Quantum Monte Carlo for quantum systems on a lattice

(finite-T calculations)

so far:

-> exact diagonalization

-> variational MC + diffusion MC : ground states / time evolutions

-> tensor-network techniques : " / " / thermodynamics

-> PIMC : thermodynamics of systems in continuum space

=> PIMC / QMC for lattice models $\neq$ $\perp$ $\vec{p}, \vec{x}$

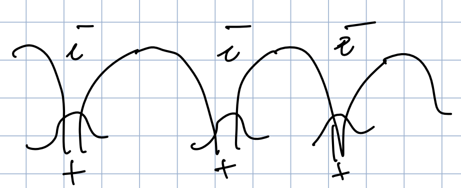
-> quantum spin models : localized electrons / quantum magnetism / quantum simulators based on cold atoms / SC circuit (ensembles of qubits)

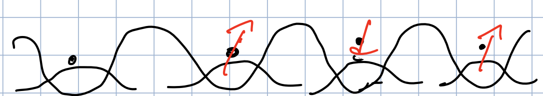
-> itinerant identical particles on a lattice : • electrons in a solid

• cold atoms in optical lattices

-> fermions

-> bosons





limitation: sign problem

fermionic systems $(d > 1)$

frustrated quantum magnets

1) PIMC ←

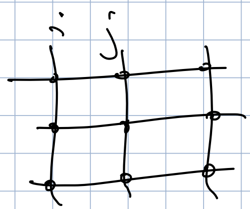
2) stochastic series expansion ←

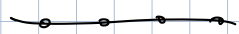
(transverse-field)

PIMC for quantum Ising model

$$H = -J\left(\sum_{\langle ij\rangle} \sigma_i^z \sigma_j^z + \frac{g}{J} \sum_i \sigma_i^x\right)$$

FM interactions





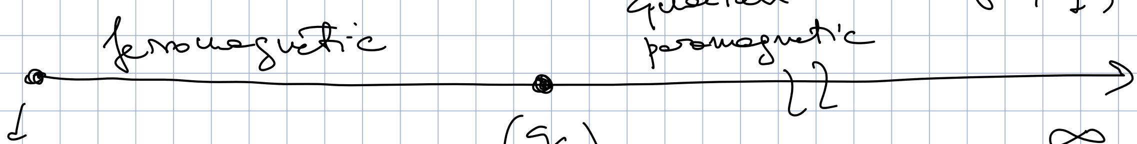
$\sigma_i = \pm 1$

$$\begin{cases} \sigma^z |\uparrow\rangle = |\uparrow\rangle \\ \sigma^z |\downarrow\rangle = -|\downarrow\rangle \end{cases}$$

$\sigma^x |\uparrow\rangle = |\downarrow\rangle$

$\sigma^x |\downarrow\rangle = |\uparrow\rangle$

ground-state phase diagram



$(g/J)_c$

quantum phase transition

$|\uparrow\uparrow \dots \uparrow\rangle$

$|\downarrow\downarrow \dots \downarrow\rangle$ deg. 2

deg. 1 : $|\rightarrow_x \rightarrow_x \dots \rightarrow_x\rangle$

$$|\rightarrow_x\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$$

$d=1$: exactly solvable $\longleftrightarrow$ $d=2$ classical Ising transition

d quantum Ising model $\longleftrightarrow$ $(d+1)$ classical Ising model

Trotter-Suzuki mapping $\rightarrow$ PIMC

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

$H_J = -J \sum_{\langle ij\rangle} \sigma_i^z \sigma_j^z$ $\leftarrow$

$H_g = -g \sum_i \sigma_i^x$

$$= \mathrm{Tr}\left(e^{-\beta(H_J + H_g)} \right)$$

$$= \lim_{M\to\infty} \mathrm{Tr}\left(\left(e^{-\beta/M\, H_J} \wedge e^{-\beta/M\, H_g} \right)^M \right) \qquad \text{Trotter–We decomposition}$$

$$\underbrace{\mathbb{1} = \sum_{\vec\sigma} |\vec\sigma\rangle\langle\vec\sigma|}$$

$$= \lim_{M\to\infty} \sum_{\vec\sigma_1} \langle \vec\sigma_1 | \left(\qquad \right)^M | \vec\sigma_1 \rangle$$

$$|\vec\sigma\rangle = |\sigma_1\, \sigma_2 \, \dots \, \sigma_N\rangle \qquad |\vec\sigma_k\rangle = |\sigma_{1,k}\, \sigma_{2,k} \dots \sigma_{N,k}\rangle$$

$$\sigma_i^z |\sigma_i\rangle = \sigma_i |\sigma_i\rangle$$

$$\left[e^{-\beta/M\, H_J} e^{-\beta/M\, H_g} = \sum_{\vec\sigma_k} e^{-\beta/M\, \hat H_J} |\vec\sigma_k\rangle\langle\vec\sigma_k| e^{-\beta/M\, \hat H_g} \qquad \mathbb{1} \right.$$

$$\left. = \sum_{\vec\sigma_k} e^{-\beta/M \sum_{\langle ij\rangle} \sigma_{i,k}\sigma_{j,k}} |\vec\sigma_k\rangle\langle\vec\sigma_k| e^{-\beta/M\, \hat H_g} \right]$$

$$= \lim_{M\to\infty} \sum_{\vec\sigma_1, \vec\sigma_2 \dots \vec\sigma_M} \langle\vec\sigma_1| e^{-\beta/M\, H_J} |\vec\sigma_2\rangle\langle\vec\sigma_2| e^{-\beta/M\, H_g} |\vec\sigma_3\rangle$$

$$\dots \langle\vec\sigma_M| e^{-\beta/M\, H_g} |\vec\sigma_1\rangle$$

$$e^{-\frac{\beta}{M}\sum_{k=1}^{M}\sum_{\langle ij\rangle} \sigma_{i,k}\sigma_{j,k}}$$

$$\&$$

$$\langle\vec\sigma_k| \underbrace{e^{+\beta/M\, g \sum_i \sigma_i^x}} |\vec\sigma_{k+1}\rangle$$

$$= \prod_i \underbrace{\langle \sigma_{i,k} | e^{\frac{\beta g}{M}\sigma_i^x} | \sigma_{i,k+1}\rangle}$$

$$\langle \sigma | \underbrace{e^{\frac{\beta g}{M}\sigma^x}} | \sigma' \rangle$$

$$= \langle\sigma| \left[\cosh\left(\frac{\beta g}{M}\right)\mathbb{1} + \sinh\left(\frac{\beta g}{M}\right)\sigma^x\right]|\sigma'\rangle$$

$$= \cosh\left(\frac{\beta g}{M}\right)\left[\delta_{\sigma\sigma'} + \tanh\left(\frac{\beta g}{M}\right)\left(1-\delta_{\sigma\sigma'}\right)\right] \leftarrow$$

$$= \cosh\left(\frac{\beta g}{M}\right) e^{(-)\frac{1}{2}(\sigma\sigma'-1)\log\left[\tanh\left(\frac{\beta g}{M}\right)\right]}$$

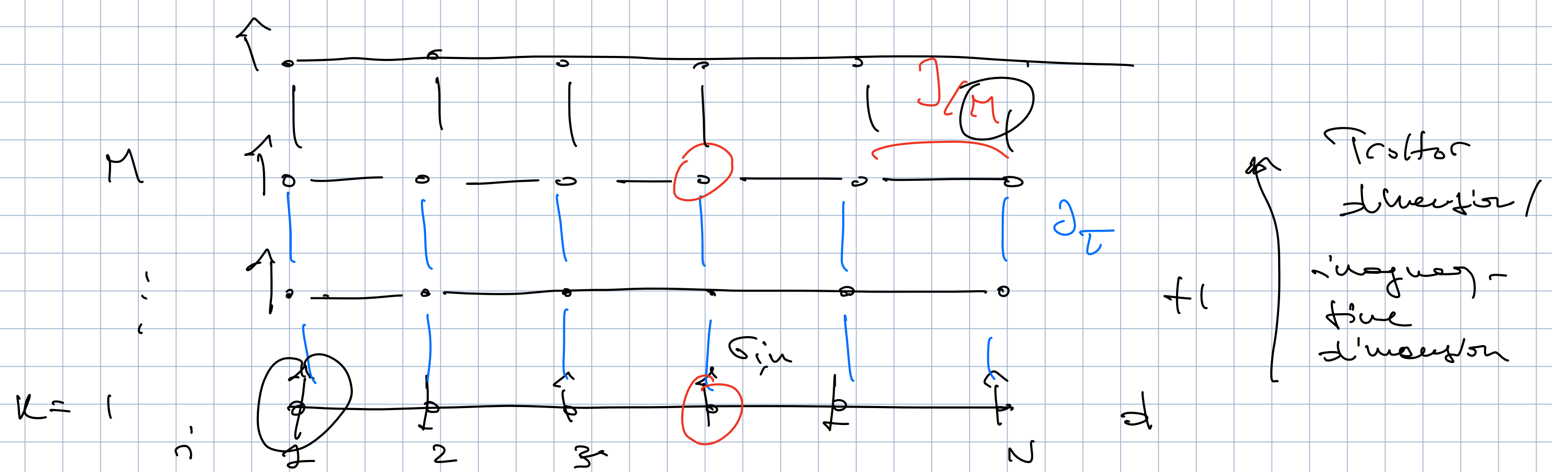
$$\frac{\beta g}{M} \ll 1$$

$$= \underbrace{\cosh\left(\frac{\beta g}{M}\right)} e^{\overbrace{\frac{1}{2}\left|\log\left[\tanh\left(\frac{\beta g}{M}\right)\right]\right|}^{\beta J_\tau}(\sigma\sigma'-1)}$$

Putting everything together

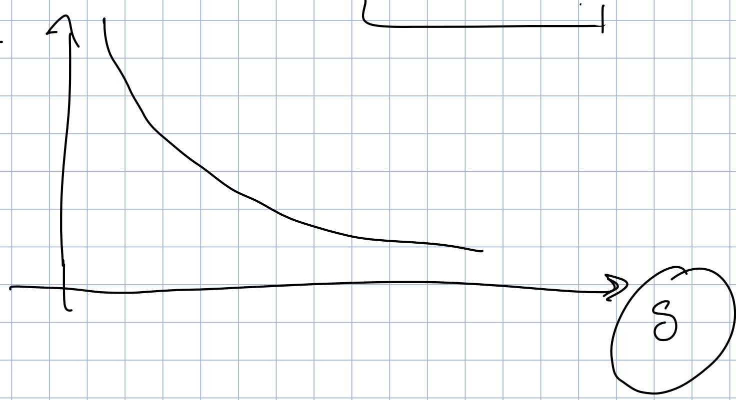
$$Z = \lim_{M\to\infty}\left[\cosh\left(\frac{\beta g}{M}\right)\right]^{NM}\sum_{\vec{\sigma}_1,\vec{\sigma}_2\dots\vec{\sigma}_M} e^{-\beta H_{eff}(\{\vec{\sigma}_k\})}$$

$$H_{eff}(\{\vec{\sigma}_k\}) = -\frac{J}{M}\sum_{k=1}^{M}\sum_{\langle ij\rangle}\sigma_{ik}\sigma_{jk} - J_\tau\sum_i\sum_k\left(\sigma_{ik}\sigma_{i,k+1}-1\right)$$

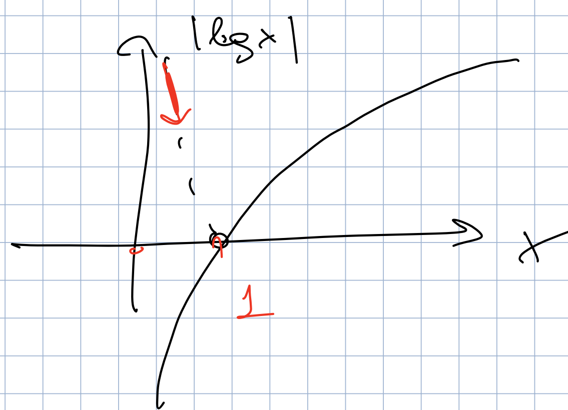


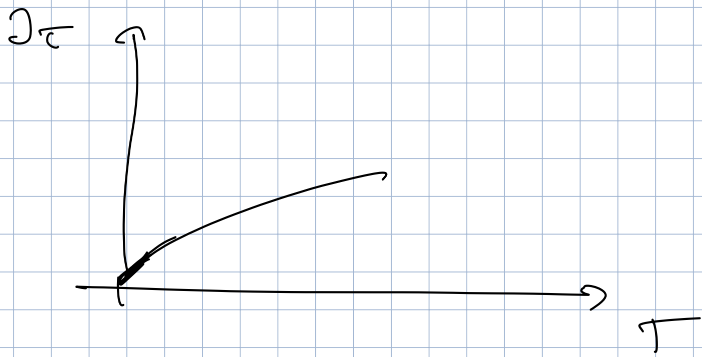
(spatially anisotropic) (d+1)-dimensional Ising model

$$J_\tau = \frac{k_B T}{2} \left| \log \left[\tanh\left(\frac{\beta \delta}{M} \right) \right] \right|$$



$\frac{\beta\delta}{M} \ll 1$





- $g \to 0$
- $T \to \infty$

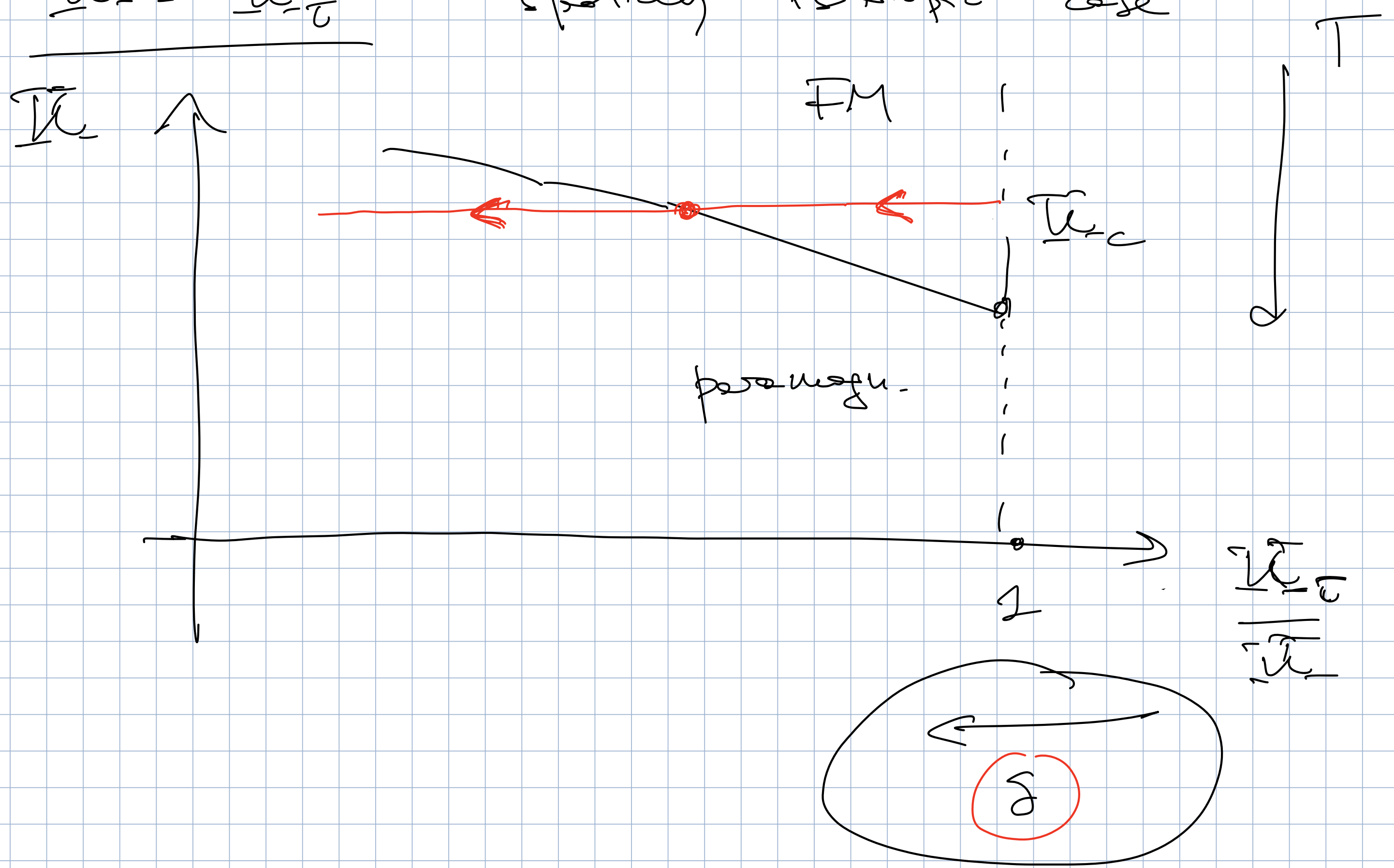
$J_\tau = \infty$

classical limit of a d-dimensional system

(d+1)-dimensional classical Ising model

$$\beta H_{eff} = -\overset{\beta J/M}{\tilde{K}} \sum_u \sum_{\langle ij\rangle} \sigma_{iu}\sigma_{ju} - \underset{\beta J_\tau}{\tilde{K}_\tau} \sum_u \sum_i \left(\sigma_{iu}\sigma_{i,u+1} - 1\right)$$

$\underline{K_- = K_{-\tau}}$ spatially isotropic case



$M \to \infty$

ground state physics $\beta \to \infty$ $(T \to 0)$

$J\,\delta\tau = \frac{\beta J}{M} = \text{const}$ $\quad \beta \to \infty,\ M \to \infty$

$\ll 1$

K_-

increasing g: classical $(d+1)$-dim. Ising transition

= quantum PT for the quantum Ising model

Generalization

$$H = -\sum_i h_i \sigma_i^z - \sum_{ij} J_{ij}\,\sigma_i^z\sigma_j^z$$

$$- \sum_{ijl} Q_{ijl}\,\sigma_i^z\sigma_j^z\sigma_l^z$$

$$\underbrace{- \sum_{ijlm} P_{ijlm}\,\sigma_i^z\sigma_j^z\sigma_l^z\sigma_m^z}_{\text{lattice gauge theories}} - \sum_i g_i\,\sigma_i^x$$

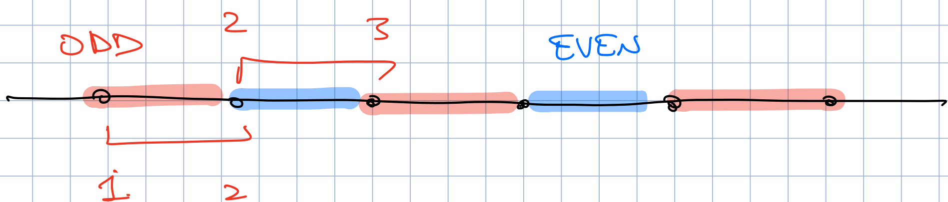
$$+ \dots$$

PIMC to XXZ model $(S = 1/2)$

$$H = -\underset{=}{J}\sum_{\langle ij\rangle}\Big(\underbrace{S_i^x S_j^x + S_i^y S_j^y}_{H^{xy}_{ij}} + \underbrace{\underset{=}{\Delta}\, S_i^z S_j^z}_{H^z_{ij}}\Big)$$

$$S^z|\sigma\rangle = \frac{\sigma}{2}|\sigma\rangle \qquad \sigma = \pm 1$$

$$Z = \sum_{\vec\sigma}\langle\vec\sigma|\, e^{-\beta\sum_{\langle ij\rangle}(H^{xy}_{ij} + H^z_{ij})}\,|\vec\sigma\rangle$$



$$[H^{xy}_{12}, H^{xy(z)}_{23}] \neq 0$$

$$H = \overbrace{\sum_{\langle ij\rangle\ \text{even}} \underbrace{\left(H^{xy}_{ij} + H^{z}_{ij}\right)}_{H_{ij}}}^{H_{even}} + \overbrace{\sum_{\langle ij\rangle\ \text{odd}} \left(H^{xy}_{ij} + H^{z}_{ij}\right)}^{H_{odd}}$$

$[H_{ij}, H_{lm}] = 0$ $\quad (ij)\ (lm)$ are both even sites / odd

$$Z =$$

$$\mathrm{Tr}\left[e^{-\beta H}\right] = \lim_{M\to\infty} \mathrm{Tr}\left[\left(e^{-\frac{\beta}{M} H_e}\, e^{-\frac{\beta}{M} H_{odd}}\right)^{M}\right]$$

$$= \lim_{M\to\infty} \mathrm{Tr}\left[\left(\left[\prod_{\langle ij\rangle\text{even}} e^{-\frac{\beta}{M}\left(H^{xy}_{ij} + H^{z}_{ij}\right)}\right]\left[\prod_{\langle ij\rangle\text{odd}} e^{-\frac{\beta}{M}\left(H^{xy}_{ij} + H^{z}_{ij}\right)}\right]\right)^{M}\right]$$

$$= \lim_{M\to\infty} \mathrm{Tr}\left[\left\{\prod_{\langle ij\rangle\text{even}}\left(e^{-\frac{\beta}{M} H^{xy}_{ij}} \underbrace{\wedge}_{\sum_{\vec\sigma} |\vec\sigma\rangle\langle\vec\sigma|} e^{-\frac{\beta}{M} H^{z}_{ij}}\right)\prod_{\langle ij\rangle\text{odd}}\left(e^{-\frac{\beta}{M} H^{xy}_{ij}} \underbrace{\wedge}_{\sum_{\vec\sigma} |\vec\sigma\rangle\langle\vec\sigma|} e^{-\frac{\beta}{M} H^{z}_{ij}}\right)\right\}^{M}\right]$$

$$= \lim_{M\to\infty} \sum_{\{\vec\sigma_u\}} \langle\vec\sigma_1| \prod_{\langle ij\rangle\text{even}} e^{-\frac{\beta}{M} H^{xy}_{ij}} |\vec\sigma_2\rangle\langle\vec\sigma_2| \prod_{\langle ij\rangle\text{odd}} e^{-\frac{\beta}{M} H^{xy}_{ij}} |\vec\sigma_3\rangle$$

$$\langle\vec\sigma_3| \prod_{\langle ij\rangle\text{even}} e^{-\frac{\beta}{M} H^{xy}_{ij}} |\vec\sigma_4\rangle \quad ---$$

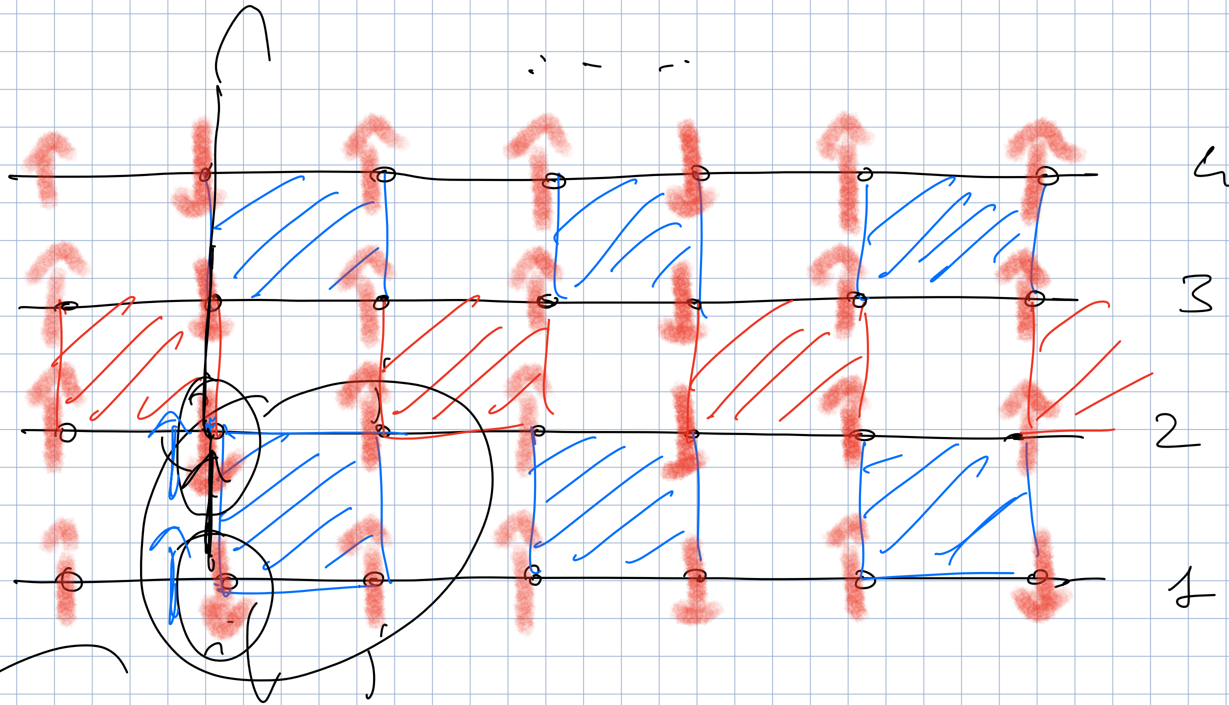
$$\langle\vec\sigma_{2M}| \prod_{\langle ij\rangle\text{odd}} e^{-\frac{\beta}{M} H^{xy}_{ij}} |\vec\sigma_1\rangle$$

$$e^{+\frac{\Delta J}{4M}\beta \sum_{\langle ij\rangle} \sum_{u=1}^{2M} \sigma_{iu}\sigma_{ju}}$$

$$\langle\vec\sigma_u| e^{-\frac{\beta}{M}\sum_{\langle ij\rangle\text{even}} H^{xy}_{ij}} |\vec\sigma_{u+1}\rangle$$

"vertex"

$$= \prod_{\langle ij\rangle\text{even}} \langle\sigma_{iu}\sigma_{ju}| e^{-\frac{\beta}{M} H^{xy}_{ij}} |\sigma_{i,u+1}\, \sigma_{j,u+1}\rangle$$



I J

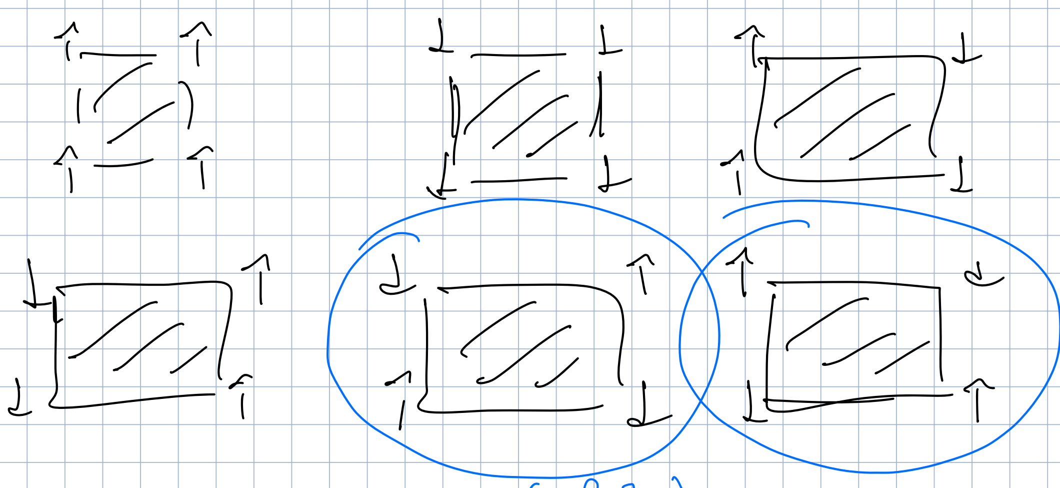
$$\langle \sigma_{i,n}\sigma_{j,n}| e^{-\beta/M\, H^{xy}_{ij}} | \sigma_{i,n+1}\sigma_{j,n+1}\rangle = W(\sigma_{i,n},\sigma_{j,n};\sigma_{i,n+1},\sigma_{j,n+1})$$

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

I

x

$W \neq 0$

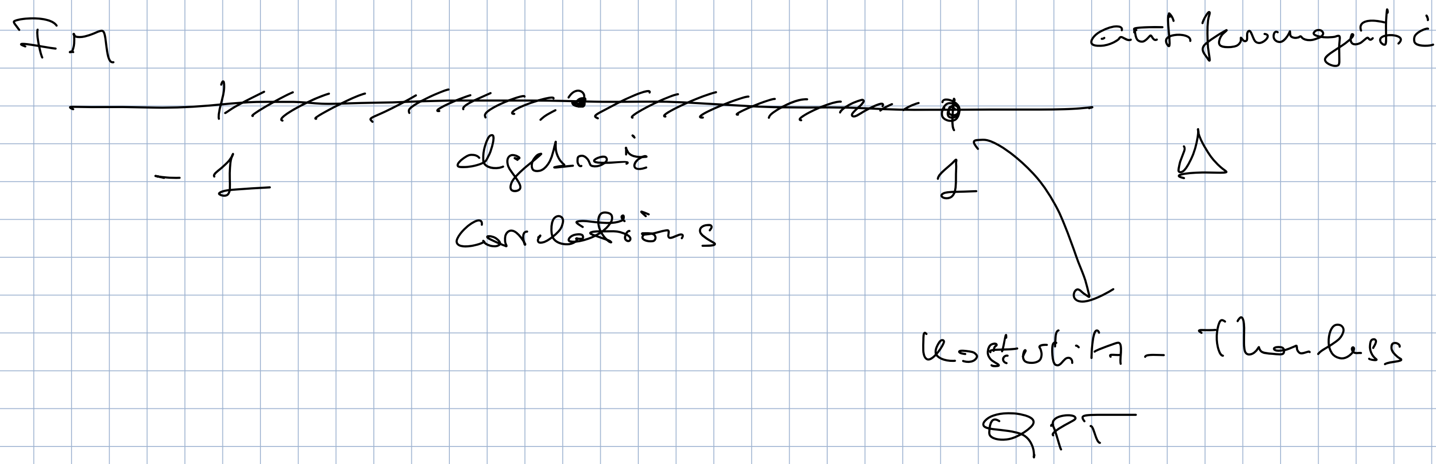


$\sinh\left(\frac{\beta J}{2M}\right)$

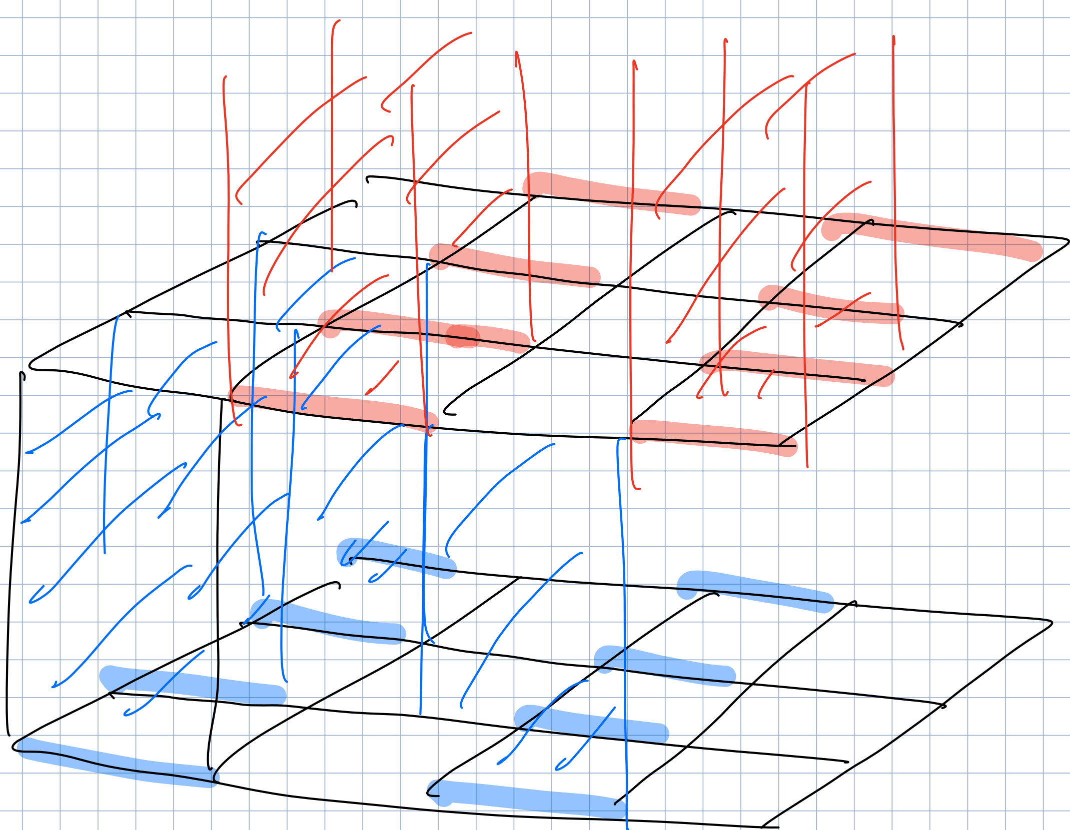
6-vertex model

quantum XXZ model in d dimensions $\Longleftrightarrow$ classical 6-vertex model in $(d+1)$ dimensions

$d = 1$



3d 6-vertex model



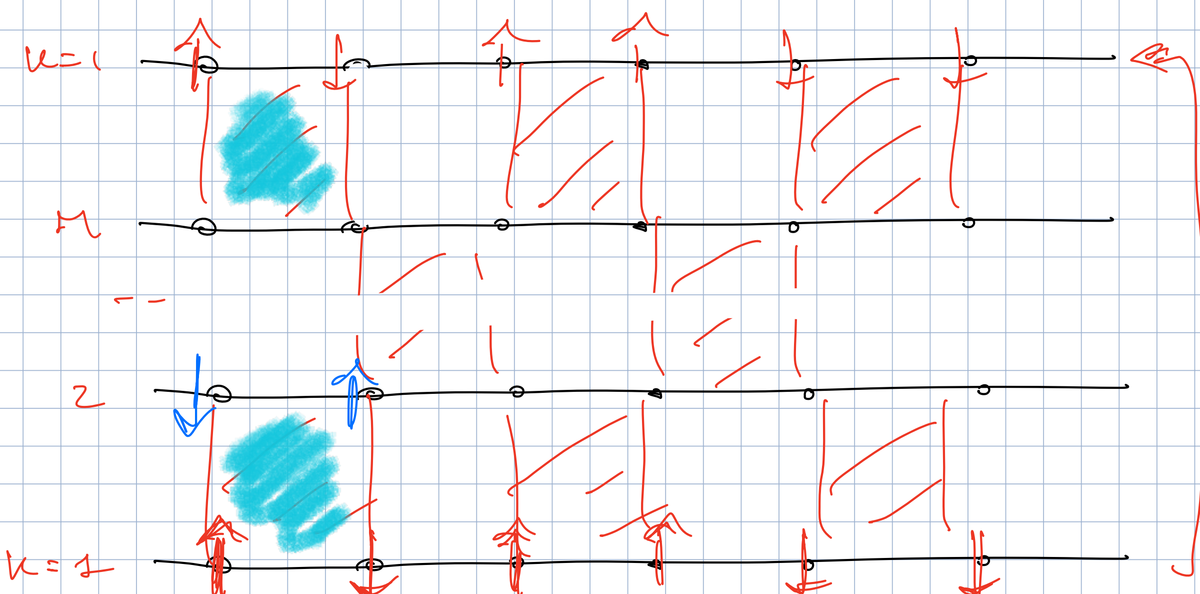
$$Z = \lim_{M\to\infty} \mathrm{Tr}\left[\left(\qquad \right)^M \right]$$

$$\simeq Z_M \, \mathrm{Tr}\left[\left(\qquad \right)^M \right] + \underbrace{O\left(\frac{\beta^2}{M}\right)}_{\text{Trotter error}}$$

$J<0 \qquad \sinh\left(\frac{\beta J}{2M}\right) < 0 \quad \to \quad$ sign problem ?

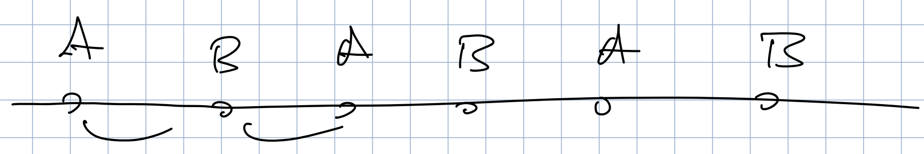
sign problem $\qquad Z = \sum_c W_c \qquad W_c \geq 0$, $\; W_c < 0$

sign problem arises when odd number of off-diagonal vertices with negative sign

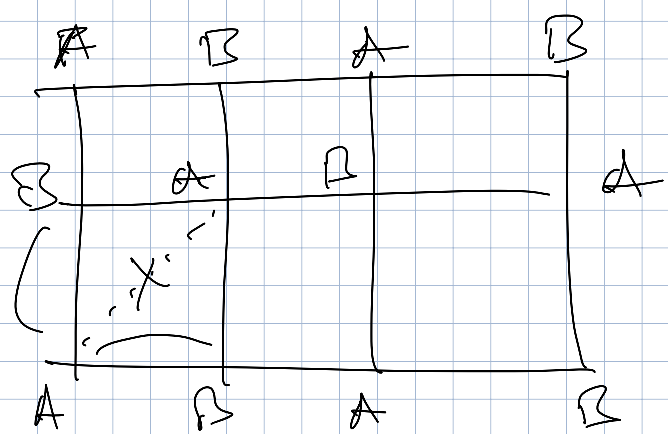


$$H = J \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)$$

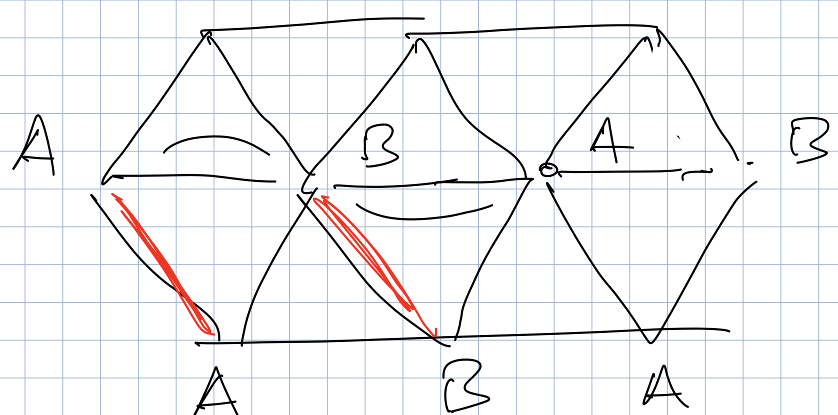
Bipartite lattice: divisible into two sublattices A, B such that there is no interaction within the same sublattice



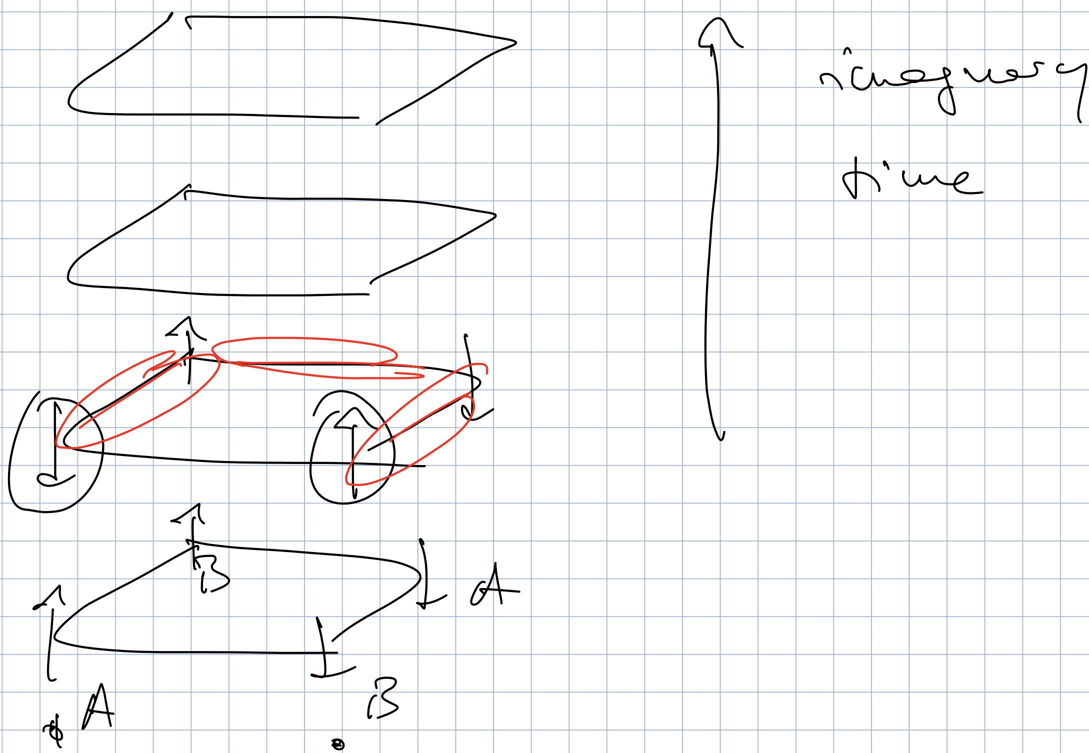
$d = 2$ ✓



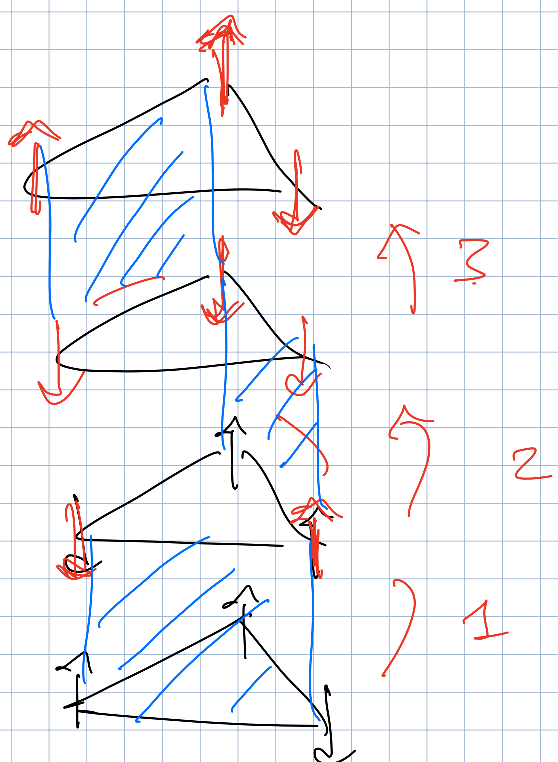
$d = 2$ ✓



✗



XYZ



odd number of anti-aligned vertices

=> neg. "probability"

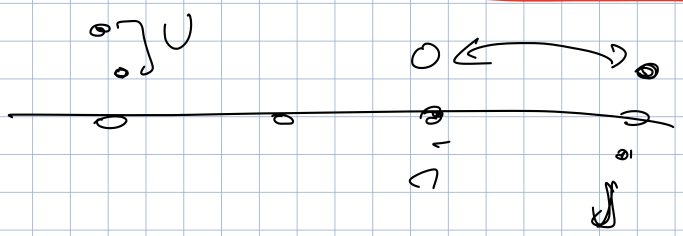
=> PIMC for quantum spins with anti-ferromagnetic interactions works on BIPARTITE LATTICES ~ when you have AF interactions between at least two spin components.

Some sign problem : bosons in a gauge field

Bose-Hubbard model

$t > 0$ diagonal

$$H = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + U \sum_i \underbrace{\tfrac{1}{2} n_i (n_i - 1)}_{\text{\# of pairs of bosons on a site}}$$



(atoms in optical lattices)

d

$$\frac{(\vec{p} + e\vec{A})^2}{2m}$$

$t < 0$

magnetic field $\Rightarrow$ $t \to t e^{i\phi}$

$t \not> 0$

Fermions : sign problem $d > 1$

or hopping going beyond nearest neighbor

QMC solvable	sign problem
bosons, quantum magnetism, ... (with only one frustrated component)	· fermions · frustrated magnetism · bosons in a gauge field ...

quantum many-body problems

PIMC in discrete imaginary time (old)
(world-line Monte Carlo)

more modern formulations

→ continuous imaginary time

gets rid of the Trotter error

→ stochastic series expansion

$$\mathrm{Tr}\left(e^{-\beta H}\right) = \sum_n \frac{\beta^n}{n!} \mathrm{Tr}\left[(-H)^n\right]$$

alternative to PIMC

Stochastic Series Expansion for lattice quantum models with two-site interactions

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}\left[(-H)^n\right]$$

$|\alpha\rangle$ basis for Hilbert space

$$= \sum_{n=0}^{\infty} \sum_{\alpha} \underbrace{\frac{\beta^n}{n!} \langle\alpha| (-H)^n |\alpha\rangle}_{W(\alpha;\, n)}$$

$$= \sum_c W_c \, ?$$

they must be efficiently computable!

otherwise:

$$Z = \sum_\alpha \underbrace{\langle\alpha| e^{-\beta H} |\alpha\rangle}$$

$$H = \sum_b H_b$$

ex. XXZ model

$$H = \sum_{b=\langle ij\rangle} \Big(\underbrace{-J\left(S_i^x S_j^x + S_i^y S_j^y\right)}_{-H_b^{(OD)}} \underbrace{- J\Delta S_i^z S_j^z + C_b \mathbb{1}}_{-H_b^{(D)}} \Big)$$

$$= -\sum_b \left(H_b^{(OD)} + H_b^{(D)}\right)$$

$$(-H)^n = \Big[\overbrace{\sum_b \left(H_b^{(D)} + H_b^{(OD)}\right)}\Big]^n$$

$$= \sum_{S_n} \prod_{p=0}^{n-1} H_{b_p}^{(A_p)} \qquad A = D,\ OD$$

sum over sequences of length n

$$(x_1+x_2)^n = xx\cdots x + yxx\cdots x + xyx\cdots x$$

$$\uparrow \quad \uparrow$$

$$x_1 x_2 \; x_1 \; x_1$$

$$Z = \sum_\alpha \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{S_n} \underbrace{\langle\alpha| \prod_{p=0}^{n-1} H^{(A_p)}_{b_p} |\alpha\rangle}_{}$$

$\downarrow$

strings of bond operators

this can be calculated efficiently

$$|\alpha\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \cdots |\sigma_N\rangle$$

$\downarrow$

ex. eigenstates of S^z_i $\quad i = 1, \dots, N$

$$H^{(A)}_b |\alpha\rangle \sim |\alpha'\rangle \; (\text{or } 0) \; ?$$

$$H^{(D)}_b |\alpha\rangle \sim |\alpha\rangle$$

$$H^{(OD)}_b |\alpha\rangle = \underbrace{(S^x_{i_b} S^x_{j_b} + S^y_{i_b} S^y_{j_b})}_{} |\alpha\rangle$$

xxz

$$\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \; |\sigma_1\sigma_2 \ldots \sigma_i \sigma_j \ldots\rangle$$

$$\uparrow \quad \downarrow$$

$$\downarrow \quad \uparrow$$

$$\prod_{p=0}^{n-1} H^{(A_p)}_{b_p} |\alpha\rangle \quad \text{defines a sequence of basis states}$$

$$\neq \quad \langle\alpha_1| \, e^{-\beta H} \, |\alpha_1\rangle$$

$$= \sum_{\alpha_1 \alpha_2 \ldots \alpha_M} \langle \alpha_1 | e^{-\beta/M\, H} | \alpha_2 \rangle \langle \alpha_2 | e^{-\beta/M\, H} | \alpha_3 \rangle \cdots \langle \alpha_M | e^{-\beta/M\, H} | \alpha_1 \rangle$$

In practice

$$Z \simeq Z_L = \sum_{n=0}^{L} \frac{\beta^n}{n!} \sum_\alpha \sum_{S_n} \langle \alpha | \prod_{p=0}^{n-1} H_{b_p}^{(A_p)} | \alpha \rangle$$

the truncation to finite order has NO consequence if $L \sim O(N\beta)$.

$S_n \xrightarrow{\text{extension}} S_L$ by inserting identities

$$\underbrace{H_{b_1}^{(A_1)} H_{b_2}^{(A_2)} \cdots H_{b_n}^{(A_n)}}_{n} \to \underbrace{\mathbb{1}\, H_{b_1}^{(A_1)}\, \mathbb{1} \cdots}_{L}$$

inserting $L-n$ identities

insertion schemes $\dfrac{L!}{(L-n)!\, n!}$

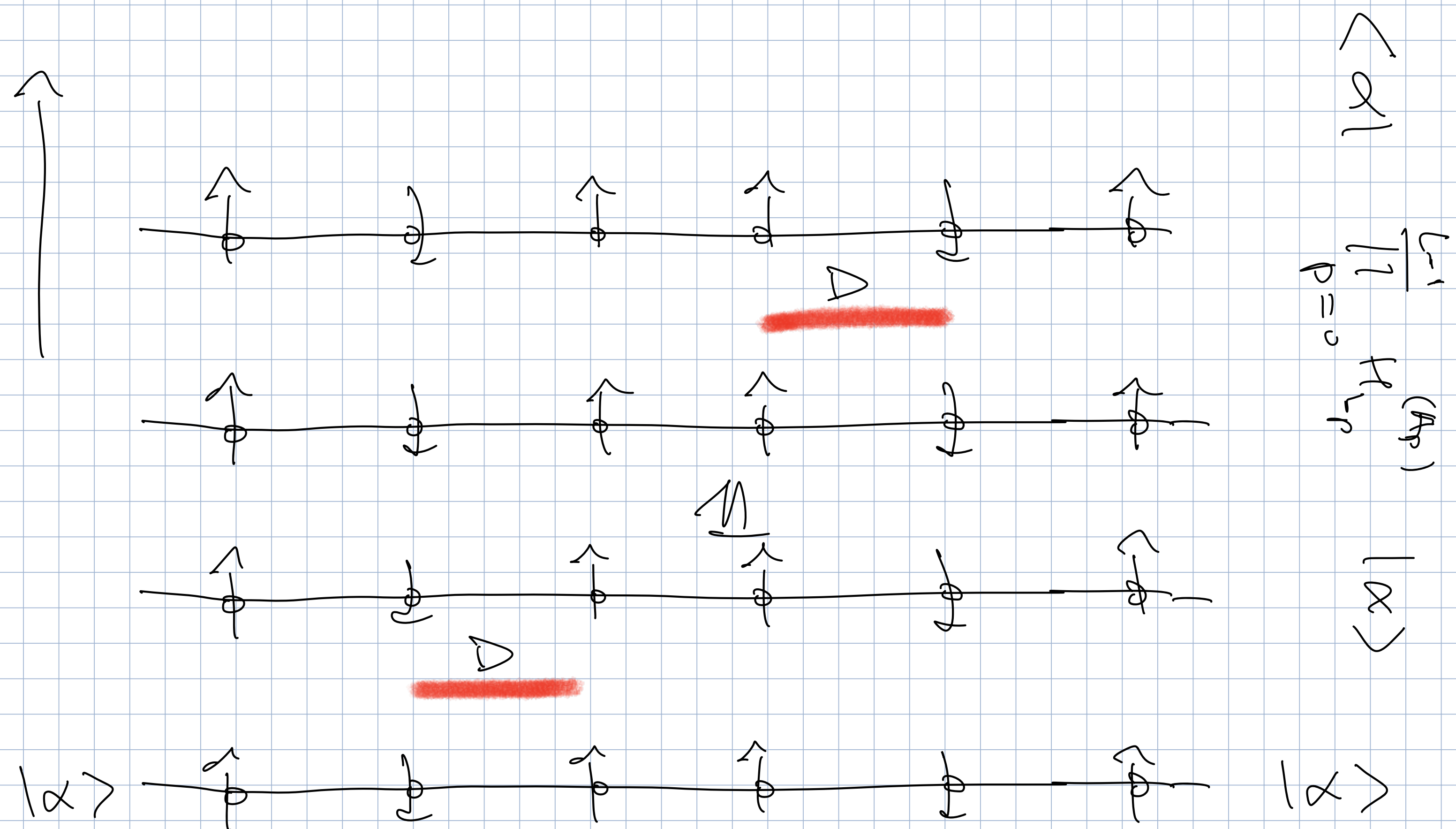
# of non-identity operators

$$Z_L = \sum_\alpha \sum_{S_L} \frac{\beta^{n(S_L)}}{\cancel{n(S_L)!}} \frac{\cancel{n(S_L)!}\,(L-n(S_L))!}{L!} \langle \alpha | \prod_{p=0}^{L-1} H_{b_p}^{(A_p)} | \alpha \rangle$$

$A_p = D, OD, \mathbb{1}$

$$= \sum_{(\alpha, J_L)} w(\alpha; J_L) \rightarrow C$$

effective classical system



$$A_p = D, \ \mathbb{1}$$

What about the truncation of the series?

$$\langle H \rangle = E = \frac{\partial(\beta F)}{\partial \beta}$$

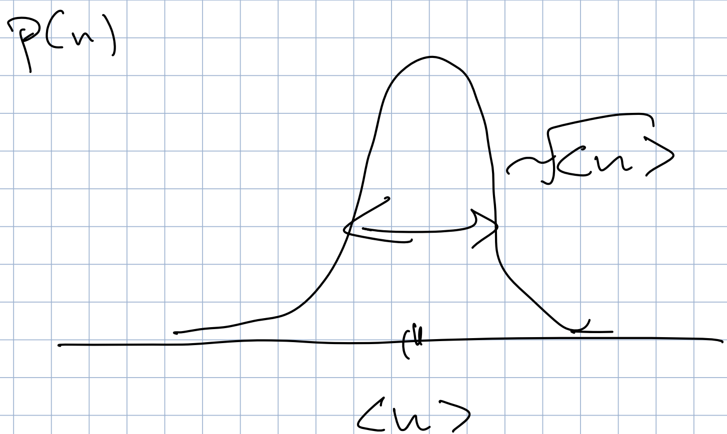
$$= \frac{\partial}{\partial \beta}\left(\cancel{\beta} \cdot (-\cancel{k_B T}) \log Z\right) = -\frac{\partial}{\partial \beta}(\log Z) = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$$

$$\overset{L=\infty}{=} - \frac{\sum_{S_L,\alpha} \frac{n(S_L)}{\beta} \overbrace{\frac{\beta^{n(S_L)}}{L!}(L-n)!\, \langle\alpha|\prod C\ \ |\alpha\rangle}^{w(S_L,\alpha)}}{\sum_{S_L} w(S_L,\alpha)}$$

$$= - \left\langle \frac{n}{\beta} \right\rangle_W$$

$$\langle n \rangle = \beta\,(\underbrace{-\langle H\rangle}_{\sim O(N)}) \sim \underline{O(N\beta)}$$

$$\langle n^2 \rangle - \langle n \rangle^2 \sim O(N)$$



In pratica $\qquad L \simeq \langle n\rangle + m\sqrt{\langle n\rangle}$