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

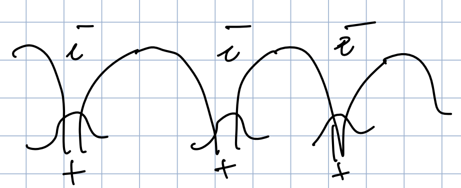
-> PIMC : thermodynamics of systems in continuum space

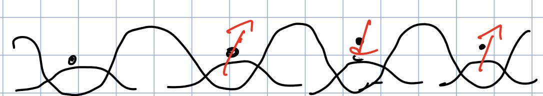
=> PIMC / QMC for lattice models ≠ ⊥ $\vec{p}, \vec{x}$

-> 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 ←

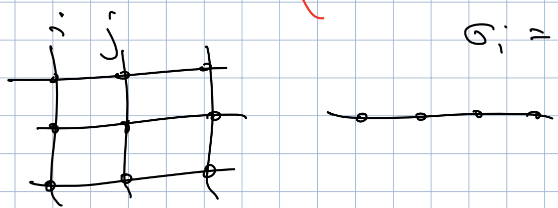
PIMC for quantum Ising model

(transverse-field)

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

FM interactions

$\sigma_i = \pm 1$

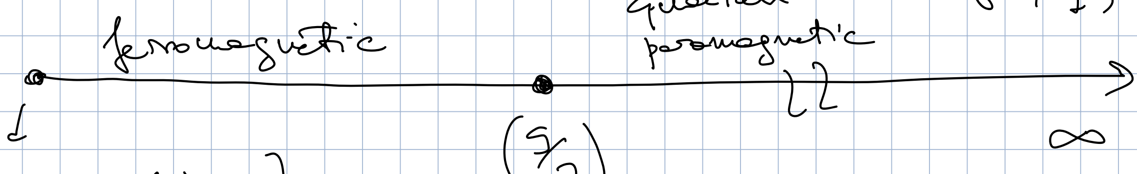


$$\begin{cases} \sigma^z|\uparrow\rangle = |\uparrow\rangle \\ \sigma^z|\downarrow\rangle = -|\downarrow\rangle \end{cases}$$

ground-state phase diagram

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

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



$$\left.\begin{matrix} |\uparrow\uparrow \ldots \uparrow\rangle \\ |\downarrow\downarrow \ldots \downarrow\rangle \end{matrix}\right] \text{deg. } 2$$

quantum phase transition

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

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

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

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

Trotter-Suzuki mapping $\rightarrow$ PIMC

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

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

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

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

$$= \lim_{M\to\infty} \mathrm{Tr}\left(\left(e^{-\beta/M\, H_J} \underbrace{\wedge}_{\mathbb{1} = \sum_{\vec\sigma} |\vec\sigma\rangle\langle\vec\sigma|} e^{-\beta/M\, H_g} \right)^M \right)$$

Trotter–We decomposition

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

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

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

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

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

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

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

$$e^{-\frac{\beta}{M}\sum_{k=1}^{M}\sum_{\langle ij\rangle} \sigma_{ik}\sigma_{jk}}$$

$$\&$$

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

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

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

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

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

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

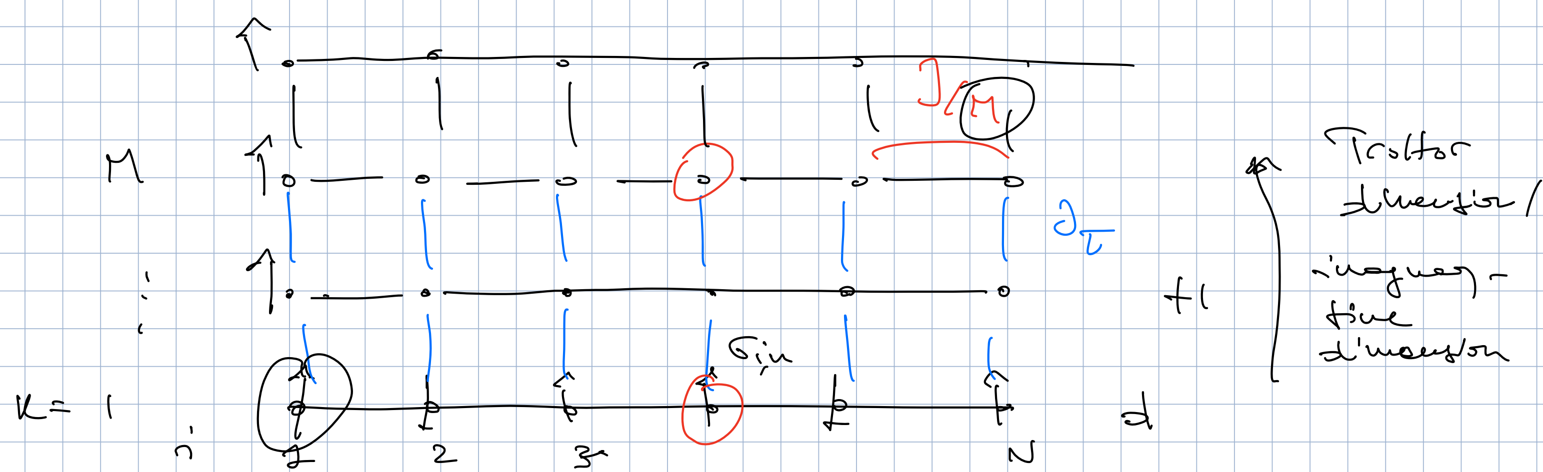
$$\frac{\beta g}{M} \ll 1$$

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

Putting everything together

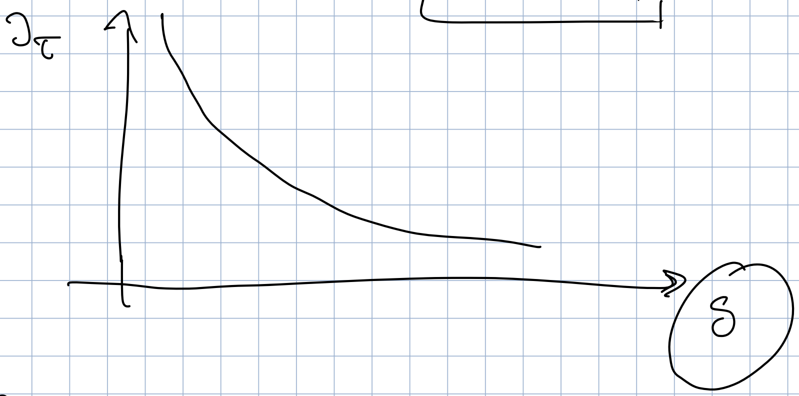
$$Z = \lim_{M \to \infty} \left[\cosh\left(\frac{\beta g}{M}\right)\right]^{NM} \sum_{\vec{\sigma}_1, \vec{\sigma}_2 \dots \vec{\sigma}_M} e^{-\beta H_{eff}(\{\vec{\sigma}_k\})}$$

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

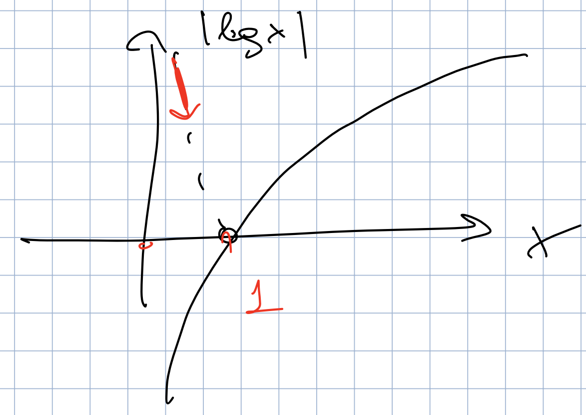


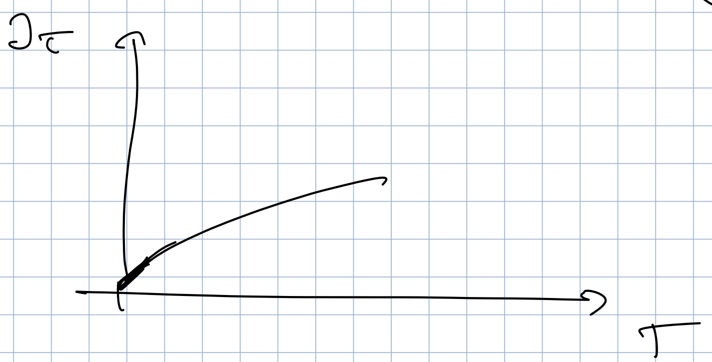
(spatially anisotropic) $(d+1)$-dimensional Ising model

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



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





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

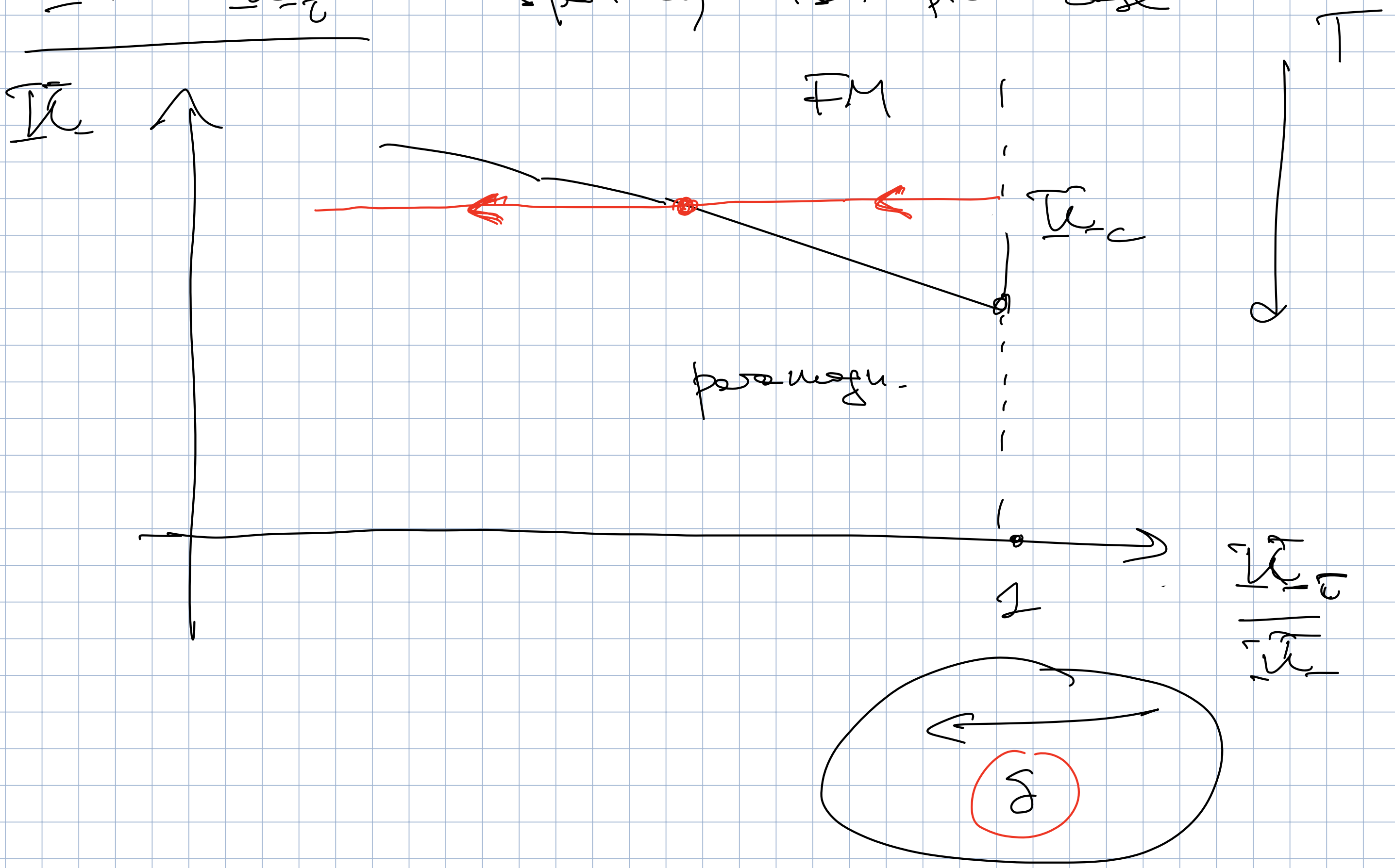
$J_\tau = \infty$

classical limit of a d-dimensional system

$(d+1)$-dimensional classical Ising model

$$\beta H_{eff} = -\underbrace{\frac{\beta J}{M}}_{} \sum_u \sum_{\langle ij \rangle} \sigma_{i,u}\sigma_{j,u} - \underbrace{K_\tau}_{\beta J_\tau} \sum_u \sum_i (\sigma_{i,u}\sigma_{i,u+1} - 1)$$

$\tilde{K}_- = \tilde{K}_{-\tau}$ spatially isotropic case



$M \to \infty$

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

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

$\ll 1$

$\tilde{K}_-$

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

= quantum PT for the quantum Ising model

Generalization $\perp$ $\perp$

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

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

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

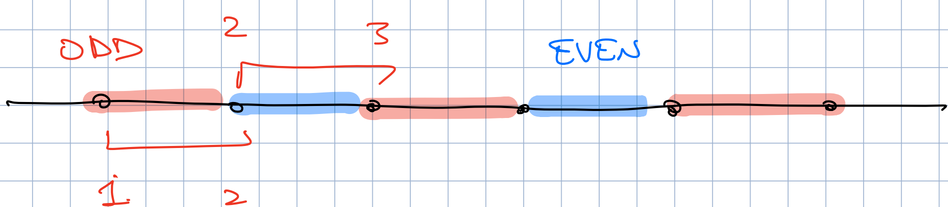
$$+ \dots$$

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

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

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

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



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

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

$$[H_{ij}, H_{lm}] = 0 \qquad (ij)\ (lm) \text{ are both even bonds (odd)}$$

$$Z =$$

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

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

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

$$= \lim_{M\to\infty} \sum_{\{\vec\sigma_k\}} \langle\vec\sigma_1| \prod_{\langle ij\rangle \text{even}} e^{-\beta/M\, H_{ij}^{xy}} |\vec\sigma_2\rangle\langle\vec\sigma_2| \prod_{\langle ij\rangle \text{odd}} e^{-\beta/M\, H_{ij}^{xy}} |\vec\sigma_3\rangle$$

$$\langle\vec\sigma_3| \prod_{\langle ij\rangle \text{even}} e^{-\beta/M\, H_{ij}^{xy}} |\vec\sigma_4\rangle \quad ---$$

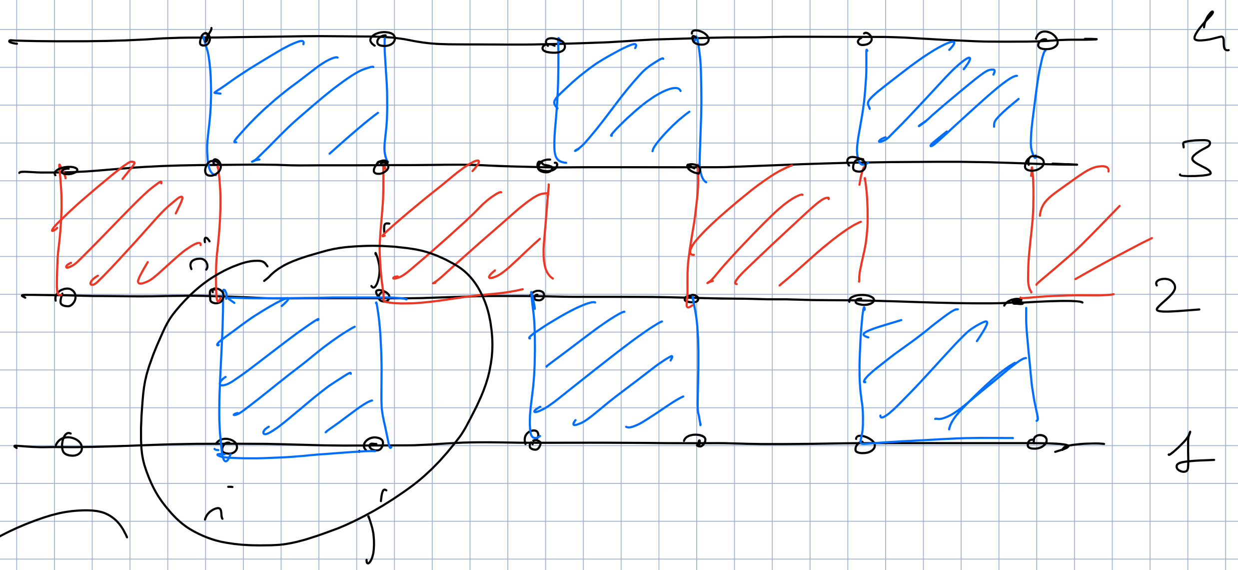
$$\langle\vec\sigma_{2M}| \prod_{\langle ij\rangle \text{odd}} e^{-\beta/M\, H_{ij}^{xy}} |\vec\sigma_1\rangle$$

$$e^{-\frac{J}{4M}\beta \sum_{\langle ij\rangle} \sum_{k=1}^{2M} \sigma_{ik}\sigma_{jk}}$$

$$\langle\vec\sigma_k| e^{-\beta/M \sum_{\langle ij\rangle \text{even}} H_{ij}^{xy}} |\vec\sigma_{k+1}\rangle$$

"vertex"

$$= \prod_{\langle ij\rangle \text{even}} \langle\sigma_{ik}\sigma_{jk}| e^{-\beta/M\, H_{ij}^{xy}} |\sigma_{ik+1}\ \sigma_{jk+1}\rangle$$



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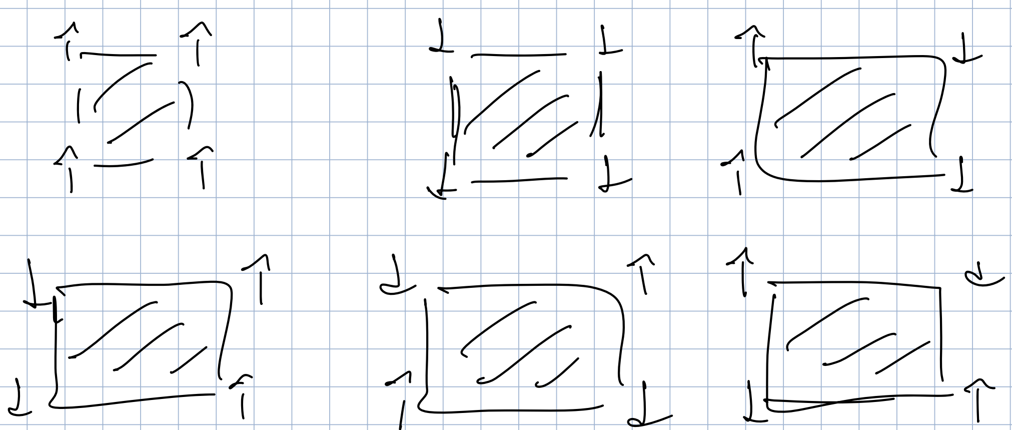
$$\langle \sigma_{ik}\sigma_{jk} | e^{-\beta/M \, H^{xy}_{ij}} | \sigma_{i,k+1}\, \sigma_{j,k+1} \rangle = W(\sigma_{ik}, \sigma_{jk}; \sigma_{i,k+1}, \sigma_{j,k+1})$$

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

I

$W \neq 0$



6-vertex model

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

$d = 1$