

Assignment - 1

1) Given $\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$

The Partition function is given by,

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

$$\Rightarrow \left(\frac{\partial Z}{\partial \beta} \right)_h = \text{Trace}(-\mathcal{H} e^{-\beta \mathcal{H}})$$

$$\Rightarrow -\frac{1}{Z} \left(\frac{\partial Z}{\partial \beta} \right)_h = \frac{\text{Trace}(\mathcal{H} e^{-\beta \mathcal{H}})}{Z} = \langle \mathcal{H} \rangle$$

$$\Rightarrow \boxed{\langle \mathcal{H} \rangle = - \left[\frac{\partial \ln(Z)}{\partial \beta} \right]_h}$$

$$\& \left(\frac{\partial^2 Z}{\partial \beta^2} \right)_h = \text{Trace}(\mathcal{H}^2 e^{-\beta \mathcal{H}})$$

$$\Rightarrow \frac{1}{Z} \left(\frac{\partial^2 Z}{\partial \beta^2} \right)_h = \frac{\text{Trace}(\mathcal{H}^2 e^{-\beta \mathcal{H}})}{Z} = \langle \mathcal{H}^2 \rangle$$

Now,

$$\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = \frac{1}{Z} \left(\frac{\partial^2 Z}{\partial \beta^2} \right)_h - \left[\frac{1}{Z} \left(\frac{\partial Z}{\partial \beta} \right)_h \right]^2$$

$$\Rightarrow \langle H^2 \rangle - \langle H \rangle^2 = \frac{1}{Z} \left[\frac{\partial}{\partial \beta} \left(\frac{\partial Z}{\partial \beta} \right) \right]_h + \left(\frac{\partial Z}{\partial \beta} \right)_h \left[\frac{\partial}{\partial \beta} \left(\frac{1}{Z} \right) \right]_h$$

$$= \left[\frac{\partial}{\partial \beta} \left(\frac{1}{Z} \left(\frac{\partial Z}{\partial \beta} \right) \right) \right]_h = \frac{\partial}{\partial \beta} \left[\frac{\partial \ln(Z)}{\partial \beta} \right]_h$$

$$\Rightarrow \langle H^2 \rangle - \langle H \rangle^2 = \left(\frac{\partial^2}{\partial \beta^2} \ln(Z) \right)_h = \frac{\partial}{\partial \beta} \left[\frac{\partial \ln(Z)}{\partial \beta} \right]_h$$

$$\Rightarrow \langle H^2 \rangle - \langle H \rangle^2 = - \left[\frac{\partial \langle \hat{H} \rangle}{\partial \beta} \right]_h$$

Now the free energy is given by,

$$F = -\frac{1}{\beta} \ln(Z), \quad dF = -SdT - Mdh$$

$$\Rightarrow \ln(Z) = -\beta F$$

$$\text{But } \langle H \rangle = - \left(\frac{\partial \ln(Z)}{\partial \beta} \right)_h = \left(\frac{\partial (\beta F)}{\partial \beta} \right)_h$$

$$\Rightarrow \langle H \rangle = F + \beta \left(\frac{\partial F}{\partial \beta} \right)_h = F + \beta \left(\frac{\partial T}{\partial \beta} \right) \left(\frac{\partial F}{\partial T} \right)_h$$

$$\Rightarrow \langle H \rangle = F - T \underbrace{\left(\frac{\partial F}{\partial T} \right)_h}_{-S} \quad \left(\frac{\partial T}{\partial \beta} = \frac{-1}{k\beta^2} \right)$$

$$\Rightarrow \langle \mathcal{H} \rangle = F + TS \Rightarrow d\langle \mathcal{H} \rangle = TdS - Md\hbar$$

where $dQ = TdS \Rightarrow$ Heat exchanged. Then the heat capacity for the entire system is,

$$C_h = \left(\frac{dQ}{dT} \right)_h = \left[\frac{\partial \langle \mathcal{H} \rangle}{\partial T} \right]_h$$

$$\Rightarrow C_h = -k_B \beta^2 \left(\frac{\partial \langle \mathcal{H} \rangle}{\partial \beta} \right)_h \quad \left[\frac{\partial \beta}{\partial T} = -k_B \beta^2 \right]$$

$$\Rightarrow \langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = - \left(\frac{\partial \langle \mathcal{H} \rangle}{\partial \beta} \right)_h = \left(\frac{C_h}{k_B \beta^2} \right)$$

$$\Rightarrow \boxed{C_h = k_B \beta^2 [\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2]}$$

$$\text{Now, } \mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - \hbar \sum_i S_i$$

where $S_i = S_{\vec{r}_i} \Rightarrow$ located on the lattice site ' i ' with $\vec{r}_i$ as the position lattice vector. $\Rightarrow \vec{r}_i = [x_i^{(1)}, x_i^{(2)}, \dots, x_i^{(d)}], x_i^{(k)} \in \mathbb{Z}^+$. for ' j ' to be the nearest neighbour of ' i ' in a d -dimensional cubic lattice, there are $2d$ - number of possibilities for ' j '.

$$\vec{x}_j = \begin{cases} [x_i^{(1)} \pm 1, x_i^{(2)}, x_i^{(3)}, \dots, x_i^{(d)}] \\ \text{or} \\ [x_i^{(1)}, x_i^{(2)} \pm 1, x_i^{(3)}, \dots, x_i^{(d)}] \\ \vdots \\ \text{or} [x_i^{(1)}, x_i^{(2)}, x_i^{(3)}, \dots, x_i^{(d)} \pm 1] \end{cases}$$

$$\sum_{\langle ij \rangle} = \frac{1}{2} \sum_i \sum_{j \in n(i)} \quad \begin{matrix} \downarrow \\ \text{(To remove} \\ \text{double counting)} \end{matrix} \quad \begin{matrix} \underbrace{\hspace{1cm}} \\ \text{(2d terms)} \end{matrix}$$

($n(i) \Rightarrow$ is the set of nearest neighbours of 'i')

$$\Rightarrow \sum_{j \in n(i)} 1 = 2d$$

$$\begin{aligned} \Rightarrow \sum_{\langle ij \rangle} S_i &= \frac{1}{2} \sum_i \sum_{j \in n(i)} S_i = \frac{1}{2} \sum_i S_i \sum_{j \in n(i)} (1) \\ &= \frac{2d}{2} \sum_i S_i = d \sum_i S_i \end{aligned}$$

$$\Rightarrow \sum_i S_i = \frac{1}{d} \sum_{\langle ij \rangle} S_i$$

$$\& \sum_j S_j = \frac{1}{d} \sum_{\langle ij \rangle} S_j$$

$$\& \sum_i S_i = \frac{\sum_i S_i + \sum_j S_j}{2}$$

$$\Rightarrow \sum_i S_i = \frac{1}{2} \left[\frac{1}{d} \sum_{\langle ij \rangle} S_i + \frac{1}{d} \sum_{\langle ji \rangle} S_j \right]$$

$$\Rightarrow \sum_i S_i = \frac{1}{2d} \sum_{\langle ij \rangle} (S_i + S_j) \quad \left(\text{since } \sum_{\langle ij \rangle} = \sum_{\langle ji \rangle} \right)$$

$$\Rightarrow \mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

$$\Rightarrow \mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - \frac{h}{2d} \sum_{\langle ij \rangle} (S_i + S_j)$$

$$\Rightarrow \mathcal{H} = \sum_{\langle ij \rangle} \left[-J S_i S_j - \frac{h}{2d} (S_i + S_j) \right]$$

defining $e_{ij} = -J S_i S_j - \frac{h}{2d} (S_i + S_j),$

$$\Rightarrow \boxed{\mathcal{H} = \sum_{\langle ij \rangle} e_{ij}}$$

$$\Rightarrow \langle \mathcal{H} \rangle = \sum_{\langle ij \rangle} \langle e_{ij} \rangle$$

$$\Rightarrow \underbrace{\langle \mathcal{H} \rangle^2 = \sum_{\langle ij \rangle} \langle e_{ij} \rangle \sum_{\langle kl \rangle} \langle e_{kl} \rangle = \sum_{\langle ij \rangle} \sum_{\langle kl \rangle} \langle e_{ij} \rangle \langle e_{kl} \rangle}$$

$$\mathcal{H}^2 = \sum_{\langle ij \rangle} \sum_{\langle kl \rangle} e_{ij} e_{kl}$$

$$\Rightarrow \langle \mathcal{H}^2 \rangle = \sum_{\langle ij \rangle} \sum_{\langle kl \rangle} \langle e_{ij} e_{kl} \rangle$$

Now $C_h = k_B \beta^2 [\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2]$
 is the Heat Capacity of entire
 System. But Specific heat capacity
 is $c_h = \frac{C_h}{N_s}$ (heat capacity per spin)

$$\Rightarrow c_h = \frac{k_B \beta^2 [\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2]}{N_s}$$

$$\Rightarrow c_h = \frac{k_B \beta^2}{N_s} \sum_{\langle ij \rangle \langle kl \rangle} [\langle e_{ij} e_{kl} \rangle - \langle e_{ij} \rangle \langle e_{kl} \rangle]$$

2)

$$\mathcal{H}_{\text{crystal field}} = -\Delta \sum_{i=1}^N (S_i^z)^2$$

$$S_i^z = \{1, 0, -1\}$$

$$(a) \quad \mathcal{Z} = \text{Trace} \left[e^{-\beta \mathcal{H}} \right]$$

$$\mathcal{Z} = \sum_{\{S_i^z\}} e^{\beta \Delta \sum_i (S_i^z)^2}$$

$$= \sum_{\{S_i^z\}} e^{\beta \Delta (S_1^z)^2} e^{\beta \Delta (S_2^z)^2} \dots e^{\beta \Delta (S_N^z)^2}$$

$$\mathcal{Z} = \sum_{S_1^z} e^{\beta \Delta (S_1^z)^2} \sum_{S_2^z} e^{\beta \Delta (S_2^z)^2} \dots \sum_{S_N^z} e^{\beta \Delta (S_N^z)^2}$$

Consider $\sum_{S_i^z = \{-1, 0, 1\}} e^{\beta \Delta (S_i^z)^2} = e^{\beta \Delta} + 1 + e^{\beta \Delta}$
 $= 1 + 2e^{\beta \Delta}$

$$\Rightarrow \mathcal{Z} = (1 + 2e^{\beta \Delta})^N \Rightarrow \ln(\mathcal{Z}) = N \ln(1 + 2e^{\beta \Delta})$$

$$\langle \mathcal{H} \rangle = - \left[\frac{\partial \ln(\mathcal{Z})}{\partial \beta} \right]_N = -N \frac{\partial \ln(1 + 2e^{\beta \Delta})}{\partial \beta}$$

$$\langle \mathcal{H} \rangle = \frac{-N (2\Delta e^{\beta\Delta})}{1 + 2e^{\beta\Delta}}$$

$$\langle \mathcal{H} \rangle = \frac{-2N\Delta}{2 + e^{-\beta\Delta}}$$

$$C = \frac{\partial \langle \mathcal{H} \rangle}{\partial T} = \left(\frac{\partial \beta}{\partial T} \right) \frac{\partial \langle \mathcal{H} \rangle}{\partial \beta}$$

$$C = -k_B \beta^2 \frac{\partial}{\partial \beta} \left(\frac{-2N\Delta}{2 + e^{-\beta\Delta}} \right)$$

$$C = 2Nk_B \Delta \beta^2 \frac{(-1)(-\Delta)e^{-\beta\Delta}}{(2 + e^{-\beta\Delta})^2}$$

$$C = \frac{2Nk_B (\beta\Delta)^2 e^{-\beta\Delta}}{(2 + e^{-\beta\Delta})^2}$$

$$C = \frac{2Nk_B \left(\frac{\Delta}{k_B T} \right)^2 e^{-\frac{\Delta}{k_B T}}}{\left(2 + e^{-\frac{\Delta}{k_B T}} \right)^2}$$

For $\beta \rightarrow 0$ i.e. $T \rightarrow \infty$

$$C \rightarrow \lim_{\beta \rightarrow 0} \frac{2Nk_B (\beta \Delta)^2 e^{-\beta \Delta}}{(2 + e^{-\beta \Delta})^2}$$

$$C \rightarrow \frac{2Nk_B (\beta \Delta)^2 (1 - \beta \Delta)}{(3 - \beta \Delta)^2}$$

regardless of $\Delta > 0$ or $\Delta < 0$,

$C \rightarrow 0$ as $\beta \rightarrow 0$

For $\beta \rightarrow \infty$ i.e. $T \rightarrow 0$

If $\Delta > 0$

$$\lim_{\beta \rightarrow \infty} \frac{2Nk_B (\beta \Delta)^2 e^{-\beta \Delta}}{(2 + e^{-\beta \Delta})^2}$$

$$C \approx 2Nk_B (\beta \Delta)^2 e^{-\beta \Delta} \rightarrow 0$$

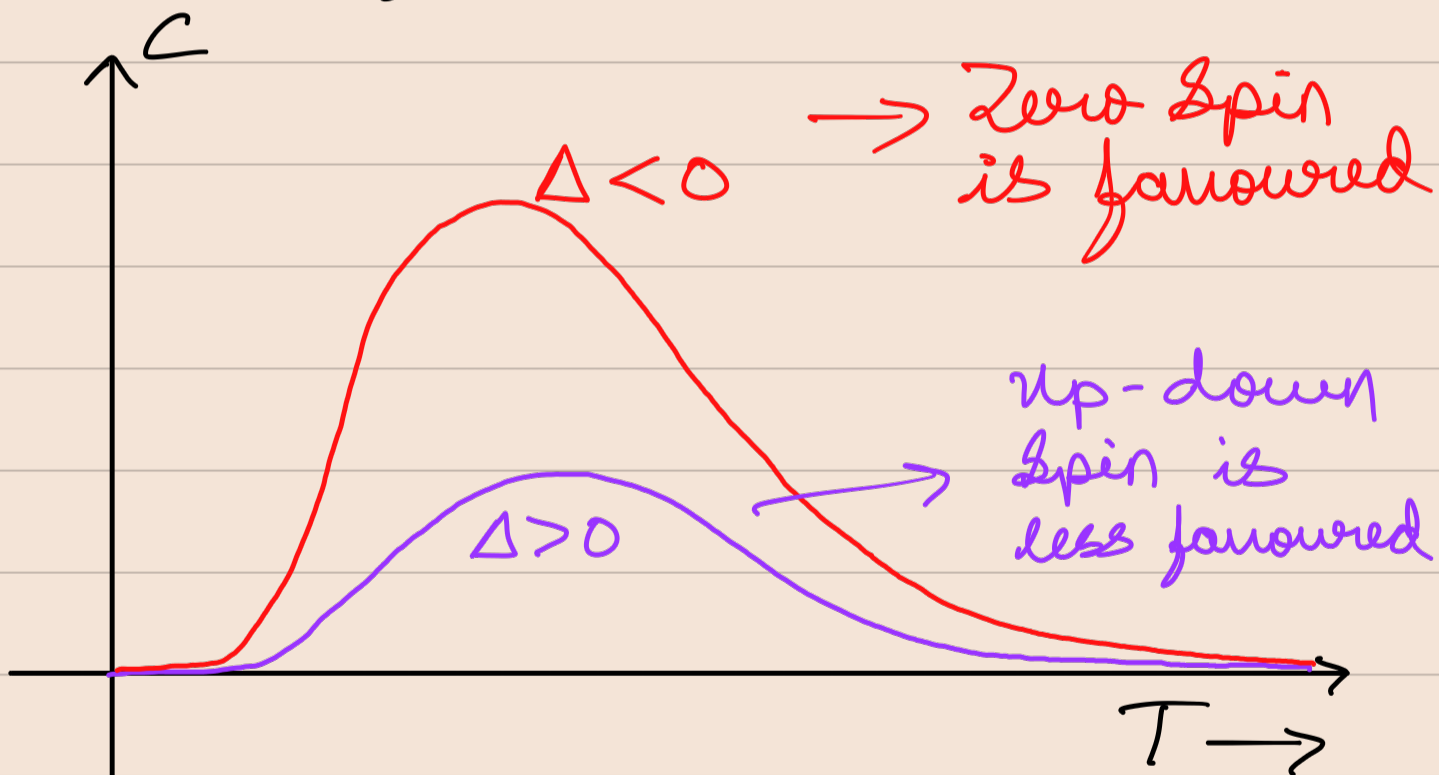
$\Rightarrow C \rightarrow 0$ as $\beta \rightarrow \infty$ if $\Delta > 0$

If $\Delta < 0$ i.e. $\Delta \rightarrow -\epsilon, \epsilon > 0$

$$C = \frac{2Nk_B (\beta\epsilon)^2 e^{\beta\epsilon}}{(2 + e^{\beta\epsilon})^2}$$

if $\beta \rightarrow \infty$, then
 $C \rightarrow 2Nk_B (\beta\epsilon)^2 e^{-\beta\epsilon}$

Thus even here $C \rightarrow 0$ in the same fashion as in $\Delta > 0$ case.



This means that extreme temperature behaviour for both $\Delta > 0$ or $\Delta < 0$ case is similar. But for mid range, $\Delta < 0$ case has more ' C ' compared to $\Delta > 0$ case.

2b) $m = \langle S_i^z \rangle$

$$\langle S_i^z \rangle = \frac{\sum_{\{S_j^z\}} S_i^z e^{-\beta \mathcal{H}}}{Z}$$

$$= \frac{\sum_{S_1^z} e^{\beta \Delta (S_1^z)^2} \sum_{S_2^z} e^{\beta \Delta (S_2^z)^2} \dots \sum_{S_i^z} S_i^z e^{\beta \Delta (S_i^z)^2} \dots \sum_{S_n^z} e^{\beta \Delta (S_n^z)^2}}{}$$

$$\sum_{S_1^z} e^{\beta \Delta (S_1^z)^2} \sum_{S_2^z} e^{\beta \Delta (S_2^z)^2} \dots \sum_{S_i^z} e^{\beta \Delta (S_i^z)^2} \dots \sum_{S_n^z} e^{\beta \Delta (S_n^z)^2}$$

$$= \frac{\sum_{S_i^z = \{0, \pm 1\}} S_i^z e^{\beta \Delta (S_i^z)^2}}{\sum_{S_i^z = \{0, \pm 1\}} e^{\beta \Delta (S_i^z)^2}}$$

$$\langle S_i^z \rangle = \frac{(0 + e^{\beta \Delta} - e^{\beta \Delta})}{(1 + e^{\beta \Delta} + e^{\beta \Delta})} = 0$$

When $h \rightarrow 0$ $\langle S_i^z \rangle = 0$

But to get the behaviour as $h \rightarrow 0^+$ we add external field 'h' & then take limit as $h \rightarrow 0$.

$$\Rightarrow \mathcal{H} \rightarrow -\Delta \sum_i (S_i^z)^2 - h \sum_i S_i^z$$

$$\Rightarrow Z = \text{Trace}(e^{-B\mathcal{H}})$$

$$Z = \sum_{\{S_i^z\}} e^{B(\Delta \sum_i (S_i^z)^2 + h \sum_i S_i^z)}$$

$$Z = \left[\sum_{S_i^z = \pm 1} e^{B[\Delta (S_i^z)^2 + h S_i^z]} \right]^N$$

(as spins are independent)

$$\Rightarrow Z = \left[e^{B[\Delta + h]} + 1 + e^{B[\Delta - h]} \right]^N$$

$$Z = \left[1 + e^{B\Delta} (e^{Bh} + e^{-Bh}) \right]^N$$

$$Z = \left[1 + 2e^{B\Delta} \cosh(Bh) \right]^N$$

Net Magnetization is given by

$$\langle M \rangle = \sum_i \langle S_i \rangle = \langle \sum_i S_i \rangle$$

$$= \frac{\text{Trace} \left[\left(\sum_i S_i \right) e^{-\beta H} \right]}{Z}$$

$$= \frac{\left[\frac{1}{\beta} \left[\frac{\partial}{\partial h} (Z) \right] \right]_{\beta}}{Z}$$

$$\Rightarrow \langle M \rangle = \frac{1}{\beta} \left[\frac{\partial \ln(Z)}{\partial h} \right]_{\beta}$$

$$\langle M \rangle = \frac{N}{\beta} \left(\frac{\partial \ln[1 + 2e^{\beta \Delta} \cosh(\beta h)]}{\partial h} \right)_{\beta}$$

$$\langle M \rangle = \frac{N}{\beta} \left[\frac{2e^{\beta \Delta} \sinh(\beta h) \times \beta}{[1 + 2e^{\beta \Delta} \cosh(\beta h)]} \right]$$

$$m = \frac{\langle M \rangle}{N} = \frac{2e^{\beta \Delta} \sinh(\beta h)}{[1 + 2e^{\beta \Delta} \cosh(\beta h)]}$$

$$\left(\frac{\partial m}{\partial h}\right) = 2e^{\beta\Delta} \left[\frac{B \cosh(\beta h)}{[1 + 2e^{\beta\Delta} \cosh(\beta h)]} - \frac{\sinh(\beta h) [2\beta e^{\beta\Delta} \sinh(\beta h)]}{[1 + 2e^{\beta\Delta} \cosh(\beta h)]^2} \right]$$

$$\chi_{\text{(per spin)}} = 2\beta e^{\beta\Delta} \left[\frac{\cosh(\beta h)}{[1 + 2e^{\beta\Delta} \cosh(\beta h)]} - \frac{2e^{\beta\Delta} \sinh^2(\beta h)}{[1 + 2e^{\beta\Delta} \cosh(\beta h)]^2} \right]$$

As $h \rightarrow 0^+$ $\sinh(\beta h) \rightarrow 0$
 $\cosh(\beta h) \rightarrow 1$

$$\Rightarrow \chi = \frac{2\beta e^{\beta\Delta}}{(1 + 2e^{\beta\Delta})} = \frac{2\beta}{(2 + e^{-\beta\Delta})}$$

• If $\Delta > 0$

$\rightarrow$ for $\beta \rightarrow 0$, i.e. $T \rightarrow \infty$

$$\chi \sim \frac{2\beta}{(2+1)} \sim \frac{2\beta}{3} \rightarrow \text{goes to '0'}$$

$(\chi \rightarrow 0)$

→ for $\beta \rightarrow \infty$, i.e. as $T \rightarrow 0$

$$\chi \sim \frac{2\beta}{2} = \beta$$

$$\Rightarrow \underline{\chi \rightarrow \infty \text{ as } T \rightarrow 0}$$

• If $\Delta < 0$ i.e. for $\Delta = -\varepsilon$
 $\varepsilon > 0$

$$\chi = \frac{2\beta}{(2 + e^{\beta\varepsilon})}$$

→ For $\beta \rightarrow 0$, i.e. as $T \rightarrow \infty$

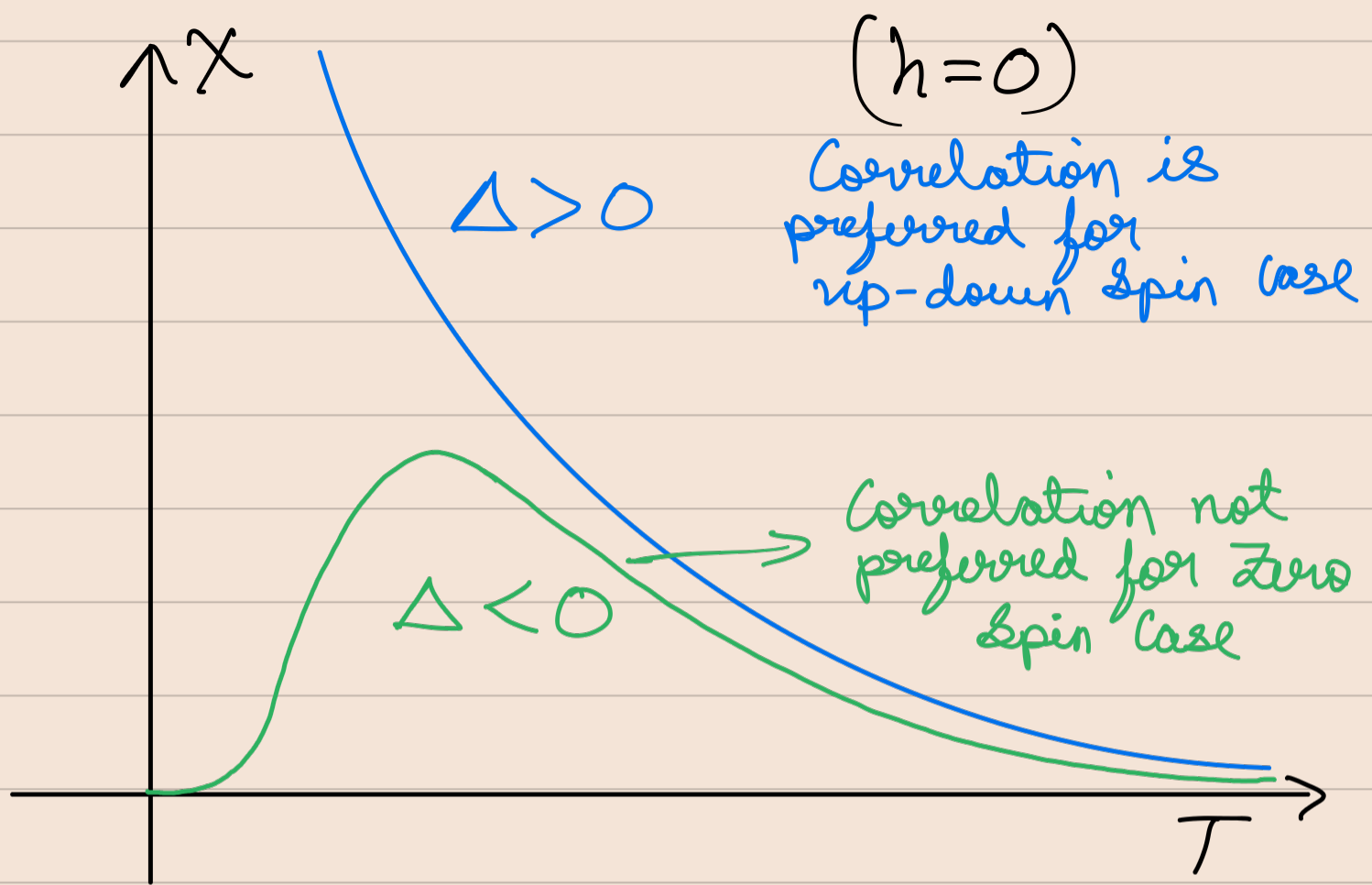
$$\chi = \frac{2}{3} \beta \rightarrow 0$$

Thus $\chi \rightarrow 0$ as $T \rightarrow \infty$.

→ For $\beta \rightarrow \infty$, i.e. as $T \rightarrow 0$

$$\chi \sim 2\beta e^{-\beta\varepsilon} \rightarrow 0$$

Even here $\chi \rightarrow 0$ as $T \rightarrow \infty$.



Thus we observe phase transition when $\Delta > 0$ whose critical temperature is at absolute zero.

But for $\Delta < 0$ there is no divergence at any 'T', hence no phase transition.

3) q -state Potts model in 1D is defined by the Hamiltonian

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

where $S_i = \{1, 2, 3, 4, \dots, q\}$

Boundary conditions $\Rightarrow$ Periodic Boundary conditions.

a) To find the partition function,

$$\mathcal{Z} = \text{Trace}(e^{-\beta \mathcal{H}}) = \text{Trace}\left[e^{\beta J \sum_i \Delta_{S_i, S_{i+1}}}\right]$$

$$\mathcal{Z} = \sum_{\{S_i\}} \left(e^{\beta J \sum_i \Delta_{S_i, S_{i+1}}} \right)$$

$$\mathcal{Z} = \sum_{S_1, S_2, \dots, S_N} e^{\beta J \Delta_{S_1, S_2}} e^{\beta J \Delta_{S_2, S_3}} \dots e^{\beta J \Delta_{S_N, 1}}$$

$$\mathcal{Z} = \sum_{S_1, S_2, \dots, S_N} \langle S_1 | T | S_2 \rangle \langle S_2 | T | S_3 \rangle \dots \langle S_N | T | S_1 \rangle$$

$$\Rightarrow \mathcal{Z} = \sum_{S_1} \langle S_1 | T^N | S_1 \rangle \Rightarrow \mathcal{Z} = \text{tr}(T^N)$$

where $T = e^{\beta J \Delta \hat{\sigma}_{z_i}, \hat{\sigma}_{z_{i+1}}}$

$$\Rightarrow T = \begin{bmatrix} e^{\beta J} & 1 & 1 & \dots & 1 \\ 1 & e^{\beta J} & 1 & \dots & 1 \\ 1 & 1 & e^{\beta J} & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & e^{\beta J} \end{bmatrix}_{q \times q}$$

3b) To find the eigen values of T .
 The outer product of a vector $|\psi\rangle$
 Such that $|\psi\rangle = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{q \times 1}$ with

itself gives $|\psi\rangle\langle\psi| = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{bmatrix}$

$$\Rightarrow T = |\psi\rangle\langle\psi| - \hat{I}_{q \times q} + e^{\beta J} \hat{I}_{q \times q}$$

$$\Rightarrow T = |\psi\rangle\langle\psi| + (e^{\beta J} - 1)\hat{I}$$

Since any vector can be an eigen vector for Identity, we should find eigen vector of $|\psi\rangle\langle\psi|$ which can be $|\psi\rangle$ itself.

$$\Rightarrow T|\psi\rangle = |\psi\rangle(\langle\psi|\psi\rangle) + (e^{\beta J} - 1)|\psi\rangle$$

$$T|\psi\rangle = \underbrace{\{\langle\psi|\psi\rangle + (e^{\beta J} - 1)\}}_{\text{eigen value}} |\psi\rangle$$

$$\langle\psi|\psi\rangle = [1 \ 1 \ 1 \dots 1]_{1 \times q} \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{q \times 1} = \underline{\underline{q}}$$

$$\Rightarrow T|\psi\rangle = \underbrace{(q + e^{\beta J} - 1)}_{\text{one of the eigen value.}} |\psi\rangle$$

Now any vector orthogonal to $|\psi\rangle$ can be another eigen vector.

i.e. for $T|\phi\rangle = |\psi\rangle\langle\psi|\phi\rangle + (e^{\beta J} - 1)|\phi\rangle$

If $\langle\psi|\phi\rangle = 0 \Rightarrow \hat{T}|\phi\rangle = (e^{\beta J} - 1)|\phi\rangle$
Hence $(e^{\beta J} - 1)$ is also an eigen value.

For a q -dim vector $|\psi\rangle$, there can be $(q-1)$ number of orthogonal vectors to it.
Thus the eigenvalue spectrum for T is,

$$\lambda_0 = (q + e^{\beta J} - 1) \Rightarrow |\lambda_0\rangle = \frac{1}{\sqrt{q}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \sum_{k=1}^q \frac{|e_k\rangle}{\sqrt{q}}$$

$(|e_k\rangle \Rightarrow \text{Standard Basis})$

$$\lambda_k = \underbrace{(e^{\beta J} - 1)}_{(q-1) \text{ fold degenerate.}} \quad (k = 1, 2, \dots, q-1)$$

$$\lambda_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \lambda_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \dots, \lambda_{q-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}$$

$$\lambda_k = \frac{-|e_1\rangle + |e_{k+1}\rangle}{\sqrt{2}} \Rightarrow \text{eigen vectors of } \lambda_k$$

$k = \{1, 2, \dots, q-1\}$

But if you notice, $\{|\lambda_k\rangle\}$ for $k = \{1, 2, 3, \dots, q-1\}$ is not orthogonal to each other. We should orthogonalize the set $\{|\lambda_k\rangle\}$. $k = \{1, 2, \dots, q-1\}$. After doing gram-schmidt orthogonalization, $|\lambda_k\rangle$ is.

$$\begin{array}{lcl}
 1 & \cdots & \frac{-1}{\sqrt{k(k+1)}} \rightarrow 1^{\text{st}} \text{ position} \\
 2 & \cdots & 0 \\
 & & \vdots \\
 q-k & \cdots & 0 \left. \vphantom{\begin{array}{c} 0 \\ \vdots \\ 0 \end{array}} \right\} (q-k-1) \text{ zeros} \\
 (q-k+1) & \cdots & \sqrt{\frac{q}{q+1}} \rightarrow (q-k+1)^{\text{th}} \text{ position} \\
 (q-k+2) & \cdots & \frac{-1}{\sqrt{k(k+1)}} \rightarrow (q-k+2)^{\text{th}} \text{ position} \\
 \vdots & & \vdots \\
 q-2 & \cdots & \frac{-1}{\sqrt{k(k+1)}} \rightarrow (q-k+k-2)^{\text{th}} \text{ position} \\
 q-1 & \cdots & \frac{-1}{\sqrt{k(k+1)}} \rightarrow [q-k+(k-1)]^{\text{th}} \text{ position} \\
 q & \cdots & \frac{-1}{\sqrt{k(k+1)}} \rightarrow q^{\text{th}} \text{ position}
 \end{array}$$

$$\Rightarrow Z = \text{Trace}(T^N) = \sum_{k=0}^{q-1} (\lambda_k)^N$$

$$\Rightarrow Z = (q + e^{\beta J} - 1)^N + (q-1)(e^{\beta J} - 1)^N$$

$$\Rightarrow Z = (q + e^{\beta J} - 1)^N \left\{ 1 + (q-1) \left[\frac{(e^{\beta J} - 1)}{e^{\beta J} - 1 + q} \right]^N \right\}$$

Thus for any $q = 1, 2, 3, \dots$,

$$\lambda_0 = (q + e^{\beta J} - 1) > \lambda_k \quad (k \neq 0)$$

Hence in thermodynamic limit, as $N \rightarrow \infty$ only λ_0 term contributes.

$$\Rightarrow \underline{Z \approx (q + e^{\beta J} - 1)^N}$$

$$c) \langle S_i S_{i+r} \rangle = \frac{\text{Trace}[S_i S_{i+r} e^{-\beta H}]}{Z}$$

$$\Rightarrow \frac{\langle S_i S_{i+r} \rangle}{Z^{-1}} = \sum_{\{S_j\}} S_i S_{i+r} e^{\beta J \sum_j \Delta(S_j, S_{j+1})}$$

$$\frac{\langle S_i S_{i+r} \rangle}{Z^{-1}} = \sum_{\{S_j\}} \left[e^{BJ\Delta(S_1, S_2)} e^{BJ\Delta(S_2, S_3)} \dots S_i e^{BJ\Delta(S_i, S_{i+1})} \right. \\ \left. \dots S_{i+r} e^{BJ\Delta(S_{i+r}, S_{i+r+1})} \dots e^{BJ\Delta(S_N, S_1)} \right]$$

$$= \sum_{\{S_j\}} \left[\langle 1 | T | S_2 \rangle \langle S_2 | T | S_3 \rangle \langle S_3 | T | S_4 \rangle \dots \right. \\ \dots \langle S_{i-1} | T | S_i \rangle S_i \langle S_i | T | S_{i+1} \rangle \dots \\ \dots \langle S_{i+r-1} | T | S_{i+r} \rangle S_{i+r} \langle S_{i+r} | T | S_{i+r+1} \rangle \dots \\ \left. \dots \langle S_N | T | S_1 \rangle \right]$$

Defining a matrix $\hat{S} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 2 & 0 & \dots & 0 \\ 0 & 0 & 3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & q \end{bmatrix}_{q \times q}$

$$= \sum_{\{S_j\}} \left[\langle 1 | T | S_2 \rangle \langle S_2 | T | S_3 \rangle \langle S_3 | T | S_4 \rangle \dots \right. \\ \dots \langle S_{i-1} | T \hat{S} | S_i \rangle \langle S_i | T | S_{i+1} \rangle \dots \\ \dots \langle S_{i+r-1} | T | S_{i+r} \rangle \langle S_{i+r} | \hat{S} T | S_{i+r+1} \rangle \dots \\ \left. \dots \langle S_N | T | S_1 \rangle \right]$$

Using Completeness relation for each $|S_j\rangle$
i.e. $\sum_{S_j} |S_j\rangle \langle S_j| = \hat{I}$ we get,

$$\frac{\langle S_i S_{i+r} \rangle}{Z^{-1}} = \sum_{S_1, S_i, S_{i+r}} \left[\langle S_1 | T^{i-1} \hat{S} | S_i \rangle \langle S_i | T^r | S_{i+r} \rangle \right. \\ \left. \times \langle S_{i+r} | \hat{S} T^{N-i-r+1} | S_1 \rangle \right]$$

$$\begin{aligned}
\frac{\langle S_i S_{i+r} \rangle}{Z^{-1}} &= \sum_{S_1} \langle S_1 | T^{i-1} \hat{S} T^r \hat{S} T^{N-r+1-i} | S_1 \rangle \\
&= \text{trace} (T^{i-1} \hat{S} T^r \hat{S} T^{N-r+1-i}) \\
&= \text{trace} (T^{N-r} \hat{S} T^r \hat{S}) \quad (\text{cyclic property of trace})
\end{aligned}$$

$$\Rightarrow \frac{\langle S_i S_{i+r} \rangle}{Z^{-1}} = \text{trace} (T^{N-r} \hat{S} T^r \hat{S})$$

$$\text{where } T = |\lambda_0\rangle\langle\lambda_0| - \hat{\mathbb{I}}_{q \times q} + e^{\beta J} \hat{\mathbb{I}}_{q \times q}$$

$$\text{with } |\lambda_0\rangle = \frac{1}{\sqrt{q}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{q \times 1} \quad \& \quad \hat{S} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 2 & 0 & \dots & 0 \\ 0 & 0 & 3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & q \end{bmatrix}_{q \times q}$$

eigen vector for $\lambda_0 = q + e^{\beta J} - 1$

Since trace is independent of the basis, we can find $\text{trace} (T^{N-r} \hat{S} T^r \hat{S})$ in the eigen basis of T matrix.

$$\Rightarrow \frac{\langle S_i S_{i+\gamma} \rangle}{Z^{-1}} = \sum_{k=0}^{q-1} \langle \lambda_k | T^{N-\gamma} \hat{S} T^{\gamma} \hat{S} | \lambda_k \rangle$$

$$= \sum_{k=0}^{q-1} \lambda_k^{N-\gamma} \langle \lambda_k | \hat{S} T^{\gamma} \hat{S} | \lambda_k \rangle$$

$$= \sum_{k, k'} \lambda_k^{N-\gamma} \langle \lambda_k | \hat{S} | \lambda_{k'} \rangle \langle \lambda_{k'} | T^{\gamma} \hat{S} | \lambda_k \rangle$$

$$= \sum_{k, k'} \lambda_k^{N-\gamma} \lambda_{k'}^{\gamma} \langle \lambda_k | \hat{S} | \lambda_{k'} \rangle \langle \lambda_{k'} | \hat{S} | \lambda_k \rangle$$

$$= \sum_{k, k'} \lambda_k^{N-\gamma} \lambda_{k'}^{\gamma} |\langle \lambda_k | \hat{S} | \lambda_{k'} \rangle|^2$$

$$= \sum_{k'} \lambda_{k'}^{\gamma} \left[\lambda_0^{N-\gamma} |\langle \lambda_0 | \hat{S} | \lambda_{k'} \rangle|^2 + \sum_{k=1}^q \lambda_k^{N-\gamma} |\langle \lambda_k | \hat{S} | \lambda_{k'} \rangle|^2 \right]$$

$$= \sum_{k'} \lambda_{k'}^{\gamma} \lambda_0^N \left[\lambda_0^{-\gamma} |\langle \lambda_0 | \hat{S} | \lambda_{k'} \rangle|^2 + \sum_{k=1}^q \left(\frac{\lambda_k}{\lambda_0} \right)^N \lambda_k^{-\gamma} |\langle \lambda_k | \hat{S} | \lambda_{k'} \rangle|^2 \right]$$

Since in thermodynamic limit,
as $N \rightarrow \infty$, $\left(\frac{\lambda_k}{\lambda_0}\right)^N \rightarrow 0$ as $\lambda_k < \lambda_0$

we neglect those terms & we get,

$$\begin{aligned} \frac{\langle S_i S_{i+r} \rangle}{Z^{-1}} &= \sum_{k'} \lambda_{k'}^r \lambda_0^{N-r} |\langle \lambda_0 | \hat{S} | \lambda_{k'} \rangle|^2 \\ &= \lambda_0^N \sum_{k'} \left(\frac{\lambda_{k'}}{\lambda_0} \right)^r |\langle \lambda_0 | \hat{S} | \lambda_{k'} \rangle|^2 \end{aligned}$$

Since $\lambda_0^N \sim Z$ in thermodynamic limit, we get the simplified expression

$$\begin{aligned} \langle S_i S_{i+r} \rangle &= \sum_{k=0}^{q-1} \left(\frac{\lambda_k}{\lambda_0} \right)^r |\langle \lambda_0 | \hat{S} | \lambda_k \rangle|^2 \\ &= \underbrace{\left(\frac{\lambda_k}{\lambda_0} \right)^r}_{\text{Independent of 'k'}} \underbrace{\sum_{k=0}^{q-1} |\langle \lambda_0 | \hat{S} | \lambda_k \rangle|^2}_1 \end{aligned}$$

$$\Rightarrow \langle S_i S_{i+r} \rangle = \left(\frac{e^{\beta J} - 1}{e^{\beta J} - 1 + q} \right)^r$$

4a)

Arithmetic mean - Geometric mean inequality

Let $\{x_i\}$ be a set of random positive values. AM-GM inequality states that,

$$\underbrace{\frac{1}{n} \sum_i x_i}_{A.M} \geq \underbrace{\left(\prod_i x_i \right)^{1/n}}_{G.M}$$

Consider $\{x_1 \neq x_2\}$

$$\Rightarrow (\sqrt{x_1} - \sqrt{x_2})^2 = x_1 + x_2 - 2\sqrt{x_1 x_2}$$

$$\text{Since } (\sqrt{x_1} - \sqrt{x_2})^2 \geq 0$$

$$\Rightarrow x_1 + x_2 - 2\sqrt{x_1 x_2} \geq 0$$

$$\Rightarrow \underbrace{\left(\frac{x_1 + x_2}{2} \right)}_{A.M} \geq \sqrt{x_1 x_2} \quad G.M$$

Thus $A.M \geq G.M$. Which is also true for more than two numbers.

Weighted A.M - G.M inequality

Consider $\{p_i\}$ where all p_i are non-negative such that $\sum_i p_i = 1$. For a random non-negative set $X = \{x_i\}$ we can write,

$$\underbrace{\sum_i p_i x_i}_{\text{weighted A.M}} \geq \underbrace{\prod_i x_i^{p_i}}_{\text{weighted G.M}}$$

Proof

Consider $G = \prod_i x_i^{p_i}$

$$\Rightarrow \log(G) = \sum_i \log(x_i^{p_i}) = \sum_i p_i \log(x_i)$$

$$\Rightarrow \log(G) = \langle \log(X) \rangle$$

$$\text{Now } A = \sum_i p_i x_i = \langle X \rangle$$

$$\Rightarrow \log(A) = \log(\langle X \rangle)$$

Since $\log$ is a strictly concave function by Jensen's inequality we can say that $\log(\langle X \rangle) \geq \langle \log(X) \rangle$

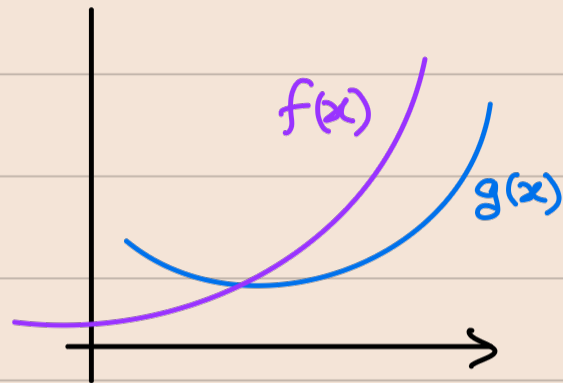
$$\Rightarrow \log(A) \geq \log(G) \Rightarrow A \geq G$$

$$\Rightarrow \boxed{\sum_i p_i x_i \geq \prod_i x_i^{p_i}}$$

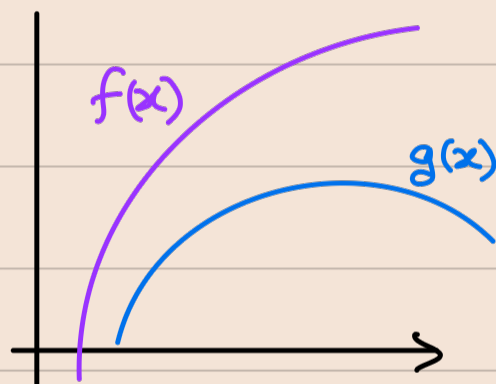
Jensen's Inequality

Jensen's inequality is a general inequality relating expectation values of a function of random variable & the function of expectation value of the random variable.

A function $f(x)$ is convex in the interval (a, b) if $f''(x) > 0$ for all $x \in (a, b)$



A function $f(x)$ is concave in the interval (a, b) if $f''(x) < 0$ for all $x \in (a, b)$



Let φ be a function whose 2nd derivative exists. Let $\langle v \rangle$ denote the expectation value of v . Then by Jensen's inequality,

$$\varphi(\langle x \rangle) \leq \langle \varphi(x) \rangle \Rightarrow \text{if } \varphi \text{ is convex}$$

$$\varphi(\langle x \rangle) \geq \langle \varphi(x) \rangle \Rightarrow \text{if } \varphi \text{ is concave}$$

(equality holds only when either φ is a constant or if x is a constant)

4b) Consider the Bogoliubov inequality

$$Z \geq Z_0 e^{-\beta \langle H - H_0 \rangle}$$

$$\Rightarrow \log(Z) \geq \log(Z_0) - \beta \langle H - H_0 \rangle$$

$$\Rightarrow \frac{-1}{\beta} \log(Z) \leq \frac{-1}{\beta} \log(Z_0) + \langle H - H_0 \rangle$$

$$F = \frac{-1}{\beta} \log(Z) \Rightarrow \text{Exact value of Free energy of true Hamiltonian}$$

$$F_0 = \frac{-1}{\beta} \log(Z_0) \Rightarrow \text{Free energy of trial Hamiltonian}$$

$$\Rightarrow F \leq F_0 + \langle H - H_0 \rangle$$

$$\text{Now } F_0 = \langle H_0 \rangle - TS_0$$

$$\langle \hat{H}_0 \rangle = \text{Trace} \left[\frac{e^{-\beta \hat{H}_0}}{Z_0} \hat{H}_0 \right]$$

But in terms of density matrix ($\hat{\rho}_0$)

$$\langle \hat{H}_0 \rangle = \text{Trace}(\hat{\rho}_0 \hat{H}_0)$$

$$\Rightarrow \hat{\rho}_0 = \frac{e^{-\beta \hat{H}_0}}{Z_0} \Rightarrow \text{density matrix}$$

Entropy S_0 , in terms of free energy is,

$$\begin{aligned} S_0 &= \frac{E_0 - F_0}{T} = k_B \beta \langle \hat{H}_0 \rangle + k_B \ln(Z_0) \\ &= k_B [\beta \text{Trace}(\rho_0 \hat{H}_0) + \ln(Z_0)] \\ &= k_B \left[\frac{\beta \text{Trace}(e^{-\beta \hat{H}_0} \hat{H}_0) + \ln(Z_0)}{Z_0} \right] \\ &= k_B \left[\frac{\beta \text{Trace}(e^{-\beta \hat{H}_0} \hat{H}_0) + \text{Trace}(e^{-\beta \hat{H}_0}) \ln(Z_0)}{Z_0} \right] \\ &= k_B \text{Trace} \left[\frac{\beta \hat{H}_0 e^{-\beta \hat{H}_0} + e^{-\beta \hat{H}_0} \ln(Z_0)}{Z_0} \right] \\ &= k_B \text{Trace} \left[\frac{e^{-\beta \hat{H}_0}}{Z_0} (\beta \hat{H}_0 + \ln(Z_0)) \right] \\ &= k_B \text{Trace} \left[\frac{e^{-\beta \hat{H}_0}}{Z_0} [-\ln(e^{-\beta \hat{H}_0}) + \ln(Z_0)] \right] \\ &= -k_B \text{Trace} \left[\frac{e^{-\beta \hat{H}_0}}{Z_0} \ln \left(\frac{e^{-\beta \hat{H}_0}}{Z_0} \right) \right] \end{aligned}$$

$$\Rightarrow \boxed{S_0 = -k_B \text{Trace}[\hat{\rho} \ln(\hat{\rho})]}$$

$$\Rightarrow F_0 = \langle \hat{H}_0 \rangle + TS_0$$

$$F_0 = \text{Trace}(\rho_0 \hat{H}) - k_B T \text{Trace}[\hat{\rho}_0 \ln(\hat{\rho}_0)]$$

Putting this value of F_0 in the Bogolioubov inequality we get,

$$F \leq \cancel{\text{Trace}(\rho_0 \hat{H})} - (k_B T) \text{Trace}[\hat{\rho}_0 \ln(\hat{\rho}_0)] + \langle (\hat{H} - \hat{H}_0) \rangle_0$$

$$\Rightarrow F \leq \text{Trace}(\rho_0 \hat{H}) - (k_B T) \text{Trace}[\hat{\rho}_0 \ln(\hat{\rho}_0)]$$

$$F \leq \langle \hat{H} \rangle_0 - TS_0 = \Phi$$

where Φ is Free energy of $\hat{H}$ found in terms of the density matrix got by eigen states of $\hat{H}_0$.

$$\underline{F = -k_B T \ln(Z)} \Rightarrow \left(\begin{array}{l} \text{for true} \\ \text{Hamiltonian} \end{array} \right)$$

$$\Phi = -k_B T \ln(Z')$$

where $Z' \Rightarrow \text{Trace}(e^{-\beta \hat{H}})$ found using eigen states of $\hat{H}_0 \Rightarrow \{|v\rangle\}$.

$$\Rightarrow -k_B T \ln(Z) \leq -k_B T \ln(Z')$$

$$\Rightarrow Z \geq Z' = \text{Trace}(e^{-\beta \hat{H}}) \text{ w.r.t } |v\rangle$$

$$\text{i.e. } Z' = \sum_v \langle v | e^{-\beta \hat{H}} | v \rangle$$

$$\Rightarrow Z' \geq \sum_v e^{-\beta \langle v | \hat{H} | v \rangle}$$

By Feynmann inequality

Proof Let $\{|n\rangle\}$ be the eigen states of $\hat{H}$ with eigen value E_n .
 $\Rightarrow \hat{H}|n\rangle = E_n|n\rangle$

So $\{|n\rangle\}$ is complete. $\Rightarrow \sum_n |n\rangle \langle n| = \hat{I}$

$$\Rightarrow |v\rangle = \sum_n (\langle n | v \rangle) |n\rangle = \sum_n c_n^{(v)} |n\rangle$$

$$\Rightarrow \langle v | \hat{H} | v \rangle = \sum_{m,n} \langle v | m \rangle \langle m | \hat{H} | n \rangle \langle n | v \rangle$$

$$\Rightarrow \langle \nu | \hat{H} | \nu \rangle = \sum_{m,n} C_m^{(\nu)*} \delta_{mn} E_m C_n^{(\nu)}$$

$$\Rightarrow \langle \nu | \hat{H} | \nu \rangle = \sum_n |C_n^{(\nu)}|^2 E_n$$

Let $p_n^{(\nu)} = |C_n^{(\nu)}|^2$. It gives the probability that the state $|\nu\rangle$ to collapse to $|n\rangle$ upon measuring. $\Rightarrow \sum_n p_n^{(\nu)} = 1$

$$\Rightarrow \langle \hat{H} \rangle_{\nu} = \sum_n p_n^{(\nu)} E_n \Rightarrow e^{\langle \hat{H} \rangle_{\nu}} = e^{\sum_n p_n^{(\nu)} E_n}$$

$$\Rightarrow e^{\langle \hat{H} \rangle_{\nu}} = \prod_n e^{p_n^{(\nu)} E_n}$$

Now we need to find expectation value of $e^{-\beta \hat{H}}$ w.r.t $|\nu\rangle$

$$\text{So } \langle \nu | e^{-\beta \hat{H}} | \nu \rangle = \sum_{m,n} C_m^{(\nu)*} C_n^{(\nu)} \langle m | e^{-\beta \hat{H}} | n \rangle$$

$$\text{Since } \hat{H} |n\rangle = E_n |n\rangle \Rightarrow \underline{f(\hat{H}) |n\rangle = f(E_n) |n\rangle}$$

$$\text{So } e^{-\beta \hat{H}} |n\rangle = e^{-\beta E_n} |n\rangle$$

$$\begin{aligned} \Rightarrow \langle \nu | e^{-\beta \hat{H}} | \nu \rangle &= \sum_{m,n} C_m^{(\nu)*} C_n^{(\nu)} \delta_{mn} e^{-\beta E_n} \\ &= \sum_n |C_n^{(\nu)}|^2 e^{-\beta E_n} \end{aligned}$$

$$\Rightarrow \langle e^{-\beta \hat{H}} \rangle_\nu = \sum_n p_n^{(\nu)} e^{-\beta E_n}$$

We can use weighted AM-GM inequality: $\sum_n p_n b_n \geq \prod_n b_n^{p_n} \left(\sum_n p_n = 1 \right)$

$$\Rightarrow \underbrace{\sum_n p_n^{(\nu)} (e^{-\beta E_n})}_{\langle e^{-\beta \hat{H}} \rangle_\nu} \geq \underbrace{\prod_n (e^{-\beta E_n})^{p_n^{(\nu)}}}_{e^{-\beta \langle \hat{H} \rangle_\nu}}$$

Thus we arrive at Feynmann's inequality which is

$$\boxed{\langle \nu | e^{-\beta \hat{H}} | \nu \rangle \geq e^{-\beta \langle \nu | \hat{H} | \nu \rangle}}$$

$$\text{Since } Z' = \sum_\nu \langle \nu | e^{-\beta \hat{H}} | \nu \rangle$$

$$Z' \geq \sum_\nu e^{-\beta \langle \nu | \hat{H} | \nu \rangle}$$

But we got previously that $Z \geq Z'$

$$\Rightarrow \boxed{Z \geq \sum_\nu e^{-\beta \langle \nu | \hat{H} | \nu \rangle}}$$