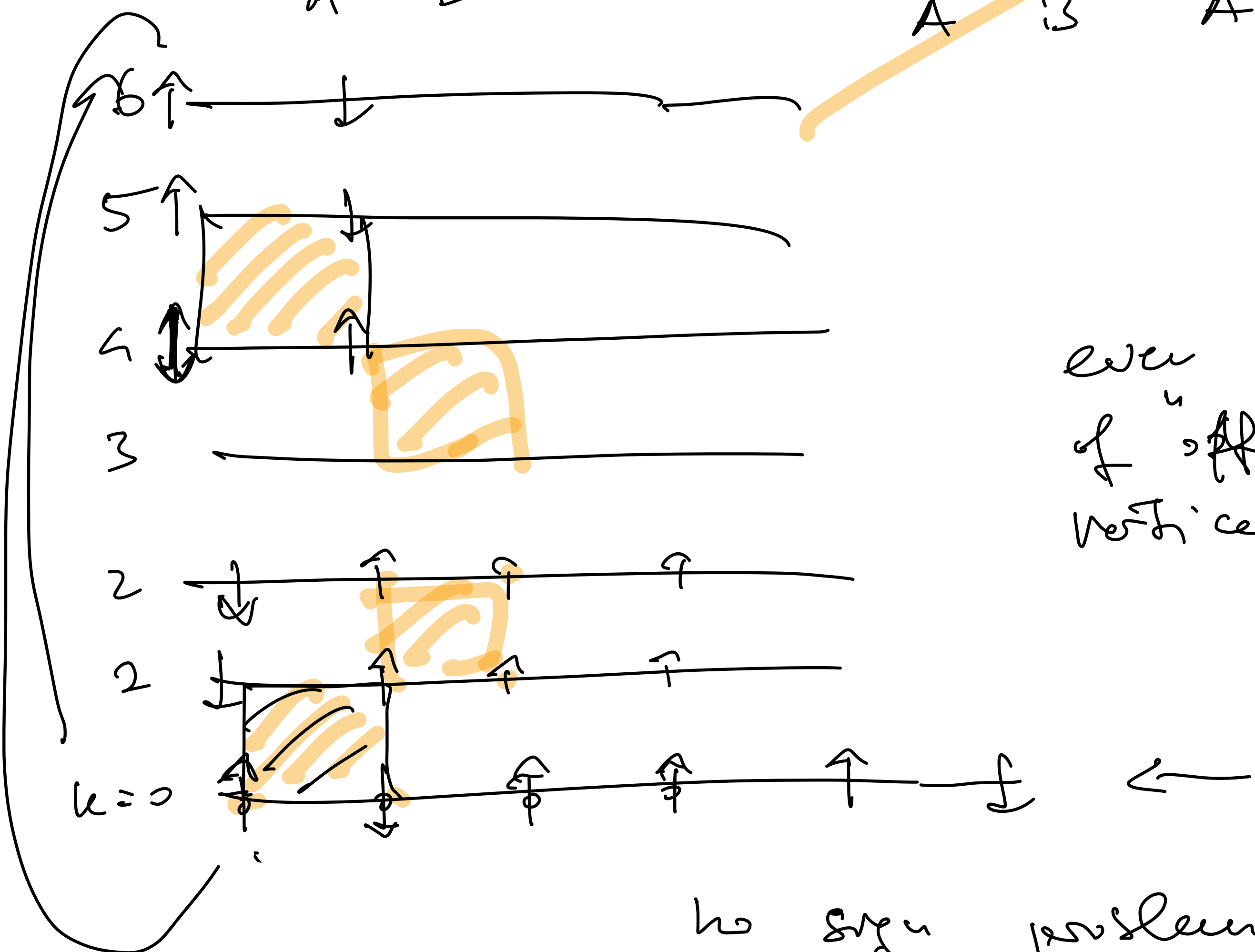
$J < 0$ $\sinh\left(\frac{\beta J}{2M}\right) < 0$

Bipartite lattice : two sublattice A & B such that there is no bond connecting a site in A(B) to a site in A(B)







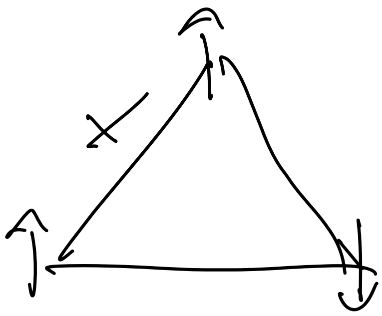


even number of "off-diagonal" vertices

no sign problem

Non-bipartite lattice

(triangular lattice, ...) $\Longrightarrow$ **SIGN PROBLEM**



Ground-state methods : **variational** MC

"Biased" approaches

choice of a variational "Ansatz"

$|\Psi\rangle$ chosen to mimic the g.s. of $\mathcal{H}$

$\mathcal{H}$: Hamiltonian

$\forall\ |\Psi\rangle$

ground state

$$E(\Psi) = \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0 = \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle$$

$$\min_{|\Psi\rangle} E(\Psi) = E_0$$

$|\vec{x}\rangle \to |x\rangle$ basis of Hilbert space $\mathcal{H}$

$$|\Psi\rangle = \sum_{\vec{x}} \psi_{\vec{x}} |\vec{x}\rangle$$

$\psi_{\vec{x}} \to \mathbb{C}$

$$\frac{\partial E}{\partial \psi_x} = 0 \quad \text{condition}$$

$$\#(\vec{x}) \sim O(\exp(N))$$

$$\to \left[\psi_{\vec{x}} =: f(\vec{x}; \vec{\alpha}) \right]$$

WORKING ASSUMPTION

"Bias"

$$\vec{\alpha} = (\alpha_1, \dots, \alpha_M) \in \mathbb{R}^M$$

$$M \sim \text{poly}(N)$$

$f(\vec{x}; \vec{\alpha})$ computable in a time $\sim \text{poly}(N)$

$\langle \Psi | \mathcal{H} | \Psi \rangle$

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

$$= \min_{\vec{\alpha}} \frac{\sum_{\vec{x}} |f(\vec{x},\vec{\alpha})|^2 \left(\sum_{\vec{x}'} \frac{f(\vec{x}';\vec{\alpha})}{f(\vec{x},\vec{\alpha})} \langle \vec{x} | \mathcal{H} | \vec{x}' \rangle \right)}{\sum_{\vec{x}} |f(\vec{x},\vec{\alpha})|^2}$$

$\Psi(\vec{x}; \vec{\alpha})$

$$= \min_{\vec{\alpha}} \sum_{\vec{x}} P(\vec{x}; \vec{\alpha}) \, E_L(\vec{x})$$

"local energy"

$$= \min_{\vec{\alpha}} \langle E_L(\vec{x}) \rangle_{|\Psi|^2}$$

→ Monte Carlo calculation

$\vec{x} \to \vec{x}' \to \vec{x}''$

Sparse matrix

$\langle \vec{x} | H | \vec{x}' \rangle$

$$\sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)$$

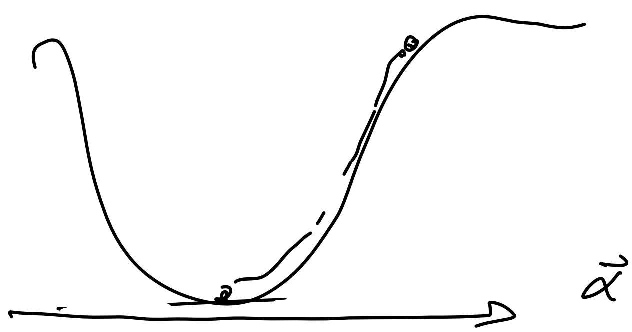
$\langle \sigma_1 \sigma_2 \dots \sigma_N | H | \sigma_1' \sigma_2' \dots \sigma_N' \rangle$

Efficiently calculate $E(\vec{\alpha})$

→ minimise w.r.t. $\vec{\alpha}$

$\vec{\nabla}_{\vec{\alpha}} E(\vec{\alpha})$ gradient

$\vec{\alpha}^{(0)}$ first guess



$$\vec{\alpha}^{(1)} = \vec{\alpha}^{(0)} - \epsilon \underline{\vec{\nabla}_{\vec{\alpha}} E(\vec{\alpha})} \qquad \epsilon \ll 1$$

$---$

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

$$O_\mu(\vec{x}) = \frac{\partial}{\partial \alpha_\mu} \log f(\vec{x};\vec{\alpha}) = \frac{\partial_{\alpha_\mu} f}{f}$$

$$O^*_\mu(\vec{x}) = \frac{\partial}{\partial \alpha_\mu} \log f^*(\quad)$$

$$\partial_{\alpha_\mu} E(\vec{\alpha}) = 2\mathrm{Re}\left[\langle O^*_\mu(\vec{x}) \, E_L(\vec{x}) \rangle_{|f|^2} - \langle O^*_\mu(\vec{x}) \rangle \langle E_L(\vec{x}) \rangle\right]$$

Examples of variational W.f.

1) Bosons $\quad |\vec{X}\rangle \to |\vec{R}\rangle = |\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\rangle$

$$|\Psi\rangle = \int d^{dN}R \; \psi(\vec{R}) \; |\vec{R}\rangle$$

$$\psi(\vec{R}) \overset{ex.}{=} \prod_i \psi_0(\vec{r}_i) \qquad \text{BEC}$$

$$\overset{ex.}{=} \prod_{i<j} \underline{u}(|\vec{r}_i - \vec{r}_j|) = e^{\sum_{i<j} w(|\vec{r}_i - \vec{r}_j|)} \qquad \text{Jastrow w.f.}$$

$$u(r) \overset{ex.}{=} \sum_q u_q \, e^{iqr}$$

$$\overset{ex.}{=} u_0 + u_1 r + u_2 r^2 + u_3 r^3 + \ldots$$

$$\alpha_0 \quad \alpha_1 \quad \alpha_2 \quad \alpha_3$$

2) Fermions

$\to$ $\phi_\beta(\vec{r}_j)$ $\chi_\beta(\sigma_j)$

$$\Phi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \ldots, \vec{r}_N\sigma_N) = \mathrm{Det}\left[\phi_{\beta_i}(\vec{r}_j)\,\chi_{\beta_i}(\sigma_j)\right]$$

Slater determinant

$$\Psi(\vec{R}, \vec{\sigma}) = \underline{\sum_\alpha c_\alpha} \; \mathrm{Det}[\quad]$$

$$\Psi(\vec{R}, \vec{\sigma}) = \mathrm{Det}[\quad] \; e^{\sum_{i<j} w(|\vec{r}_i - \vec{r}_j|)}$$