

24/02/25

Lecture 15

Spontaneous Ordering

The existence of spontaneous ordering in a many particle system, signifies the system's macroscopic state or the phase characterized by a specific level of organization or correlation between its constituent particles, which is distinguished by an order parameter.

Eg: Spontaneous magnetization where the spins align in a particular direction which is given by m_s

$$m_s = \lim_{h \rightarrow 0^+} \lim_{N \rightarrow \infty} \langle S_i \rangle$$

where $S_i \Rightarrow$ Spin at i^{th} lattice site.

If $m_s \neq 0$, then even in the absence of an external 'h', the ensemble average $\langle S_i \rangle$ of spin is not zero.

Long range Order

The presence of a long range order in the system implies that even far away remote portions of the system have correlated behaviour. This is characterized by the correlation function.

Eg: $C(r) = \langle S_i S_{i+r} \rangle$ is a correlation function. And $G(r) = \langle S_i S_{i+r} \rangle - \langle S_i \rangle \langle S_{i+r} \rangle$ is a correlation function of mean difference of S_i & S_r .

i.e.

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

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

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

Now if there is order in the system then when $T < T_c$ even at $h=0$, $\langle S_i \rangle = \langle S_{i+r} \rangle = m_s \neq 0$.

Also we had earlier seen that

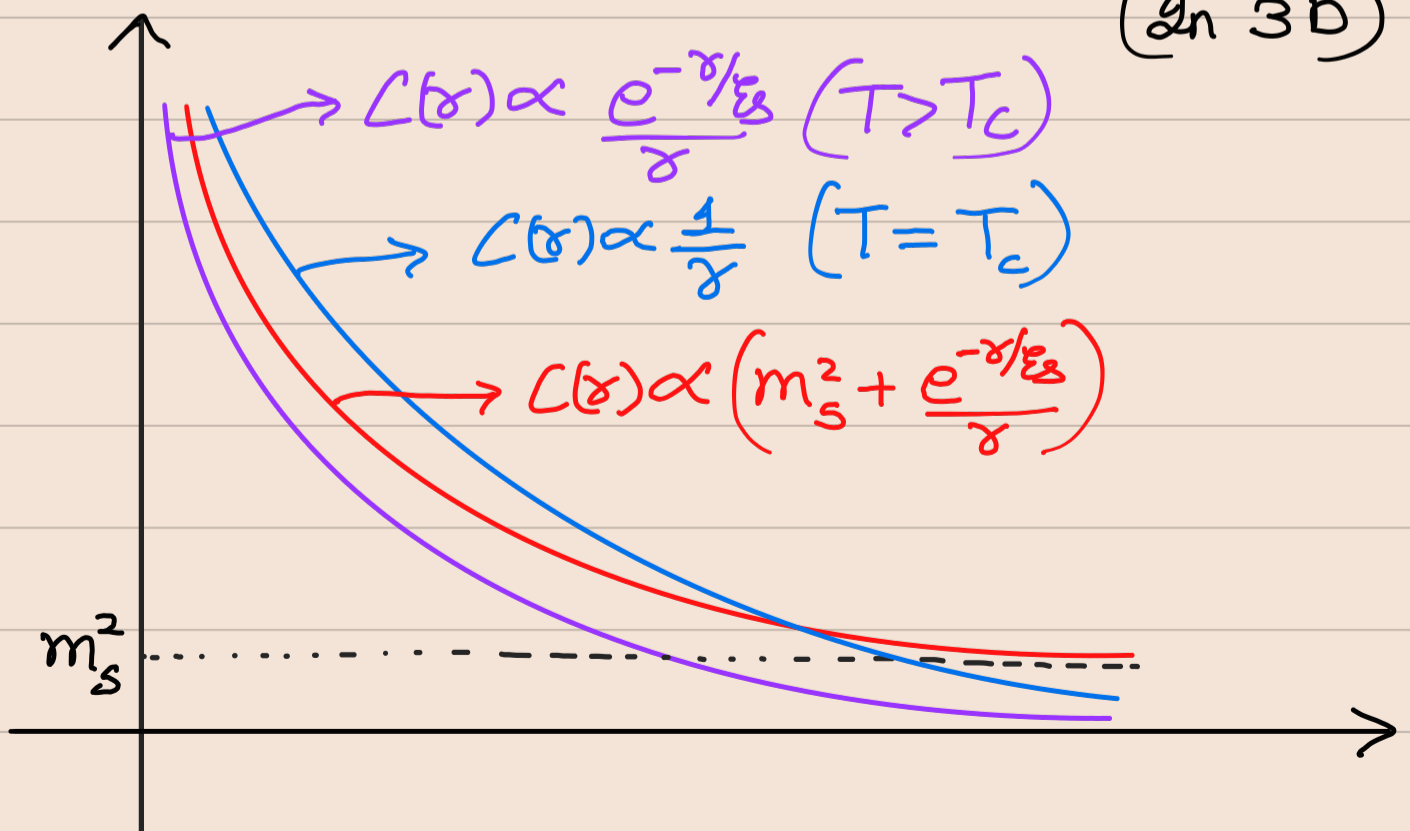
$$G(r) = \frac{e^{-r/\xi_s}}{r^{d-2+\eta}}$$

Thus as $r \rightarrow \infty \Rightarrow G(r) \rightarrow 0$
 $\Rightarrow \lim_{r \rightarrow \infty} C(r) = \langle S_i S_{i+r} \rangle = \langle S_i \rangle \langle S_{i+r} \rangle$

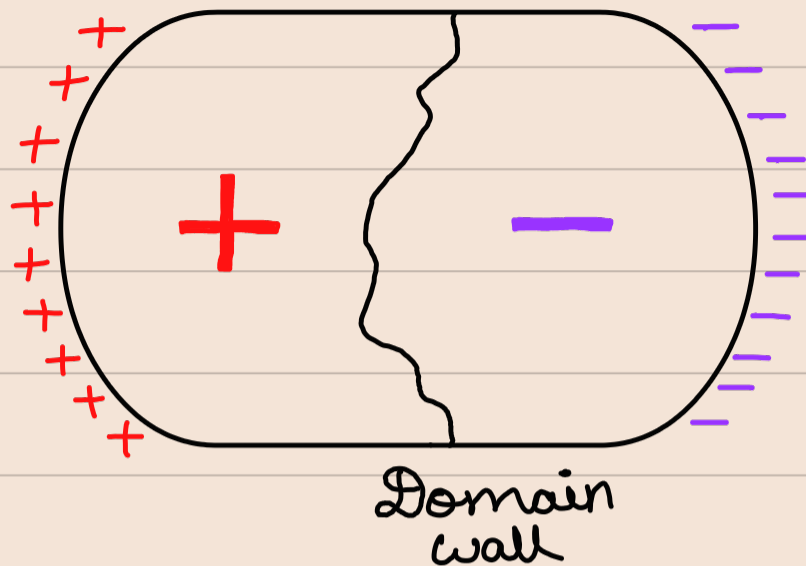
$$\Rightarrow C(r \rightarrow \infty) = m_s^2 \quad (\text{when } T < T_c)$$

Thus if there is order in the system then even for large distances the $C(r)$ correlation function is non-zero. This is the indication of long-range order.

(In 3D)



Anti-Periodic Boundary Condition



Consider a d -dim. spin system with anti-periodic boundary condition where one side is +ve and -ve on the opposite side. Mathematically this can be implemented as

$S_{i+L} = -S_i$ where L is the length of the system. If $T < T_c$, even though the translation invariance is lost, the long range order is still present since $N \rightarrow \infty$.

$$\text{i.e. } \lim_{\delta \rightarrow \infty} \lim_{N \rightarrow \infty} \langle S_i S_{i+\delta} \rangle \neq 0.$$

But due to anti periodic boundary condition, there will be a domain wall interface which separates the up-spins & down spins.

This will increase the free energy of the system when compared to the periodic boundary case.

$$\Rightarrow F_{\text{anti-periodic}} = F_{\text{periodic}} + F_{\text{interface}}$$

$L^d \Rightarrow d$ -dimensional Volume of System

$L^{d-1} \Rightarrow$ Interface area in d -dimension

$L \Rightarrow$ System's length

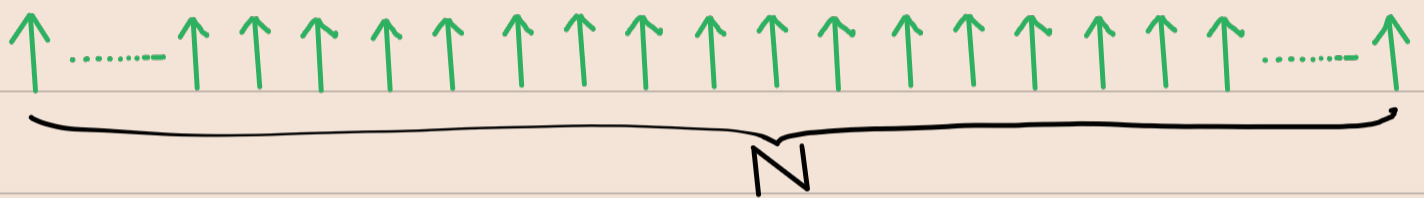
For large system the $F_{\text{interface}}$ is extensive quantity, hence it will be proportional to interface area. $\Rightarrow F_{\text{interface}} = \sigma L^{d-1}$
 $\sigma \Rightarrow$ interface tension.

$$\Rightarrow F_{\text{anti-periodic}} = f L^d + \sigma L^{d-1}$$

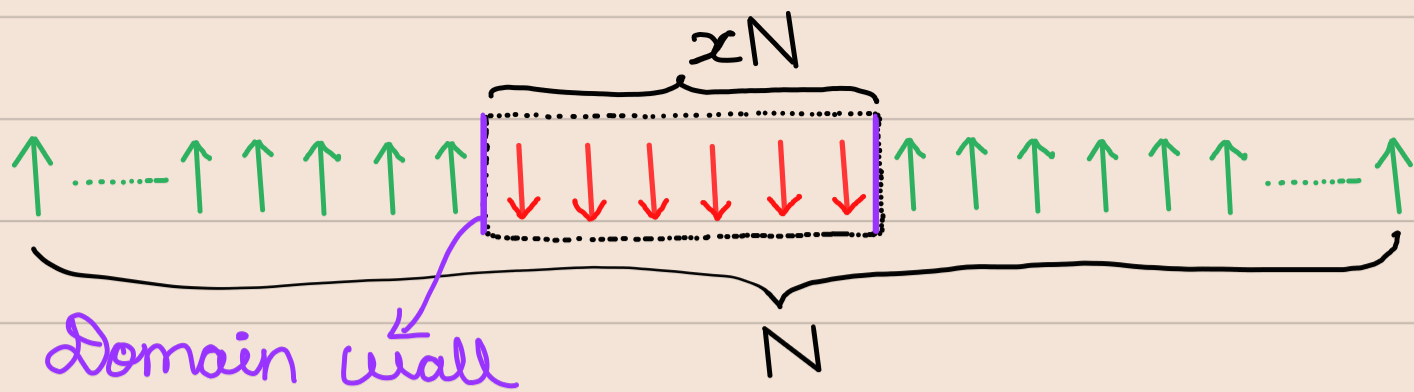
$f \Rightarrow$ free energy per spin per unit volume

Why a 1-D system with only short range interaction can have no long range order at any non-zero temperature?

Landau's Argument



Consider 'N' spins arranged in a 1D chain. Let the spins all be oriented in a particular direction at some non-zero temperature. The net magnetization per spin is m_0 . So we now have to prove that this is an unstable configuration. Even though the free energy is minimum the disorder is favoured (entropy over takes the free energy). $F_{\text{net}} = -NJ$ when all the spins are aligned at $h=0$.



Consider flipping ' x ' fractions of spins which are in some region where $\frac{1}{N} \leq x < \frac{1}{2}$. Then the new net

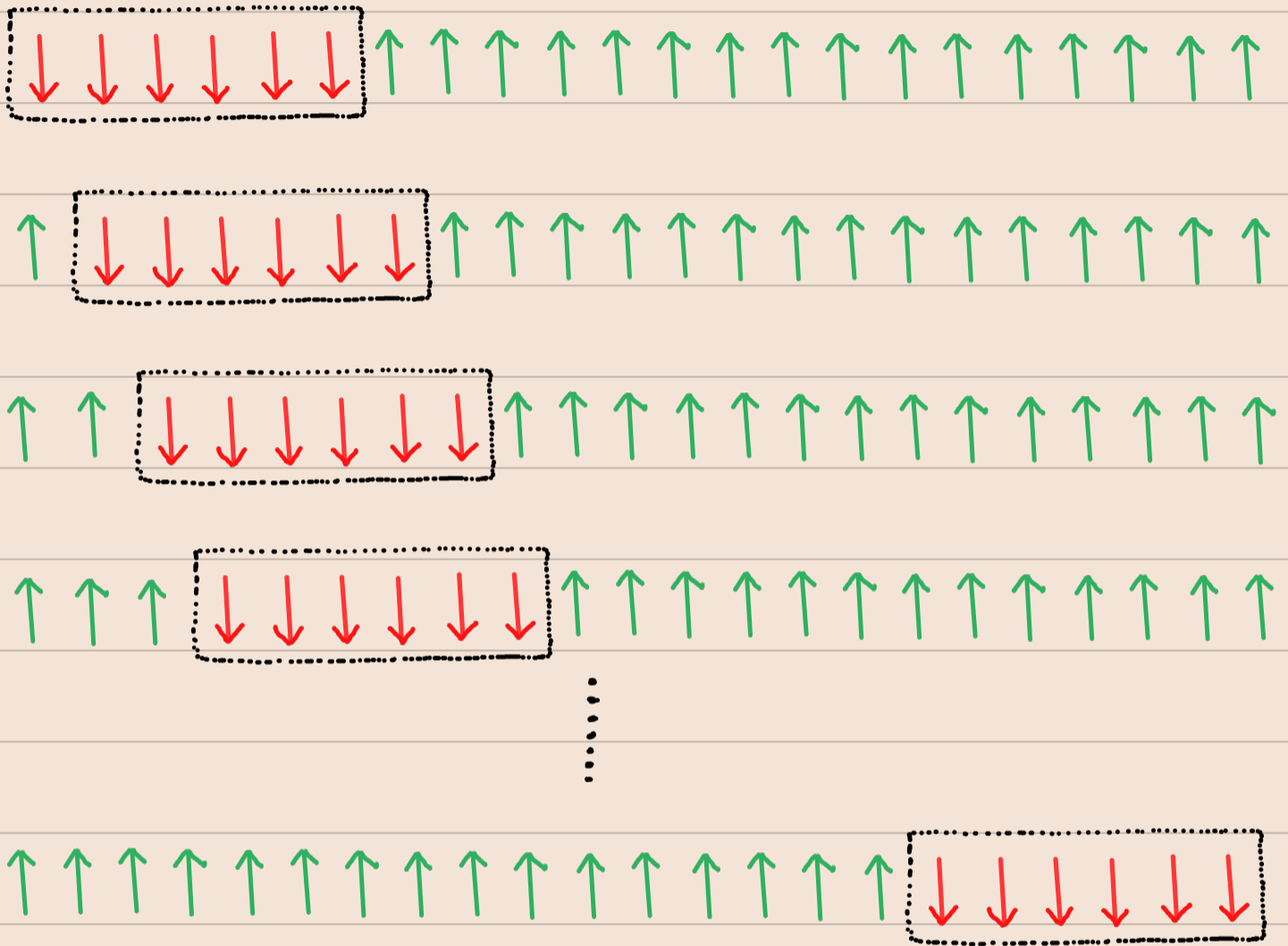
magnetization is $\underbrace{(1-x)m_0}_{\text{unaffected}} - \underbrace{xm_0}_{\text{affected}}$

$$\Rightarrow m_{\text{net}} = (1-2x)m_0$$

The change in free energy is $\Delta F = \Delta E - T\Delta S$ ($T > 0$)

$\Delta E = 2J + 2J$ as there are two interfaces with opposite spin. Each interface costs an energy of $2J$ considering the periodic boundary conditions.

$\Delta S \Rightarrow$ It is the Configurational entropy due to all possible arrangements which has same $\Delta E = 4J$.



All the above configurations have same $\Delta E = 4J$, which is $N - Nx$ number of configurations.

$$\Rightarrow \Delta S = k_B \ln[N(1-x)]$$

$$\Delta S = k_B \ln(N) + k_B \ln(1-x)$$

$$\Delta F = 4J - k_B T \left(\ln(N) - \left[x + \frac{x^2}{2} + \dots \right] \right)$$

when $N \rightarrow \infty$ the last term can be ignored.

$$\Rightarrow \Delta F = 4J - k_B T \ln(N)$$

If T is finite then ΔF will be further minimized. Hence in thermodynamic limit the presence of domain walls is thermodynamically stable. As having even a single domain wall is enough to break the long range order & as it will inevitably appear, the long 1D chain will break-up into many finite domains & hence Correlation function $C(x)$ decays exponentially.

Thus even a small amount of thermal energy ($T > 0$) is enough to create domain walls that will break any putative order.

Hence presence of $m_0 \neq 0$ at a temperature $T > 0$ will lead to disorder & equilibrium is not attained. But only when $m_0 = 0$ it can be an equilibrium state. Moreover we just saw that even if $m_0 \neq 0$, the system favours disorder & it eventually reaches a state of $m_0 = 0$.

Find mistake: Ising argument

Consider a 2D discrete Ising Spin System. It has some T_c .

now for J along $x \Rightarrow J_1$

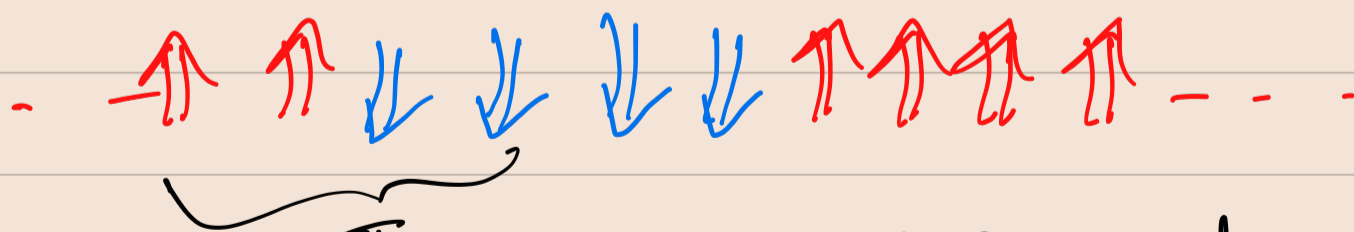
for J along $y \Rightarrow J_2$

$T_c \propto J \Rightarrow$ Make $J_2 \rightarrow \infty$

This increases T_c by a factor

Thus all spin along a Column will be the same as $J_2 \rightarrow \infty$

(spin freeze) and act as Super spin along x -axis.

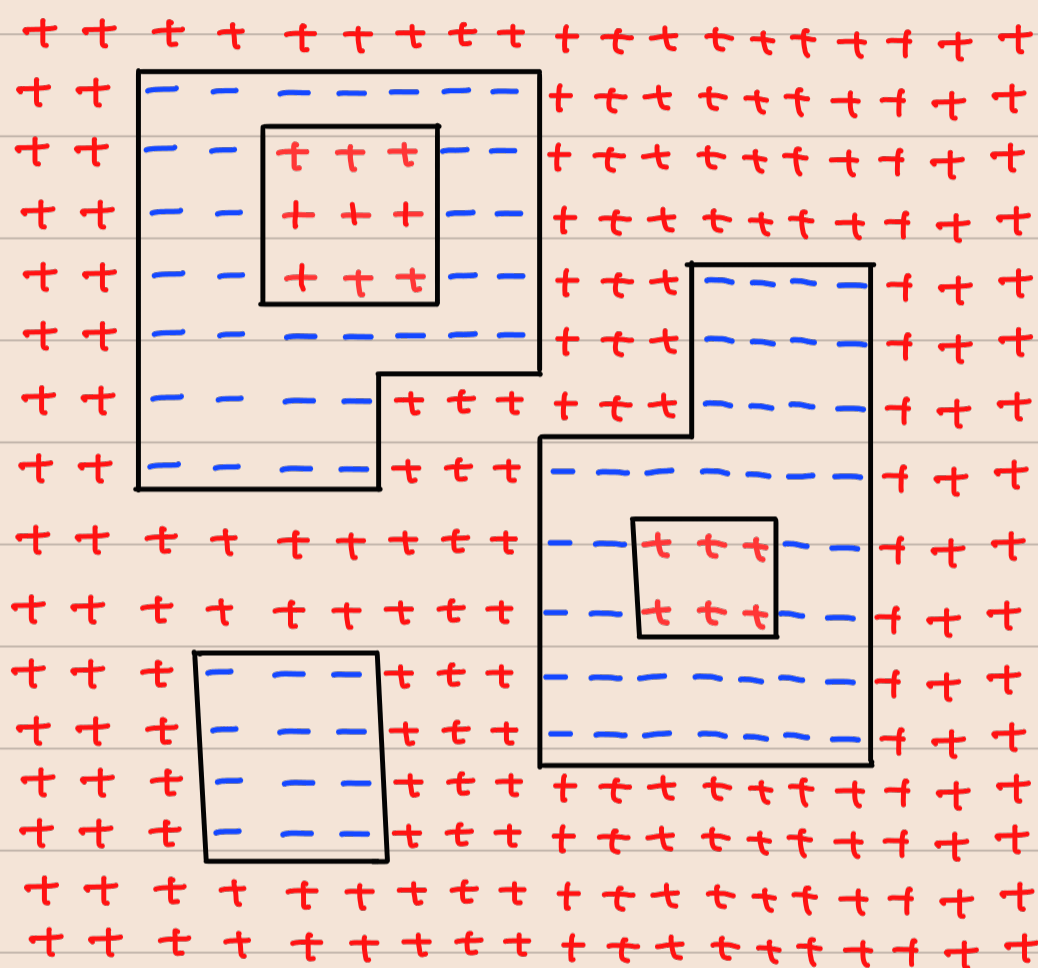


This is a 1D analogue.

Thus for this $T_c = 0$

$\Rightarrow T_c \text{ original} = 0 \Rightarrow$ No order at non zero T_c .

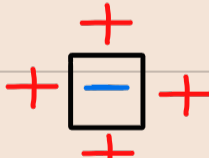
Existence of Spontaneous Magnetization in 2D Ising Spin System at non-zero Temperature with only short range Interaction. — Peierls Argument



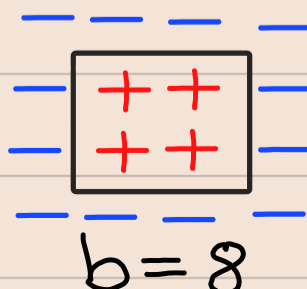
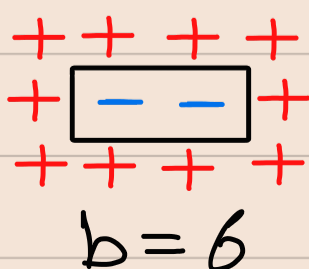
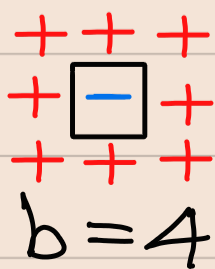
$$H = -J \sum_{\langle i,j \rangle} S_i S_j \Rightarrow \text{Short range Ising model}$$

Consider a Square lattice of Ising spins which are all up in the boundary (fixed boundary condition). Peierls showed that there exists non-zero magnetization in the bulk if the temperature is low enough.

Even though this boundary will simulate external magnetic field, it will not matter as its influence is extremely weak in the limit of an infinite lattice. Consider an arbitrary configuration of spins as shown above. We can draw a domain wall between any two unlike spins. Since the border is fixed in the boundary, every border wall has to be a closed loop whose length has to be an even number greater than 2.

 $\Rightarrow$ Smallest possible domain.

Let 'b' be the length of the domain wall border which can take values of 4, 6, 8, ...



-- So on.

A domain wall of length ' b ' is a closed polygon which is made of ' b ' number of vertical / horizontal segments.

Let $\gamma(b)$ be the number of borders of length ' b ' in the given configuration ' C '. Let $B(C)$ be the set of all borders in configuration C . A domain wall is uniquely specified by numbers ' b ' & ' i ' where ' i ' is the border index. We define an indicator function $\chi_b^{(i)}$ where

$$\chi_b^{(i)} = \begin{cases} 1, & i^{\text{th}} \text{ border of length 'b' is present in } C, \text{ i.e. } i \in B(C). \\ 0, & \text{otherwise} \end{cases}$$

Now the area of a domain wall of border size ' b ' is always less than $(\frac{b}{4})^2$. Since any domain wall of total length ' b ' will always fit inside a square of side ' $\frac{b}{4}$ '.

Notice that every '-' spin is enclosed by atleast one domain wall. So the number '-' spins in the configuration equal to the sum of areas of all the borders. But every border of length 'b' has area less than $(b/4)^2$, thus,

$$N_- \leq \sum_b \left(\frac{b}{4}\right)^2 \sum_{i=1}^{v(b)} \chi_b^{(i)}(c)$$

$\left(\frac{b}{4}\right)^2 \Rightarrow$ Upper bound on the no: of spins enclosed by a border of length 'b'.

The thermal average of $\chi_b^{(i)}$ is given by,

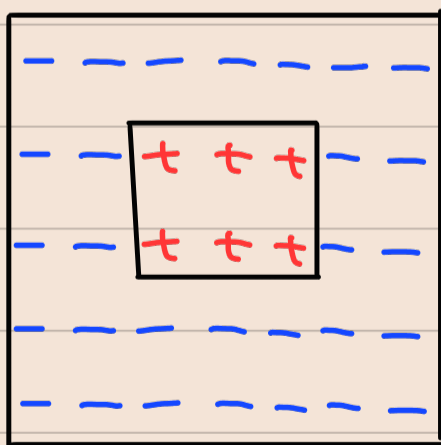
$$\langle \chi_b^{(i)} \rangle = \frac{\sum_c \chi_b^{(i)}(c) e^{-\beta E(c)}}{\sum_c e^{-\beta E(c)}}$$

Let $\mathcal{C}$ be those configurations where $\chi_b^{(i)} = 1$ then,

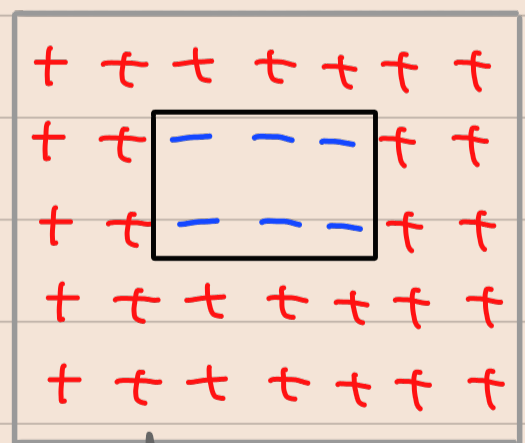
$$\Rightarrow \langle \chi_b^{(i)} \rangle = \frac{\sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})}}{\sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})}}$$

$\mathcal{C} \Rightarrow$ all possible configurations

Now, give some configuration $\mathcal{C}$ we can obtain another configuration by flipping the signs of every spin inside all the borders.

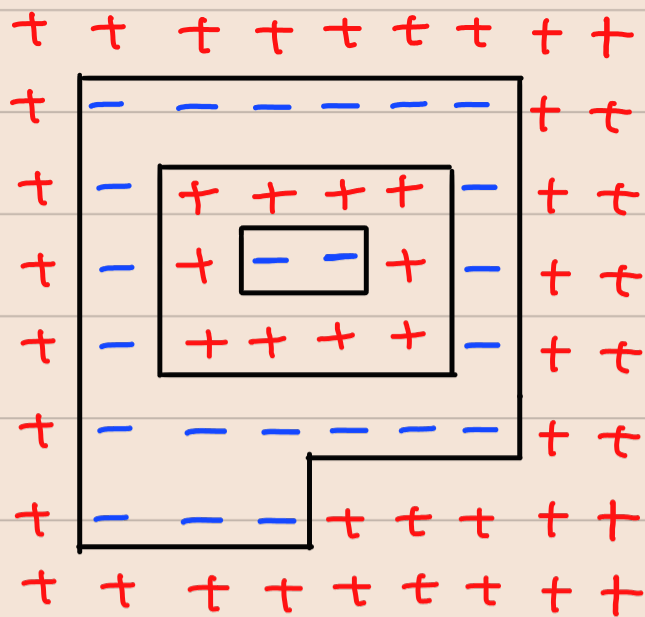


Spin flip $\rightarrow$



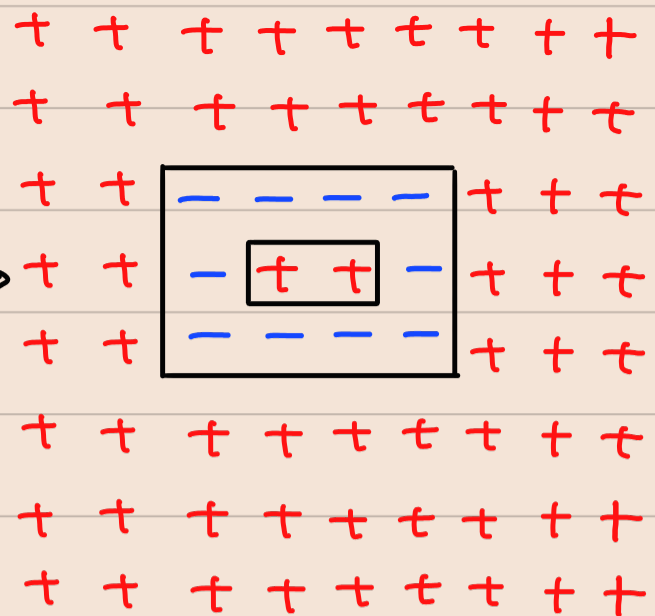
$\hookrightarrow$ i^{th} border of length 'b' belongs to $\mathcal{C}$.

This border vanishes
 $\mathcal{C}'$ doesn't have this border



Configuration: C

flip $\rightarrow$



Configuration C'

The energy change b/w $E(C)$ & $E(C')$ is given only by the border length 'b',

$$E(C') = E(C) - 2Jb$$

reduction of energy
by spin flipping

$$\Rightarrow \langle \chi_b^{(i)} \rangle = \frac{\sum_C e^{-\beta E(C)}}{\sum_C e^{-\beta E(C)}}$$

$C \Rightarrow$ all possible configurations

We replace a bigger set of all possible C by a smaller set of all C' which reduces the value of denominator.

$$\Rightarrow \langle \chi_b^{(i)} \rangle \leq \frac{\sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})}}{\sum_{\mathcal{C}'} e^{-\beta E(\mathcal{C}')}}$$

$$\Rightarrow \langle \chi_b^{(i)} \rangle \leq \frac{\sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})}}{\sum_{\mathcal{C}'=\mathcal{C}} e^{-\beta E(\mathcal{C})} e^{2\beta Jb}}$$

$$\Rightarrow \underbrace{\langle \chi_b^{(i)} \rangle}_{\text{}} \leq e^{-2\beta Jb}$$

We know that,

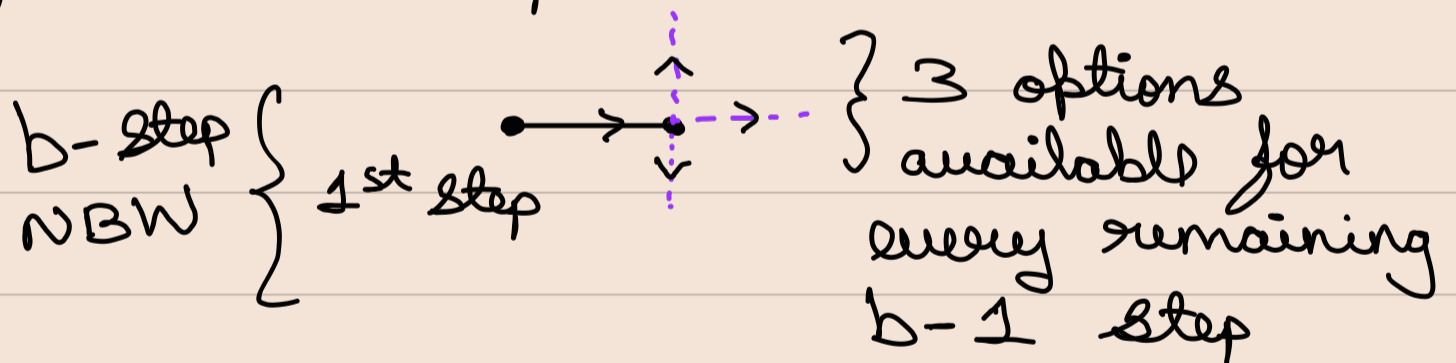
$$N_- \leq \sum_b \left(\frac{b}{4}\right)^2 \sum_{i=1}^{\nu(b)} \chi_b^{(i)}(\mathcal{C})$$

$$\Rightarrow \langle N_- \rangle \leq \sum_b \left(\frac{b}{4}\right)^2 \sum_{i=1}^{\nu(b)} \langle \chi_b^{(i)}(\mathcal{C}) \rangle$$

$$\Rightarrow \langle N_- \rangle \leq \sum_b \left(\frac{b}{4}\right)^2 \sum_{i=1}^{\nu(b)} e^{-2\beta Jb}$$

Now we need to estimate $\nu(b)$ which is the total numbers of borders of size 'b'. But we shall allow an over estimation of $\nu(b)$, by replacing it by the total numbers of possible borders of size 'b'. Thus $\langle N_- \rangle$ will be lesser than the over estimated value (upper limit)

To find this let us consider the non-back tracking walk (NBW) where the random walk to the immediate previous step is not allowed.



Thus there are 3^{b-1} total allowed options of such a walk of b -steps. And the maximum no. of allowed borders of length 'b' is less than the number of sites 'N'.

$\Rightarrow$ The upper bound for $\nu(b)$ is given by $N3^{b-1}$. Thus we shall replace $\nu(b)$ by $N3^{b-1}$ & allow borders that can't exist, but $\langle N_- \rangle$ is always less than the over estimated value.

$$\Rightarrow \langle N_- \rangle \leq \sum_b \left(\frac{b}{4}\right)^2 \sum_{i=1}^{\nu(b)} e^{-2\beta J b}$$

$$\Rightarrow \langle N_- \rangle \leq \sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta J b} \nu(b)$$

$$\Rightarrow \langle N_- \rangle \leq \sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta J b} N 3^{b-1}$$

$$\Rightarrow \frac{\langle N_- \rangle}{N} \leq \sum_b \left(\frac{b}{4}\right)^2 3^{b-1} e^{-2\beta J b}$$

$$\frac{\langle N_- \rangle}{N} \leq \frac{1}{48} \sum_{b=\{4,6,8,\dots\}} b^2 \left[3e^{-2\beta J} \right]^b$$

$$\text{Let } x = 3e^{-2\beta J}$$

$$\Rightarrow \frac{\langle N_- \rangle}{N} \leq \frac{1}{48} \sum_{b=\{4,6,8,\dots\}} b^2 x^b$$

$$\text{Put } b=2m \text{ \& } m=2,3,4,\dots$$

$$\Rightarrow \frac{\langle N_- \rangle}{N} \leq \frac{1}{48} \sum_{m=\{2,3,4,\dots\}} 4m^2 x^{2m}$$

$$\sum_{m=1}^{\infty} m^2 (x^2)^m = \frac{x^2 (1+x^2)}{(1-x^2)^3}$$

$$\Rightarrow \boxed{\frac{\langle N_- \rangle}{N} \leq \frac{1}{12} \left[\frac{x^2 (1+x^2)}{(1-x^2)^3} - x^2 \right]}$$

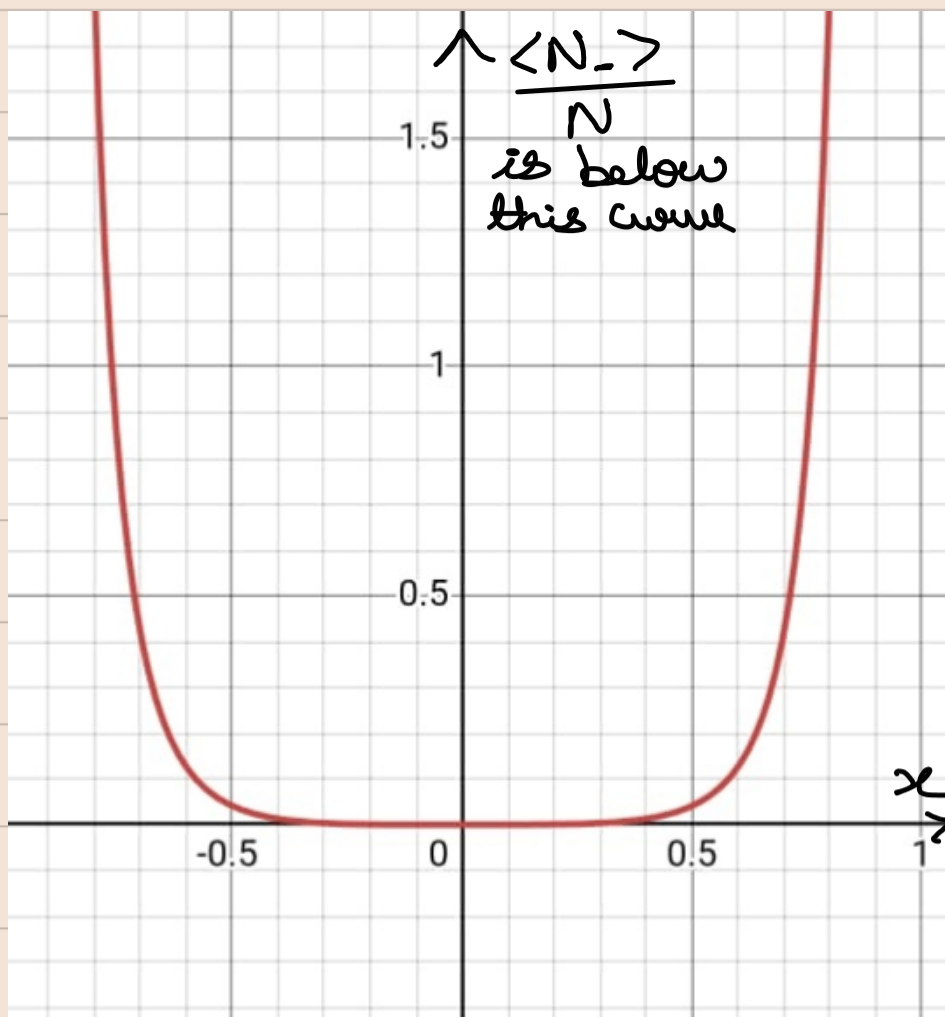
$$\text{where } x = 3e^{-2\beta J}$$

$$\Rightarrow \text{If } T \text{ is such that } x = \frac{1}{2}$$

$$\frac{\langle N_- \rangle}{N} \leq 0.0409$$

$$\Rightarrow 3e^{-2\beta J} = \frac{1}{2} \Rightarrow \beta J = \frac{1}{2} \log(6)$$

$$\Rightarrow T = \frac{2J}{k_B \log(6)} > 0. \quad \beta = \frac{\log(6)}{2J}$$



If $x < 0.71369 = x^*$, then $\frac{\langle N_- \rangle}{N}$ is lesser than 0.5.

$$\Rightarrow 3e^{-2\beta^*J} = x^* \Rightarrow e^{-2\beta^*J} = \frac{x^*}{3}$$

$$\Rightarrow -2\beta^*J = \log\left(\frac{x^*}{3}\right) \Rightarrow \beta^* = \frac{1}{2J} \log\left(\frac{3}{x^*}\right)$$

$$\Rightarrow T^* = \frac{2J}{k_B \log\left(\frac{3}{x^*}\right)}$$

For $J=1$, $k_B T^* \sim 1.392$, But Onsager found by his exact solution that $k_B T^* \sim 2.25$ for $J=1$.

Thus if T is sufficiently small i.e. $T < T^*$, then $\frac{\langle N_- \rangle}{N} < \frac{1}{2}$.

$$\text{Since } \langle N_+ \rangle + \langle N_- \rangle = N$$

$$\Rightarrow \langle N_+ \rangle - \langle N_- \rangle = N - 2\langle N_- \rangle$$

$$\Rightarrow \underbrace{\frac{\langle N_+ \rangle - \langle N_- \rangle}{N}}_{m_0} = 1 - 2\left(\frac{\langle N_- \rangle}{N}\right)$$

$$\Rightarrow m_0 = 1 - 2\frac{\langle N_- \rangle}{N}$$

Thus if $T < T^*$, then, $\frac{\langle N_- \rangle}{N} < \frac{1}{2}$

$$\Rightarrow 2\frac{\langle N_- \rangle}{N} < 1 \Rightarrow 1 - 2\frac{\langle N_- \rangle}{N} > 0$$

$$\Rightarrow \underline{m_0 > 0}$$

Hence there can be non-zero m_0 at a non-zero but low enough temperature in 2D Ising model with only short range interaction where only nearby interaction is allowed.