

Two-spin correlation function

$$\langle s_i s_{i+r} \rangle = \frac{1}{Z} \sum_{s_1} \dots \sum_{s_N} s_i s_{i+r} e^{\beta \sum_{i=1}^N (J s_i s_{i+1} + \frac{h}{2} (s_i + s_{i+1}))}$$

$$= \frac{1}{Z} \sum_{s_1} \dots \sum_{s_N} \langle s_1 | T | s_2 \rangle \dots \langle s_{i-1} | T | s_i \rangle s_i \langle s_i | T | s_{i+1} \rangle \dots$$

$$\langle s_{i+r-1} | T | s_{i+r} \rangle s_{i+r} \langle s_{i+r} | T | s_{i+r+1} \rangle \dots \langle s_N | T | s_1 \rangle$$

$$= \frac{1}{Z} \text{Tr} \left(T^{i-1} \sigma_z T^r \sigma_z T^{N-i-r+1} \right)$$

$$= \frac{1}{Z} \text{Tr} \left(S S^{-1} T^{i-1} S S^{-1} \sigma_z S S^{-1} T^r S S^{-1} \sigma_z S S^{-1} T^{N-i-r+1} S S^{-1} \right)$$

$$= \frac{1}{Z} \text{Tr} \left(S \Lambda^{i-1} S^{-1} \sigma_z S \Lambda^r S^{-1} \sigma_z S \Lambda^{N-i-r+1} S^{-1} \right)$$

$$= \frac{1}{Z} \text{Tr} \left(\Lambda^r S^{-1} \sigma_z S \Lambda^{N-i-r+1} S^{-1} S \Lambda^{i-1} S^{-1} \sigma_z S \right)$$

$$= \frac{1}{Z} \text{Tr} \left(\Lambda^r S^{-1} \sigma_z S \Lambda^{N-r} S^{-1} \sigma_z S \right) \quad \text{using cyclic property}$$

$$= \frac{1}{Z} \text{Tr} \left(\Lambda^r S^{-1} \sigma_z S \Lambda^{N-r} S^{-1} \sigma_z S \right)$$

$$= \frac{1}{Z} \text{Tr} \left(\begin{pmatrix} \lambda_+^r & 0 \\ 0 & \lambda_-^r \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_+^{N-r} & 0 \\ 0 & \lambda_-^{N-r} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right)$$

$$= \frac{1}{Z} \text{Tr} \left(\begin{pmatrix} 0 & \lambda_+^r \\ \lambda_-^r & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda_+^{N-r} \\ \lambda_-^{N-r} & 0 \end{pmatrix} \right)$$

$$= \frac{1}{Z} \text{Tr} \left(\begin{pmatrix} \lambda_+^r \lambda_-^{N-r} & 0 \\ 0 & \lambda_+^{N-r} \lambda_-^r \end{pmatrix} \right)$$

$$= \frac{\lambda_+^r \lambda_-^{N-r} + \lambda_+^{N-r} \lambda_-^r}{\lambda_+^N + \lambda_-^N}$$

$$\langle s_i s_{i+r} \rangle = \frac{\left(\frac{\lambda_-}{\lambda_+}\right)^r + \left(\frac{\lambda_-}{\lambda_+}\right)^{N-r}}{1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N} \sim \left(\frac{\lambda_-}{\lambda_+}\right)^r \quad \text{as } N \rightarrow \infty$$

$$\Rightarrow \langle s_i s_{i+r} \rangle \sim \exp(-r/\beta) \quad \text{as } N \rightarrow \infty$$

where $\beta = \frac{1}{k_B T} = \frac{1}{k_B \ln(\coth(\beta J))} \quad \begin{cases} \rightarrow 0 & \text{if } \beta J \rightarrow 0 \quad (\text{High T}) \\ \rightarrow \infty & \text{if } \beta J \rightarrow \infty \quad (\text{Low T}) \end{cases}$

Ising Model (arbitrary dimensions) in terms of long and short range order variables

$$L \equiv \frac{1}{N} \sum_i s_i = \frac{1}{N} (N_+ - N_-) \quad \dots \quad (1) \quad \text{and} \quad \sigma \equiv \frac{N_{++} - N_{\text{bonds}}/2}{N_{\text{bonds}}/2} \quad \dots \quad (2)$$

N_{++} = Number of bonds with up spins at both ends

$N_{\text{bonds}} = \gamma N/2$ = total number of bonds (γ = coordination number)

$$\gamma = \begin{cases} 2 & \text{for 1d chain} \\ 4 & \text{for 2d square lattice, 6 for cubic lattice} \\ 2d & \text{for d-dimensional hypercubic lattice} \end{cases}$$

$$\text{We know, } N_+ + N_- = N \quad \dots \quad (3)$$

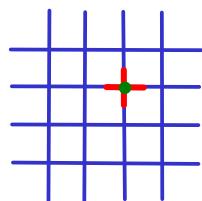
From (1) and (3), we have,

$$N_+ = \frac{N}{2} (1 + L) \quad \dots \quad (4)$$

$$\text{and } N_- = \frac{N}{2} (1 - L) \quad \dots \quad (5)$$

Let each bond be made of two half bonds that stick out of the sites.

There are γ half-bonds coming out of each site



A site is coloured green and the four half bonds are coloured red.

The number of half bonds coming from all the up spin sites is

$$\gamma N_+ = 2N_{++} + N_{+-} \quad \dots \quad (6)$$

$$\text{Similarly } \gamma N_- = 2N_{--} + N_{+-} \quad \dots \quad (7)$$

$$\text{From Eq. (2), } N_{++} = \frac{\gamma N}{4} (1 + \sigma) \quad \dots \quad (8)$$

\Rightarrow From Eqs. (6, 4)

$$N_{+-} = \frac{\gamma N}{2} (1 + L) - \frac{\gamma N}{2} (1 + \sigma)$$

$$\Rightarrow N_{+-} = \frac{\gamma N}{2} (L - \sigma) \quad \dots \quad (9)$$

$$\text{Since } N_{++} + N_{--} + N_{+-} = N_{\text{bonds}} = \gamma N/2,$$

$$N_{--} = \frac{\gamma N}{2} - \frac{\gamma N}{4} (1 + \sigma) - \frac{\gamma N}{2} (L - \sigma)$$

$$\Rightarrow N_{--} = \frac{\gamma N}{4} (1 + \sigma - 2L)$$

$$\begin{aligned}
 H &= -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \\
 &= -J(N_{++} + N_{--} - N_{+-}) - h(N_+ - N_-) \\
 &= -JN_{\text{bonds}} + 2JN_{+-} - hLN \\
 &= -J\gamma N/2 + J\gamma N(L-\sigma) - hLN
 \end{aligned}$$

$$H = -\frac{J\gamma N}{2}(2\sigma - 2L + 1) - hLN$$

$\therefore H$ depends only on L and σ .

Bragg-Williams approximation (Mean Field Theory)

Assumption \therefore No additional short range order than what can be guessed from the long range order.

$$\left(\text{Probability of finding a } ++ \text{ bond} \right) = \left(\text{Square of the probability of finding a } + \text{ bond} \right)$$

$$\Rightarrow \frac{N_{++}}{N_{\text{bonds}}} = \left(\frac{N_+}{N} \right)^2$$

$$\Rightarrow \frac{1+\sigma}{2} = \left(\frac{1+L}{2} \right)^2$$

$$\Rightarrow L^2 + 2L + 1 = 2(1+\sigma)$$

$$\Rightarrow L^2 = 2\sigma - 2L + 1$$

$$\therefore H_{\text{MF}} = -\frac{J\gamma N}{2}L^2 - hNL$$

The total number of spin configurations that correspond to a given value of L $= \binom{N}{N_+} = \frac{N!}{N_+! N_-!}$, where $N_{\pm} = \frac{N}{2}(1 \pm L)$

\therefore The partition function is,

$$Z = \text{Tr } e^{-\beta H}$$

$$= \sum_L \binom{N}{N_+} \exp \left[\beta N \left(\frac{J\gamma L^2}{2} + hL \right) \right]$$