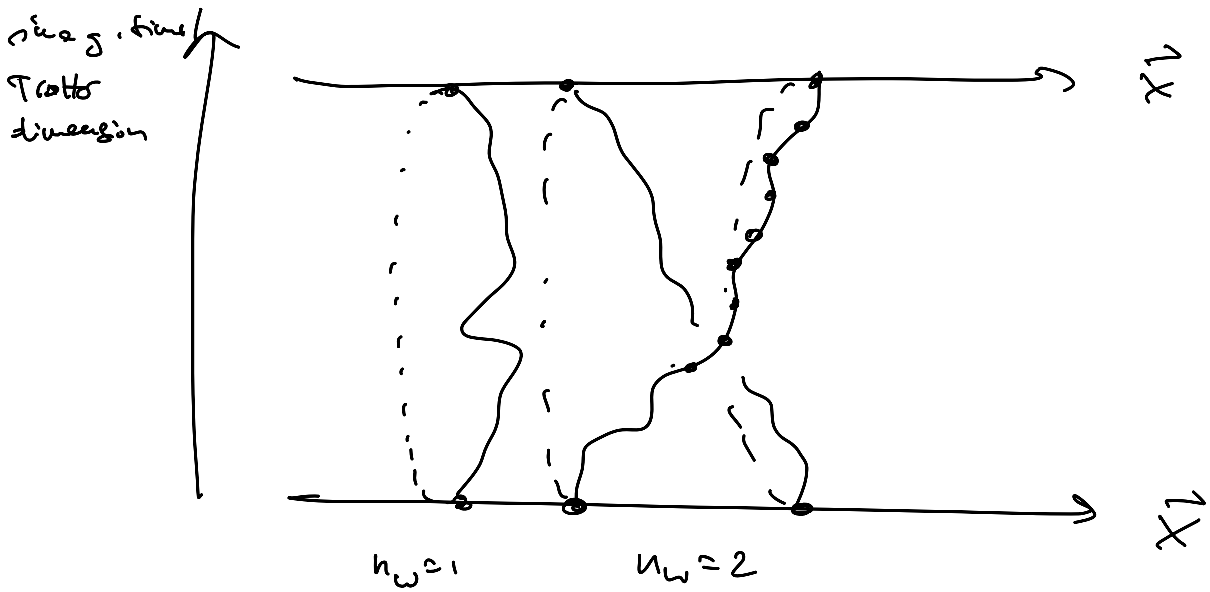
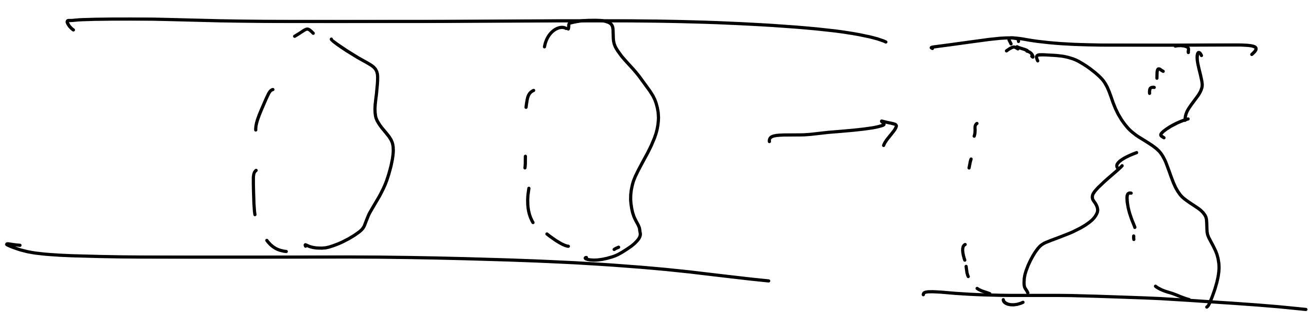
Path-integral MC for identical quantum particles

$$Z_N = \mathrm{Tr}[e^{-\beta \mathcal{H}_N}] = \int \mathcal{D}[\{\vec{x}_n\}]\, e^{-S_N[\{\vec{x}_n\}]}$$



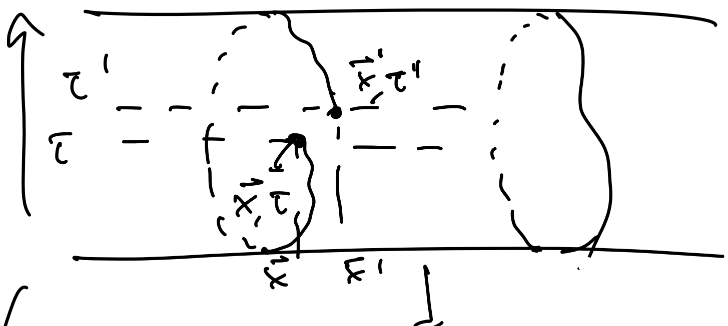
permutation cycles

sample permutation cycles



"Worm" algorithm (Boninsegni / Prokof'ev 2006)

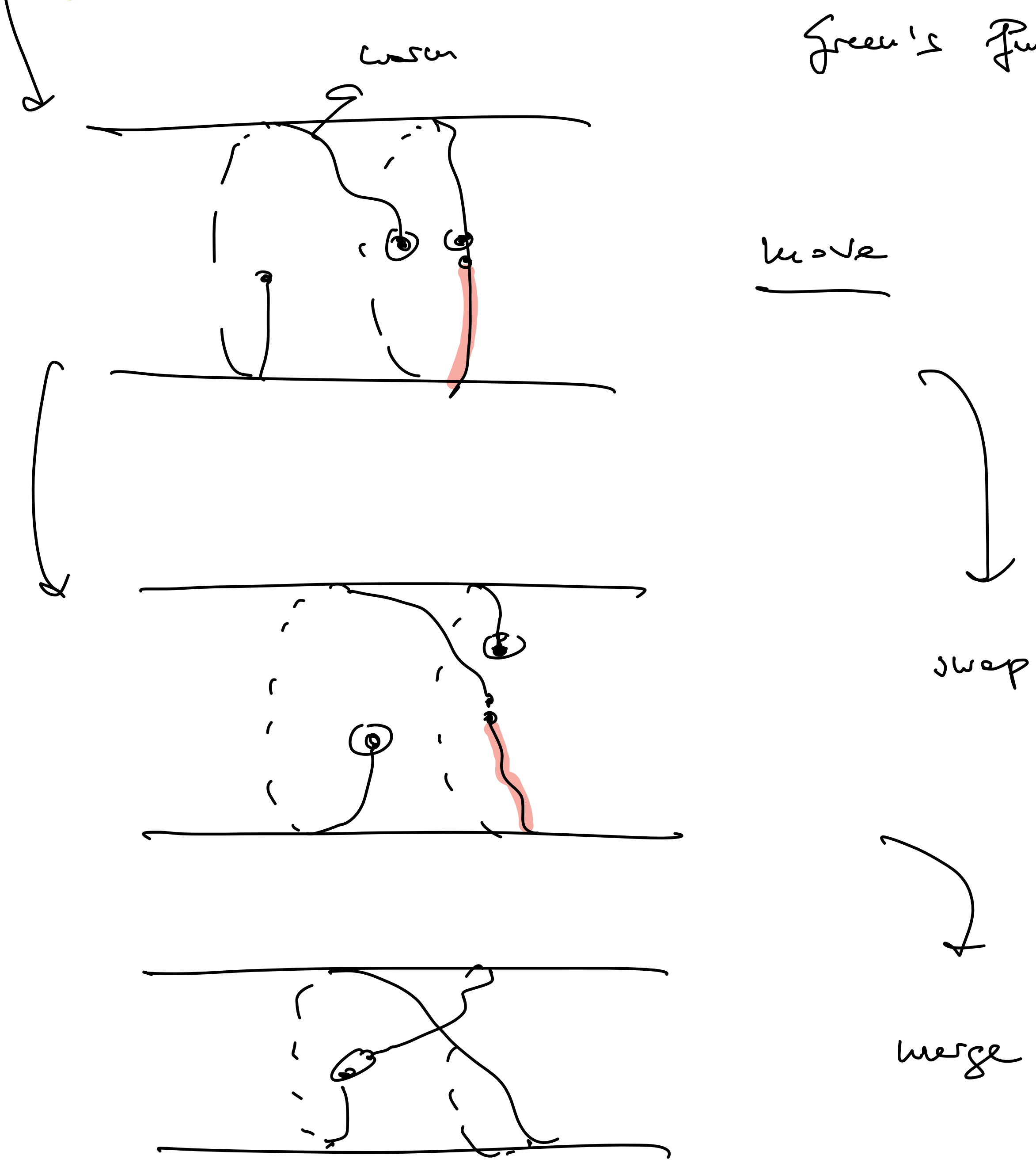
"outside" of the partition function



open

$$\langle \hat{\psi}(\vec{x},\tau)\, \psi^{\dagger}(\vec{x}',\tau') \rangle = G(\vec{x},\vec{x}';\tau,\tau')$$

Green's function



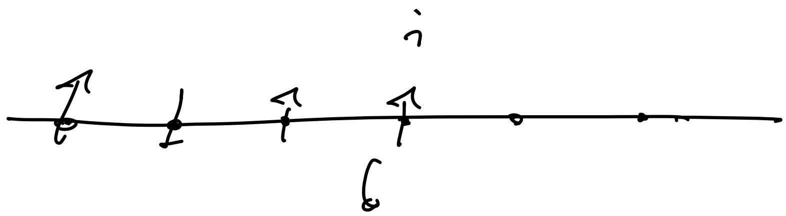
QMC (PIMC) for quantum spin lattices

→ magnetism in condensed

→ quantum statistical mechanism

↓

quantum phase transitions



$$\hat{\vec{S}}_i = \frac{1}{2}\vec{\sigma}_i \qquad \text{spin-}\tfrac{1}{2}$$

$$\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$$

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

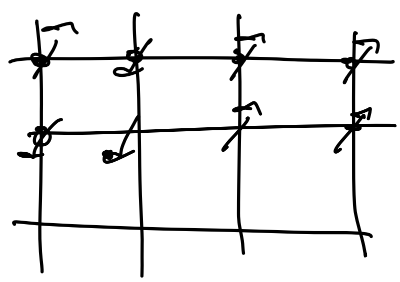
$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Transverse-field (quantum) Ising model (TFIM)

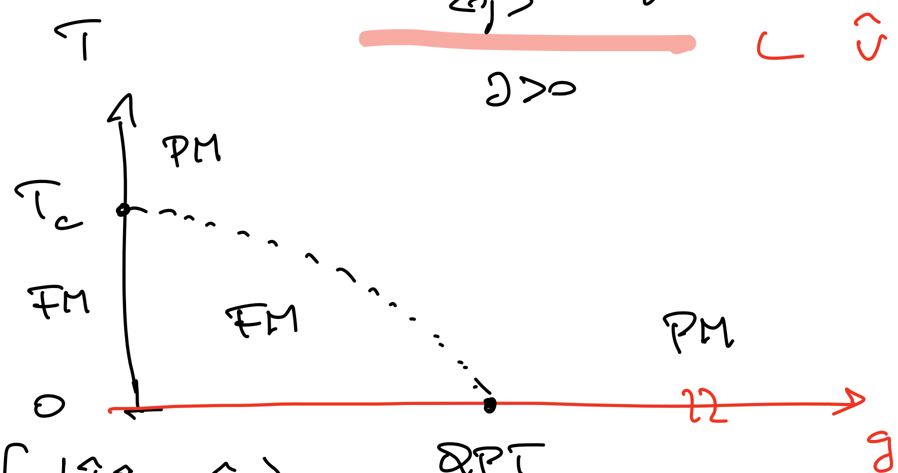
Ising model for ferromagnetism ($d=2$)

$$\hat{H} = \underbrace{-J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z}_{\hat{H}_0} \underbrace{- g \sum_i \sigma_i^x}_{\hat{V}}$$

$J>0$



$\sigma = \pm 1$



QPT
quantum phase transition

$$\left[\begin{matrix} |\uparrow\uparrow \ldots \uparrow\rangle \\ |\downarrow\downarrow \ldots \downarrow\rangle \end{matrix} \right.$$

$|\rightarrow_x \rightarrow_x \ldots \rightarrow_x\rangle$

$\sigma^z|\uparrow\rangle = |\uparrow\rangle$

$\sigma^z|\downarrow\rangle = -|\downarrow\rangle$

$$[\hat{H}_0, \hat{V}] \neq 0$$

Path-integral mapping (Trotter-Suzuki mapping) of the partition function

$$Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \sum_{c} e^{-S_c}$$

configs. of a classical $(d+1)$-dim. Ising model

$$= \sum_{|\vec\sigma\rangle} \langle\vec\sigma|\, e^{-\beta(\hat{H}_0+\hat{V})}\, |\vec\sigma\rangle$$

$|\vec\sigma\rangle = |\sigma_1\,\sigma_2\,\dots\,\sigma_N\rangle$ $\qquad \hat{\sigma}_i^z|\sigma_i\rangle = \sigma_i|\sigma_i\rangle$

$$= \lim_{M\to\infty} \sum_{|\vec\sigma\rangle} \langle\vec\sigma|\left(e^{-\beta/M\,\hat{H}_0}\, e^{-\beta/M\,\hat{V}}\right)^M |\vec\sigma\rangle$$

$$\sum_{|\vec\sigma_1\rangle} |\vec\sigma_1\rangle\langle\vec\sigma_1| = \mathbb{1}$$

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

$$\underbrace{e^{+\frac{\beta J}{M}\sum_{k=1}^{M}\sum_{\langle ij\rangle}\sigma_i^{(k)}\sigma_j^{(k)}}}_{\text{diagonal}}$$

$$\langle\vec\sigma|e^{-\beta/M\,\hat{V}}|\vec\sigma'\rangle = \langle\vec\sigma|\prod_{i=1}^{N} e^{+\frac{\beta g}{M}\sigma_i^x}|\vec\sigma'\rangle$$

$$= \prod_{i=1}^{N} \langle\sigma_i|\, e^{+\beta s/M\,\sigma_i^x}\, |\sigma_i'\rangle$$

$$\cosh\left(\frac{\beta s}{M}\right)\mathbb{1} + \sinh\left(\frac{\beta s}{M}\right)\sigma_i^x$$

$$\cosh\left(\frac{\beta s}{M}\right)\delta_{\sigma_i\sigma_i'} + \sinh\left(\frac{\beta s}{M}\right)\left(1-\delta_{\sigma_i\sigma_i'}\right)$$

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

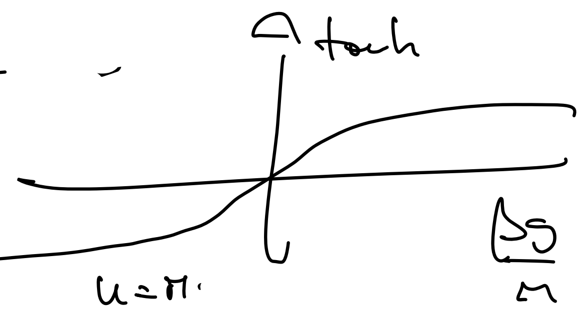
$$\cosh\left(\frac{\beta s}{M}\right) e^{-\frac{1}{2}\log\left[\tanh\left(\frac{\beta s}{M}\right)\right]\left(\sigma\sigma'-1\right)}$$

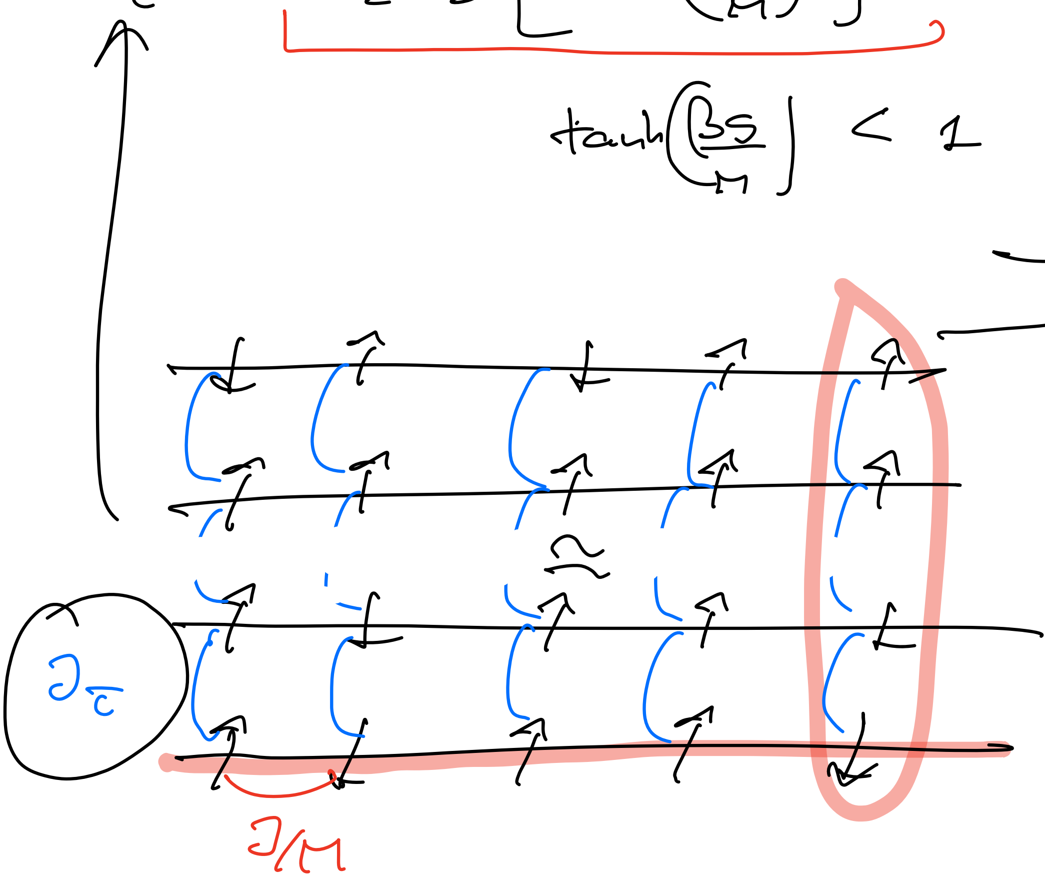
$$Z = \lim_{M\to\infty} \sum_{\vec{\sigma}_1 \ldots \vec{\sigma}_M} \left[\cosh\left(\frac{\beta s}{M}\right)\right]^{MN} e^{-\beta H_{eff}[\{\sigma_i^{(u)}\}]}$$

$$H_{eff}[\{\sigma_i^{(u)}\}] = -\frac{J}{M}\sum_{\langle ij\rangle}\sum_u \sigma_i^{(u)}\sigma_j^{(u)} - J_\tau \sum_{i=1}^{N}\sum_{u=1}^{M}\left(\sigma_i^{(u)}\sigma_i^{(u+1)} - 1\right)$$

$$J_\tau = -\frac{1}{2}\log\left[\tanh\left(\frac{\beta s}{M}\right)\right] = \frac{1}{2}\left|\log\left[\tanh\left(\frac{\beta s}{M}\right)\right]\right|$$

$$\tanh\left(\frac{\beta s}{M}\right) < 1$$





$u = M$

$u = M-1$

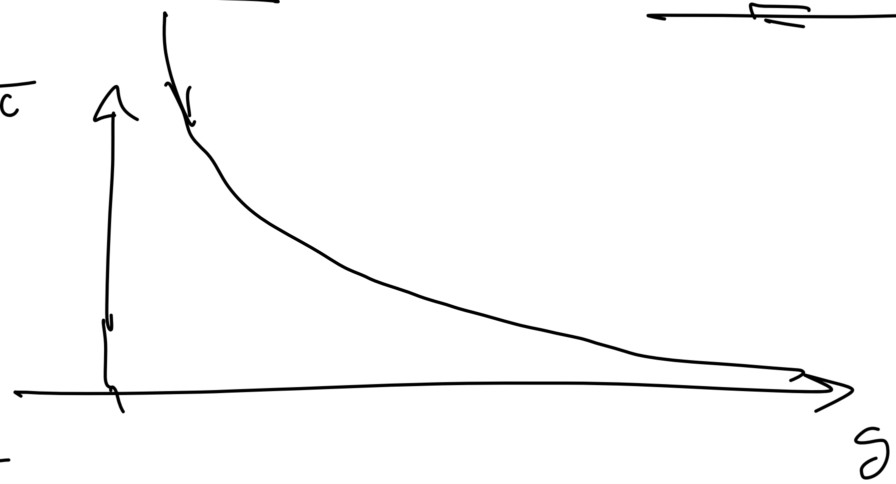
$u = 2$

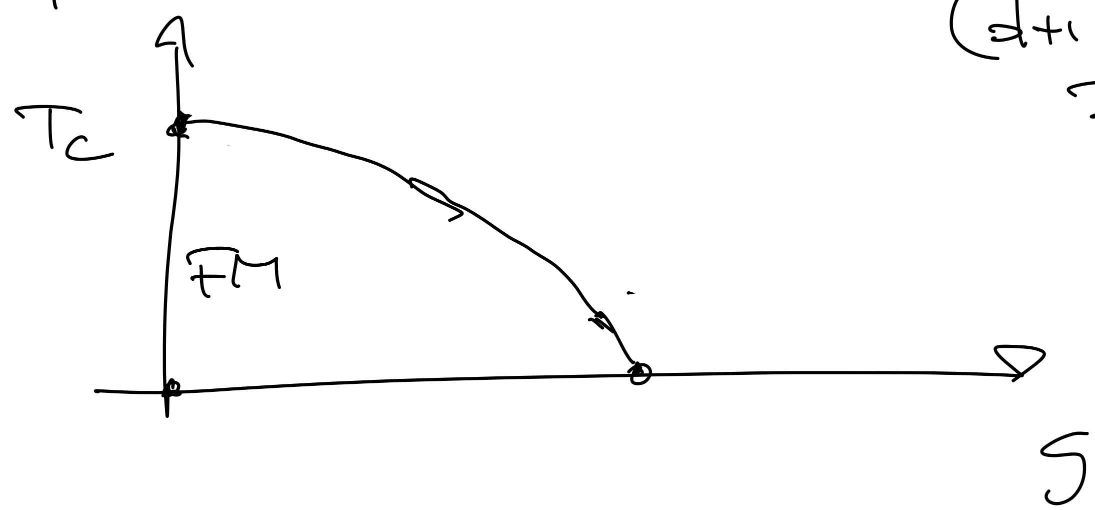
$u = 1$

(d+1) - dimensional classical Ising model

with spatial anisotropy

increase g at fixed β





(d+1) - classical Ising model

$$\lim_{\substack{M\to\infty \\ \beta\to\infty}} \frac{\beta}{M} = \epsilon \qquad \partial_\tau = \frac{1}{2}\left|\log\left[\tanh(\epsilon g)\right]\right|$$

$$S = \beta H_{eff}$$

$$= -\epsilon [J] \sum_{k}\sum_{\langle ij \rangle} \sigma_i^{(k)}\sigma_j^{(k)} + \frac{\partial_\tau}{\epsilon} \sum_k \sum_i \sigma_i^{(k)}\sigma_i^{(k+1)}$$

Fixed temperature ϵ

Generalizing the picture

$$\mathcal{H} = \sum_{ij} J_{ij}\,\sigma_i^z \sigma_j^z + \sum_{ijk} K_{ijk}\,\sigma_i^z \sigma_j^z \sigma_k^z + \dots + \sum_i h_i\,\sigma_i^z$$

$$- \sum_i g_i\,\sigma_i^x$$