

20/01/25

Lecture 5

1D Ising Model Exact Solution by Transfer Matrix Method

- Periodic Boundary Conditions
- Nearest Neighbour Interactions

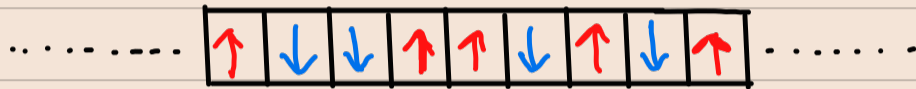
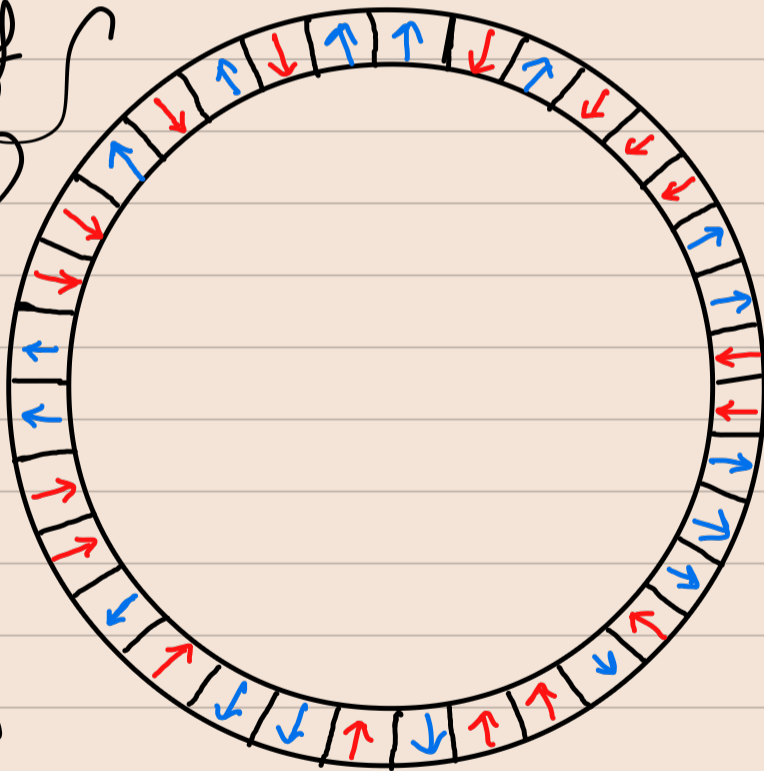


Illustration of
Periodic
Boundary
Condition

This is not
the spatial
arrangement
of spins.



A set of N spins are arranged in
in a 1D chain. Spin variable at ' i^{th} '
cell is S_i which can take values
of 1 (up spin) or -1 (down spin).

In the presence of External field 'h' (in S.I. $\mu_B h$) the Hamiltonian for the ising model becomes,

$$\mathcal{H} = -J \sum_{\substack{\langle i, j \rangle \\ j = i+1}}^N S_i S_j - h \sum_{i=1}^N S_i$$

(we used PBC) $\leftarrow \left(\frac{S_i + S_{i+1}}{2} \right)$

$$\Rightarrow \mathcal{H} = -J \sum_{i=1}^N S_i S_{i+1} - \frac{h}{2} \sum_{i=1}^N (S_i + S_{i+1})$$

$$\mathcal{Z} = \text{Trace} (e^{-\beta \hat{H}}) = \sum_{\{c\}} e^{-\beta H_c}$$

c: various configurations

$$\Rightarrow \mathcal{Z} = \sum_{\{S_1, S_2, \dots, S_N\}} e^{\beta \sum_i \left(J S_i S_{i+1} + \frac{h}{2} [S_i + S_{i+1}] \right)}$$

Let, $\beta J = K$ & $\beta h = L$

$$\Rightarrow \mathcal{Z} = \sum_{\{S_1, S_2, \dots, S_N\}} \prod_{i=1}^N e^{(K S_i S_{i+1} + \frac{L}{2} [S_i + S_{i+1}])}$$

$$Z = \prod_{i=1}^N \sum_{S_i} e^{\left[K S_i S_{i+1} + \frac{L}{2} (S_i + S_{i+1}) \right]}$$

Consider a matrix 'T' whose elements are given by

$$\langle S_i | T | S_{i+1} \rangle = e^{\left[K S_i S_{i+1} + \frac{L}{2} (S_i + S_{i+1}) \right]}$$

Since $S_i = \pm 1$, $S_{i+1} = \pm 1$,

'T' is a 2×2 matrix.

$$T = \begin{bmatrix} \langle +1 | T | +1 \rangle & \langle +1 | T | -1 \rangle \\ \langle -1 | T | +1 \rangle & \langle -1 | T | -1 \rangle \end{bmatrix}$$

$$T = \begin{pmatrix} e^{K+L} & e^{-K} \\ e^{-K} & e^{K-L} \end{pmatrix} \Rightarrow \text{Transfer Matrix}$$

$$\Rightarrow Z = \sum_{S_1, S_2, \dots, S_N} \langle S_1 | T | S_2 \rangle \langle S_2 | T | S_3 \rangle \times \dots \times \langle S_{N-1} | T | S_N \rangle \langle S_N | T | S_1 \rangle$$

$$\Rightarrow Z = \sum_{S_1 = \{\pm 1\}} \langle S_1 | T^N | S_1 \rangle$$

$$Z = \text{Trace}(T^N)$$

$$\text{Now } \text{trace}(T^N) = \lambda_0^N + \lambda_1^N$$

where λ_0 & λ_1 are eigen values of the transfer Matrix.

$$T = \begin{bmatrix} e^{K+L} & e^{-K} \\ e^{-K} & e^{K-L} \end{bmatrix}$$

Eigen values are given by

$$\begin{vmatrix} e^{K+L} - \lambda & e^{-K} \\ e^{-K} & e^{K-L} - \lambda \end{vmatrix} = 0$$

$$\Rightarrow (e^{K+L} - \lambda)(e^{K-L} - \lambda) - e^{-2K} = 0$$

$$e^{2K} + \lambda^2 - \lambda(e^{K-L} + e^{K+L}) - e^{-2K} = 0$$

$$e^{2K} + \lambda^2 - \lambda e^K (e^L + e^{-L}) - e^{-2K} = 0$$

$$\lambda^2 - 2\lambda e^K \cosh(L) + 2 \sinh(2K) = 0$$

$$\lambda = \frac{2e^K \cosh(L) \pm \sqrt{4e^{2K} \cosh^2(L) - 8 \sinh(2K)}}{2}$$

$$\lambda = e^K \cosh(L) \pm \sqrt{e^{2K} + e^{2K} \sinh^2(L) - 2\left(\frac{e^{2K} - e^{-2K}}{2}\right)}$$

$$\lambda = e^K \cosh(L) \pm \sqrt{e^{2K} \sinh^2(L) + e^{-2K}}$$

$$\lambda_0 = e^K \cosh(L) + \sqrt{e^{2K} \sinh^2(L) + e^{-2K}}$$

$$\lambda_1 = e^K \cosh(L) - \sqrt{e^{2K} \sinh^2(L) + e^{-2K}}$$

clearly $\lambda_0 > \lambda_1$ always

$$\Rightarrow Z = \lambda_0^N + \lambda_1^N$$

$$F = -k_B T \ln(\mathcal{Z}) = -k_B T \ln(\lambda_0^N + \lambda_1^N)$$

$$F = -k_B T \ln\left(\lambda_0^N \left[1 + \left(\frac{\lambda_1}{\lambda_0}\right)^N\right]\right)$$

$$F = -N k_B T \ln(\lambda_0) - k_B T \ln\left[1 + \left(\frac{\lambda_1}{\lambda_0}\right)^N\right]$$

In the limit $N \rightarrow \infty$

$$\text{Since, } \frac{\lambda_1}{\lambda_0} < 1 \Rightarrow \lim_{N \rightarrow \infty} \left(\frac{\lambda_1}{\lambda_0}\right)^N \rightarrow 0$$

Hence in thermodynamic limit,

$$\underline{F = -N k_B T \ln(\lambda_0)}$$

$$\text{where } \lambda_0 = e^{\beta J} \cosh(\beta h) + \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}$$

$$M = -\left(\frac{\partial F}{\partial h}\right)_{N,T} = \frac{N k_B T}{\lambda_0} \left(\frac{\partial \lambda_0}{\partial h}\right)$$

$$M = \frac{N}{\lambda_0} \left[e^{\beta J} \sinh(\beta h) + \frac{e^{2\beta J} \sinh(2\beta h)}{2 \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}} \right]$$

$$M = \frac{N}{\lambda_0} \left[\frac{e^{\beta J} \sinh(\beta h) + e^{\beta J} \sinh(2\beta h)}{2 \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \right]$$

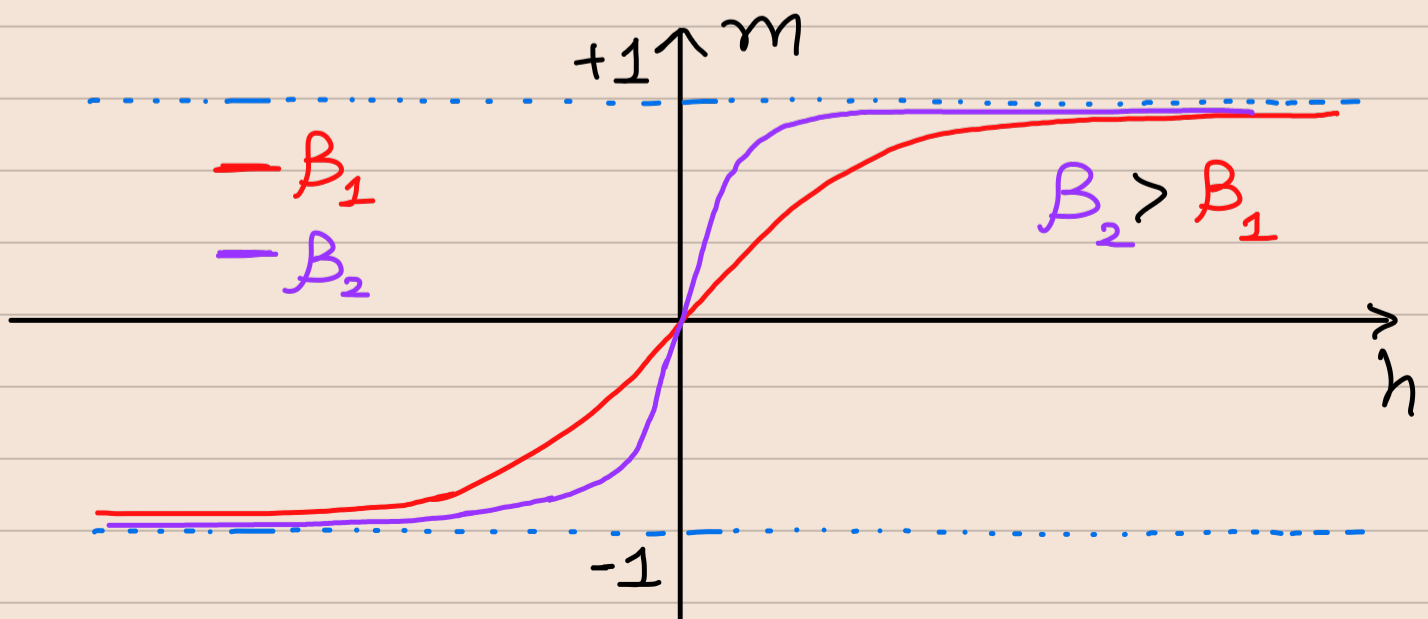
$$= \frac{N}{\lambda_0} \left[\frac{e^{\beta J} \sinh(\beta h) + e^{\beta J} \cosh(\beta h) \sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \right]$$

$$= \frac{N}{\lambda_0} \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \left[e^{\beta J} \cosh(\beta h) + \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}} \right]$$

$\Rightarrow$ using $m = \frac{M}{N}$ we get

$$m = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$$

$m(h=0) = 0 \Rightarrow$ There is no spontaneous magnetization at any Temperature.



At very low temperature ($\beta \rightarrow \infty$)

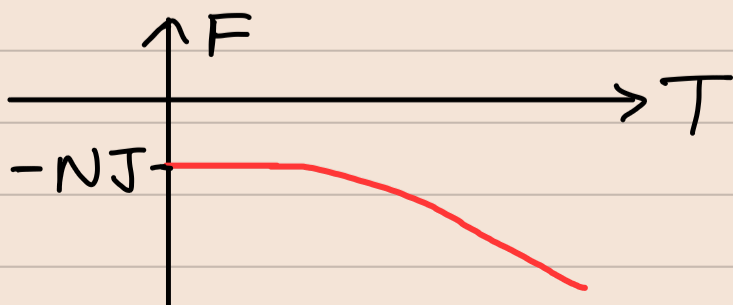
$$\sinh^2(\beta h) \gg e^{-4\beta J}$$

$$\Rightarrow \underline{m \rightarrow 1 \text{ (as } T \rightarrow 0)}$$

Hence all spins tend to align at $T=0$. But for ' T ' slightly more than zero, there is no spontaneous magnetization rather for ' T ' close to zero (but not zero) a very small ' h ' is enough to get complete alignment.

Hence ' $T=0$ ' acts as a phase transition critical temperature for 1D Ising chain.

$$F = -NJ \text{ at } T=0 \Rightarrow \left(\frac{\partial F}{\partial T} \right)_{T=0} = 0$$



So $T=0$ is a Critical point.

Susceptibility is given by,

$$\chi_m = \left(\frac{\partial M}{\partial h} \right)_B \quad \text{or} \quad \frac{\chi_m}{N} = \chi_s = \left(\frac{\partial m}{\partial h} \right)_B$$

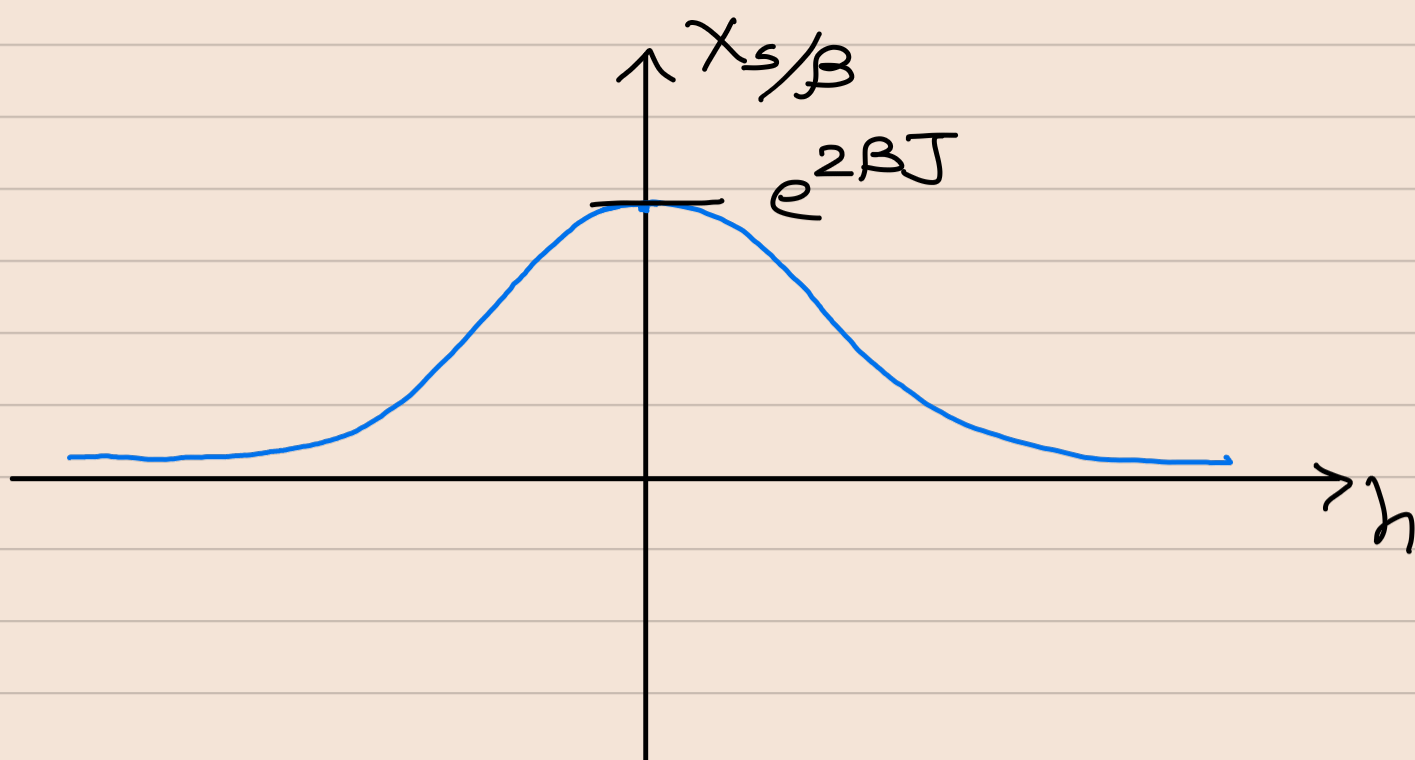
$$\chi_s = \frac{\partial}{\partial h} \left[\frac{\sinh(Bh)}{\sqrt{\sinh^2(Bh) + e^{-4BJ}}} \right]_B$$

$$\frac{\chi_s}{B} = \frac{\left\{ \frac{\left[\sqrt{\sinh^2(Bh) + e^{-4BJ}} \cosh(Bh) - \frac{\sinh(Bh) \cdot 2 \cosh(Bh) \sinh(Bh)}{2 \sqrt{\sinh^2(Bh) + e^{-4BJ}}} \right]}{\sinh^2(Bh) + e^{-4BJ}} \right\}}{1}$$

$$\chi_s = \frac{B e^{-4BJ} \cosh(Bh)}{[\sinh^2(Bh) + e^{-4BJ}]^{3/2}}$$

Note: when $J=0$, $\chi_s = B \operatorname{sech}^2(Bh)$
as $h \rightarrow 0$, $\chi_s = B$

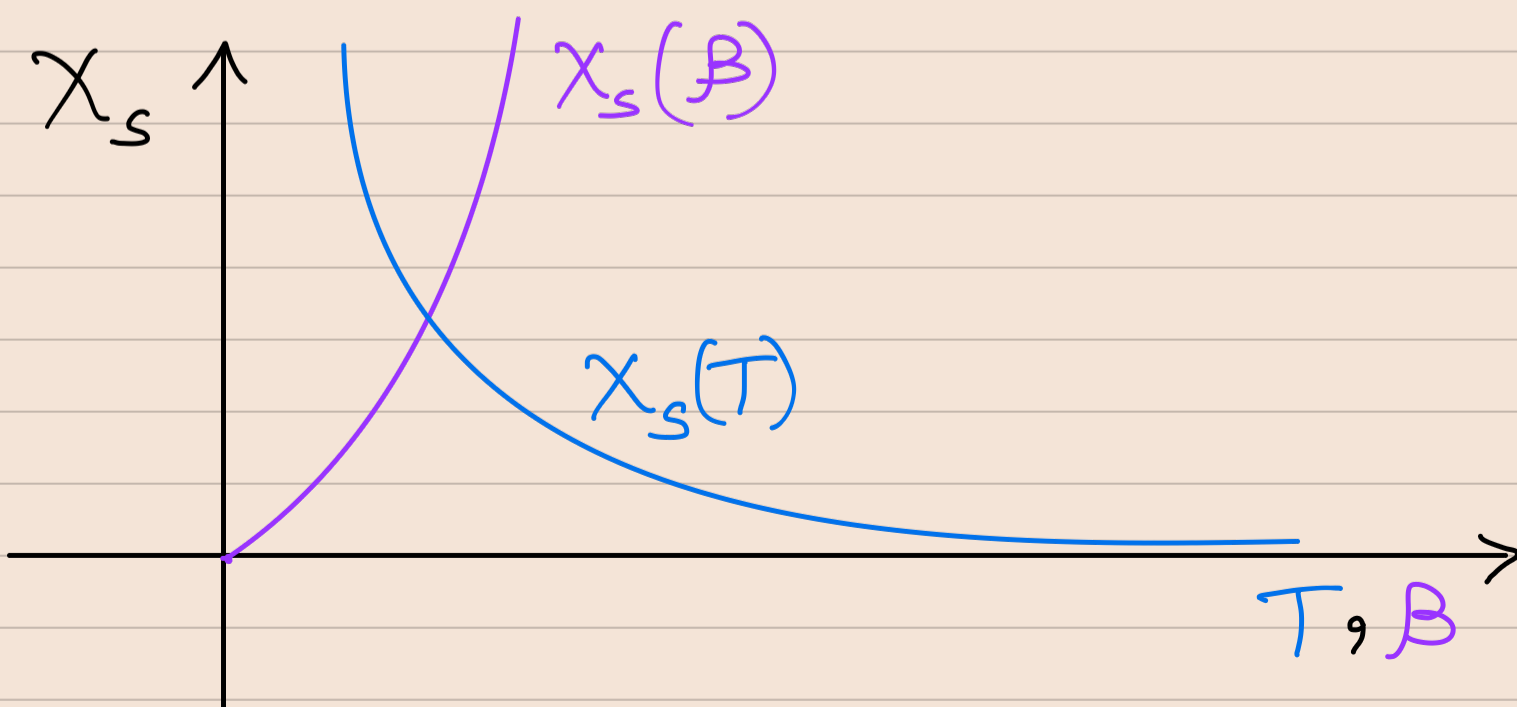
we arrive at the result obtained in the case of non-interacting spins.



as $h \rightarrow 0$, $X_s = \beta e^{2\beta J}$

$$\frac{1 + \tanh(\beta J)}{1 - \tanh(\beta J)} = \frac{\cosh(\beta J) + \sinh(\beta J)}{\cosh(\beta J) - \sinh(\beta J)} = \frac{2e^{\beta J}}{2e^{-\beta J}} = e^{2\beta J}$$

$$\Rightarrow \lim_{h \rightarrow 0} X_s = \beta \left[\frac{1 + \tanh(\beta J)}{1 - \tanh(\beta J)} \right]$$



Zero field Ising Model (1D)

Here $H = -J \sum_{i=1}^N S_i S_{i+1}$

All results are same as before except we should substitute $h=L=0$

The transfer matrix becomes,

$$T = \begin{bmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{bmatrix} = e^K \mathbb{I} + e^{-K} \sigma_x$$

Since σ_x & $\mathbb{I}$ commute, the eigen vectors of T are same as that of σ_x .

The eigen values are given by

$$\lambda = (e^K \pm e^{-K}) \begin{bmatrix} \text{eig}(\hat{\mathbb{I}}) = 1 \\ \text{eig}(\sigma_x) = \pm 1 \end{bmatrix}$$

$$\Rightarrow \lambda_0 = 2 \cosh(K)$$

$$\lambda_1 = 2 \sinh(K)$$

$$\left(\begin{array}{l} \lambda_0 > \lambda_1 \text{ for} \\ \text{all values of } K \end{array} \right)$$

The eigen vectors of T are

$$|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad |1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$\{|0\rangle, |1\rangle\}$ form a basis called m-basis.

Observe that the eigen vectors are independent of K or L . But in presence of h , The eigen vectors are dependent on K & L .

$$Z = \lambda_0^N + \lambda_1^N = 2^N [\cosh^N(K) + \sinh^N(K)]$$
$$Z = 2^N \cosh^N(K) [1 + \tanh^N(K)]$$

Now in thermodynamic limit, $N \rightarrow \infty$ but $-1 < \tanh(K) < 1$ always, so

$\tanh^N(K) \rightarrow 0$ as $N \rightarrow \infty$.

$$K = \beta J$$

$$\Rightarrow \underline{Z \sim 2^N \cosh^N(\beta J)}$$

Now $\tilde{F} = -\frac{1}{\beta} \ln(\tilde{Z})$

$$F = -\frac{N}{\beta} \ln[2 \cosh(\beta J)]$$

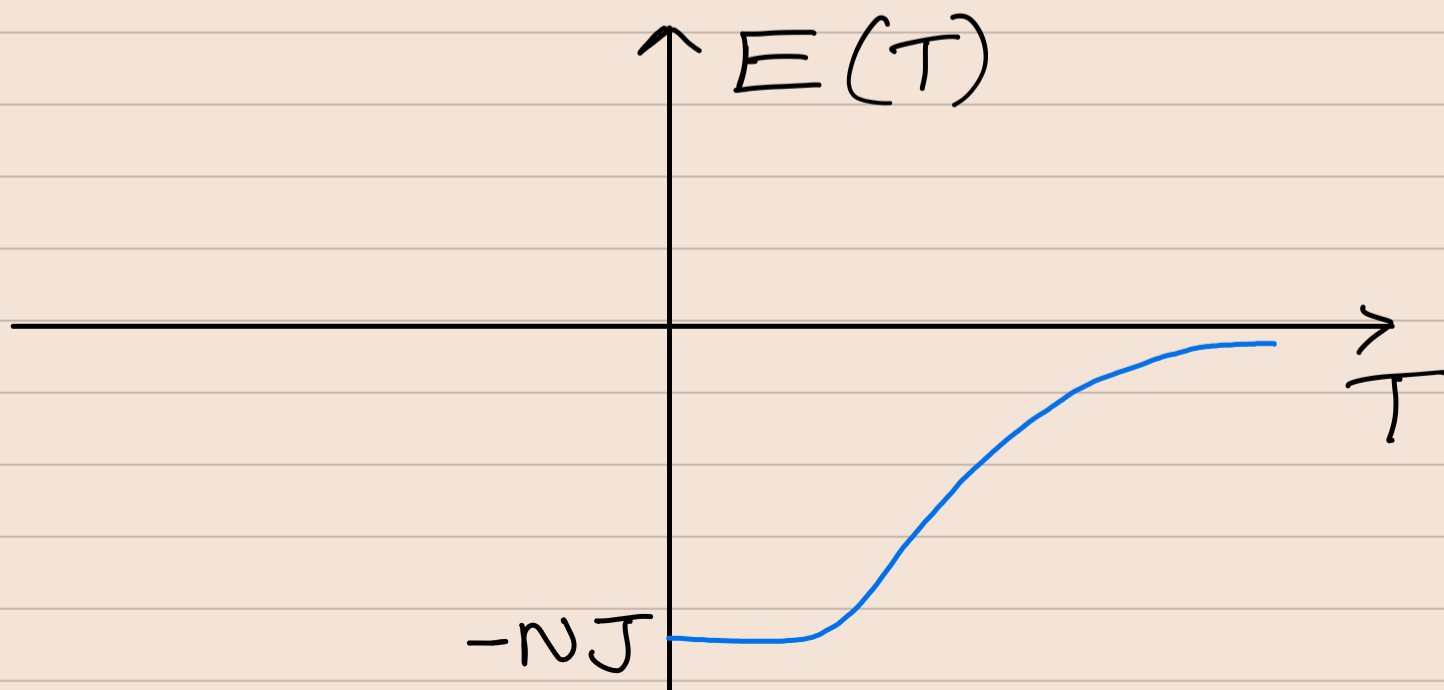
$\langle H \rangle = \text{Average energy} = E$

$$E = -\frac{\partial}{\partial \beta} \ln(\tilde{Z})$$

$$E = -N \frac{\partial}{\partial \beta} \ln[2 \cosh(\beta J)]$$

$$= -N \frac{J \sinh(\beta J)}{\cosh(\beta J)}$$

$$E = -NJ \tanh(\beta J)$$

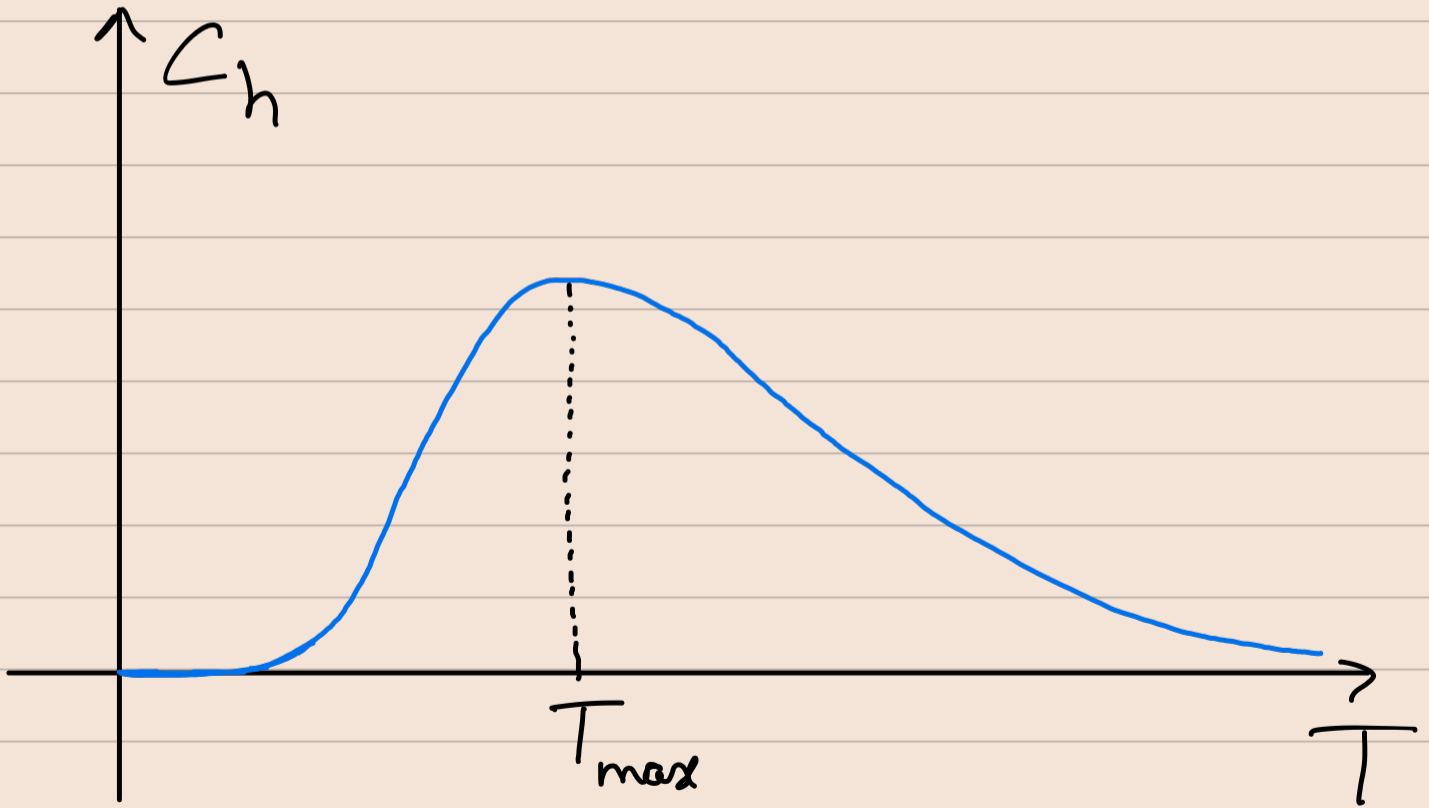


Heat Capacity

$$C_h = \frac{\partial E}{\partial T} = \frac{\partial B}{\partial T} \left(\frac{\partial E}{\partial B} \right)$$

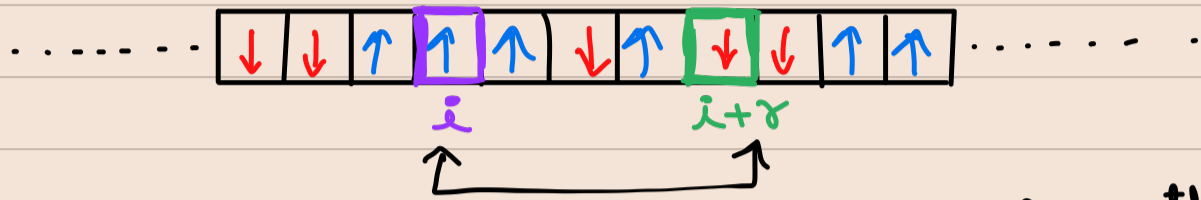
$$C_h = \frac{-1}{k_B T^2} (-NJ) J \operatorname{sech}^2(\beta J)$$

$$C_h = N k_B \left[\frac{J^2 \beta^2}{\cosh^2(\beta J)} \right]$$



$T_{\max}$ is solⁿ of $\coth\left(\frac{J}{k_B T}\right) = \frac{1}{k_B T}$

Spin-Spin Correlation Function for 1D Ising Model in the absence of an external magnetic field.



Correlation b/w i^{th} & $(i+r)^{\text{th}}$ spins

The correlation b/w spins at i^{th} & $(i+r)^{\text{th}}$ cell is defined as $\langle S_i S_{i+r} \rangle$ which is the ensemble average of product of spin variables at these lattice sites.

$$\langle S_i S_{i+r} \rangle = \frac{\text{Trace} (S_i S_{i+r} e^{-\beta \mathcal{H}})}{\text{Trace} (e^{-\beta \mathcal{H}})}$$

where $Z = \text{Trace} (e^{-\beta \mathcal{H}})$

$$\mathcal{H} = -J \sum_i S_i S_{i+1}$$

$$\text{Trace} \left[S_i S_{i+\gamma} e^{+BJ \sum_j S_j S_{j+1}} \right]$$

$$= \sum_{\{S_1, S_2, \dots, S_N\}} S_i S_{i+\gamma} \prod_{j=1}^N \underbrace{e^{BJ S_j S_{j+1}}}_{\langle S_j | T | S_{j+1} \rangle}$$

$$= \sum_{\{S_k\}} \left[\langle S_1 | T | S_2 \rangle \langle S_2 | T | S_3 \rangle \dots \right.$$

$$\dots \langle S_{i-1} | T | S_i \rangle S_i \langle S_i | T | S_{i+1} \rangle \dots$$

$$\dots \langle S_{i+\gamma-1} | T | S_{i+\gamma} \rangle S_{i+\gamma} \langle S_{i+\gamma} | T | S_{i+\gamma+1} \rangle \dots$$

$$\dots \left. \langle S_{N-1} | T | S_N \rangle \langle S_N | T | S_1 \rangle \right]$$

$$\left[\text{Using } \sum_{S_k} |S_k\rangle \langle S_k| = \hat{1} \right.$$

$$\left. \text{(completeness relation)} \right]$$

$$= \sum_{\{S_1, S_i, S_{i+\gamma}\}} \langle S_1 | T^{[(i-1)-1]+1} | S_i \rangle S_i \langle S_i | T^{[(i+\gamma-1)-i]+1} | S_{i+\gamma} \rangle$$

$$\times S_{i+\gamma} \langle S_{i+\gamma} | T^{[N-1-(i+\gamma)]+1} \times T | S_1 \rangle$$

$$(\sigma_z | S_i \rangle = S_i | S_i \rangle)$$

$$= \sum_{\{S_1, S_i, S_{i+\gamma}\}} \langle S_1 | T^{i-1} \sigma_z | S_i \rangle \langle S_i | T^\gamma | S_{i+\gamma} \rangle$$

$$\times \langle S_{i+\gamma} | \sigma_z T^{N-\gamma-i+1} | S_1 \rangle$$

(use completeness relation)

$$= \sum_{S_1} \langle S_1 | T^{i-1} \sigma_z T^r \sigma_z T^{N-r-i+1} | S_1 \rangle$$

$$= \text{tr} (T^{i-1} \sigma_z T^r \sigma_z T^{N-r-i+1})$$

(use cyclic property of trace)

$$= \text{tr} (T^{N-r} \sigma_z T^r \sigma_z)$$

$$\Rightarrow \text{Trace}(S_i S_{i+r} e^{-\beta H}) = \text{tr} (T^{N-r} \sigma_z T^r \sigma_z)$$

Since trace is independent of basis
use the basis that diagonalizes 'T'.
i.e. $|0\rangle \neq |1\rangle \equiv \{|m\rangle\}$

$$\text{tr} (T^{N-r} \sigma_z T^r \sigma_z) = \sum_m \langle m | T^{N-r} \sigma_z T^r \sigma_z | m \rangle$$

$$= \sum_m \sum_{m'} \langle m | T^{N-r} \sigma_z | m' \rangle \langle m' | T^r \sigma_z | m \rangle$$

$$\left[T |m\rangle = \lambda_m |m\rangle, (m, m' = 0, 1) \right]$$

(T is hermitian)

$$= \sum_m \sum_{m'} \lambda_m^{N-r} \langle m | \sigma_z | m' \rangle \lambda_{m'}^r \langle m' | \sigma_z | m \rangle$$

$$\mathbb{Z} \langle S_i S_{i+r} \rangle = \text{Trace}(S_i S_{i+r} e^{-\beta H}) = \text{tr} (T^{N-r} \sigma_z T^r \sigma_z)$$

$$\Rightarrow \mathbb{Z} \langle S_i S_{i+r} \rangle = \sum_m \sum_{m'} \lambda_m^{N-r} \lambda_{m'}^r \langle m | \sigma_z | m' \rangle \langle m' | \sigma_z | m \rangle$$

$$= \sum_{m'} \left[\lambda_0^{N-r} \lambda_{m'}^r \langle 0 | \sigma_z | m' \rangle \langle m' | \sigma_z | 0 \rangle \right]$$

$$+ \sum_{m'} \left[\lambda_1^{N-r} \lambda_{m'}^r \langle 1 | \sigma_z | m' \rangle \langle m' | \sigma_z | 0 \rangle \right]$$

$$= \lambda_0^N \sum_{m'} \lambda_{m'}^r \left[\lambda_0^{-r} \langle 0 | \sigma_z | m' \rangle \langle m' | \sigma_z | 0 \rangle + \underbrace{\left(\frac{\lambda_1}{\lambda_0} \right)^N}_{\text{negligible}} \lambda_1^{-r} \langle 1 | \sigma_z | m' \rangle \langle m' | \sigma_z | 0 \rangle \right]$$

In thermodynamic limit $\left(\frac{\lambda_1}{\lambda_0} \right)^N \rightarrow 0$.

$$\Rightarrow \mathbb{Z} \langle S_i S_{i+r} \rangle = \lambda_0^N \sum_{m'} \left(\frac{\lambda_{m'}}{\lambda_0} \right)^r \langle 0 | \sigma_z | m' \rangle \langle m' | \sigma_z | 0 \rangle$$

But in thermodynamic limit $\mathbb{Z} \sim \lambda_0^N$

$$\Rightarrow \langle S_i S_{i+r} \rangle = \left(\frac{\lambda_0}{\lambda_0} \right)^r \langle 0 | \sigma_z | 0 \rangle \langle 0 | \sigma_z | 0 \rangle + \left(\frac{\lambda_1}{\lambda_0} \right)^r \langle 0 | \sigma_z | 1 \rangle \langle 1 | \sigma_z | 0 \rangle$$

$$\Rightarrow \langle S_i S_{i+r} \rangle = |\langle 0 | \sigma_z | 0 \rangle|^2 + \left(\frac{\lambda_1}{\lambda_0} \right)^r |\langle 0 | \sigma_z | 1 \rangle|^2$$

(in σ_z basis)

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

(the inner products are independent of basis)

$$\langle 0 | \sigma_z | 0 \rangle = \frac{1}{2} (1 \ 1) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{2} (1 \ -1) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0$$

$$\langle 0 | \sigma_z | 1 \rangle = \frac{1}{2} (1 \ 1) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$= \frac{1}{2} (1 \ -1) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = 1$$

$$\Rightarrow \langle S_i S_{i+r} \rangle = \left(\frac{\lambda_1}{\lambda_0} \right)^r$$

In absence of external field,

$$\lambda_1 = 2 \sinh(BJ), \lambda_0 = 2 \cosh(BJ)$$

$$\Rightarrow \langle S_i S_{i+r} \rangle = [\tanh(\beta J)]^r$$

[power of any number can be written as an exponential ($a^x = e^{x \log(a)}$)]

$$\Rightarrow \langle S_i S_{i+r} \rangle = e^{r \log[\tanh(\beta J)]}$$

Since $0 < \tanh(\beta J) < 1$

$$\Rightarrow \log[\tanh(\beta J)] < 0$$

$$\Rightarrow \langle S_i S_{i+r} \rangle = e^{-r/\xi_g} \quad (\xi_g > 0)$$

where $\xi_g = \frac{-1}{\log[\tanh(\beta J)]}$

$$\Rightarrow \boxed{\langle S_i S_{i+r} \rangle = e^{-r/\xi_g}}$$

ξ_g is called correlation length

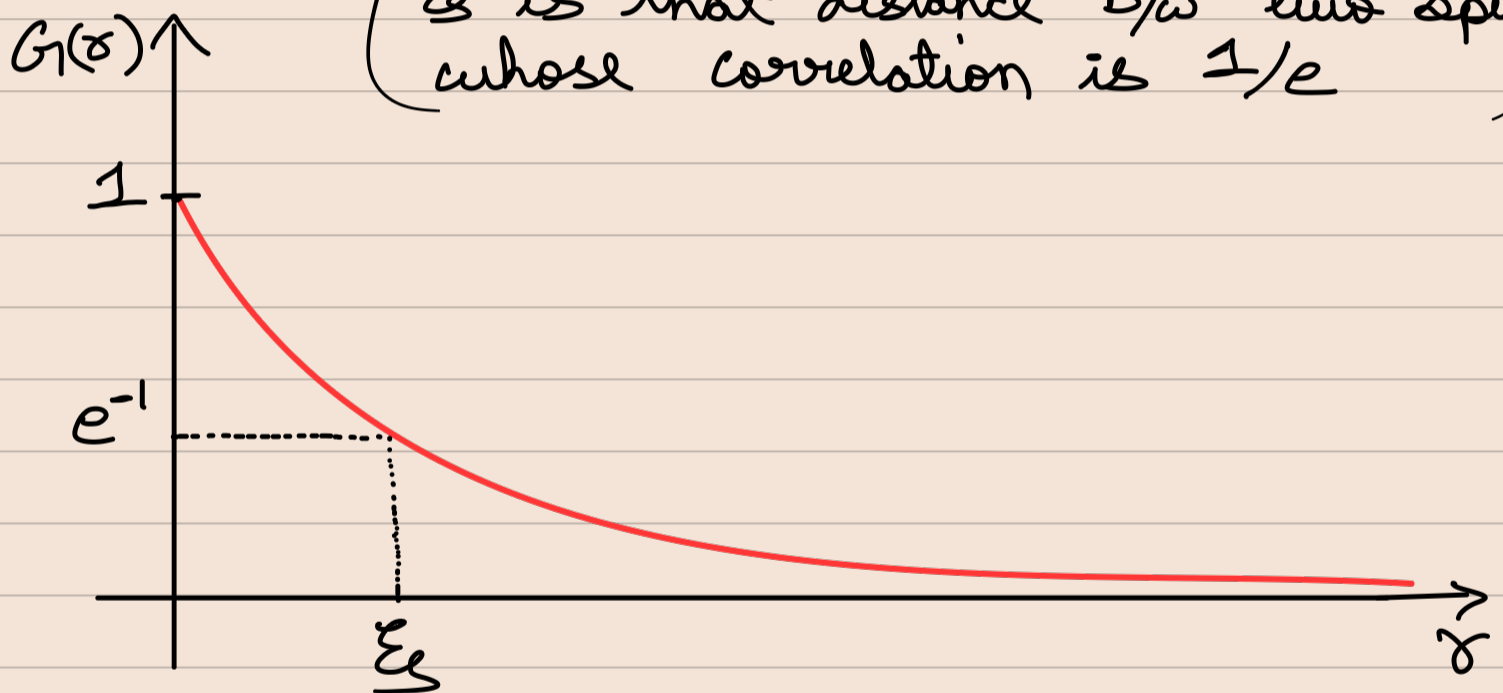
$$G(r) = \langle S_i S_{i+r} \rangle - \langle S_i \rangle \langle S_{i+r} \rangle$$

But in absence of 'h'

$$\langle S_i \rangle = \langle S_{i+r} \rangle = 0$$

$$\Rightarrow \underline{G(r) = e^{-r/\xi_c}}$$

(ξ_c is that distance b/w two spin whose correlation is $1/e$)



Correlation function decays exponentially for Ising spins. The Correlation length defines the length scale b/w which spins tend to be aligned with each other.

Magnetic Susceptibility per Spin

$$\chi_s = B \sum_{\gamma=1}^{\infty} G(\gamma)$$

$$\chi_s = B \sum_{\gamma=1}^{\infty} e^{-\gamma/\epsilon_s} = B \sum_{\gamma=1}^{\infty} (e^{-1/\epsilon_s})^{\gamma}$$

$$= B \left[\frac{1 + e^{-1/\epsilon_s}}{1 - e^{-1/\epsilon_s}} \right]$$

$$\chi_s = B \left[\frac{1 + \tanh(\beta J)}{1 - \tanh(\beta J)} \right]$$

$$\chi_s = B \left[\frac{\cosh(\beta J) + \sinh(\beta J)}{\cosh(\beta J) - \sinh(\beta J)} \right]$$

$$\chi_s = B \left(\frac{2e^{\beta J}}{2e^{-\beta J}} \right) = B e^{2\beta J}$$

$$\Rightarrow \boxed{\chi_s = B e^{2\beta J}}$$

This was the same result we got through Magnetization as $h \rightarrow 0$

3D Ising

In 3D ising model, we get

$$G(r) \propto \frac{e^{-r/\xi}}{r}$$

$$\chi_s = \beta \sum_r \frac{e^{-r/\xi}}{r}$$

Here ξ can tend to ' ∞ ' at critical temperatures. So χ_s shows some interesting features.

- If χ_m is finite $\Rightarrow \xi$ is finite
- If χ_m is infinite $\Rightarrow \xi$ is infinite
since $\sum_r \frac{1}{r}$ (is diverging series)
- If ξ is infinite, χ_m may or may not be infinite