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Lecture 7

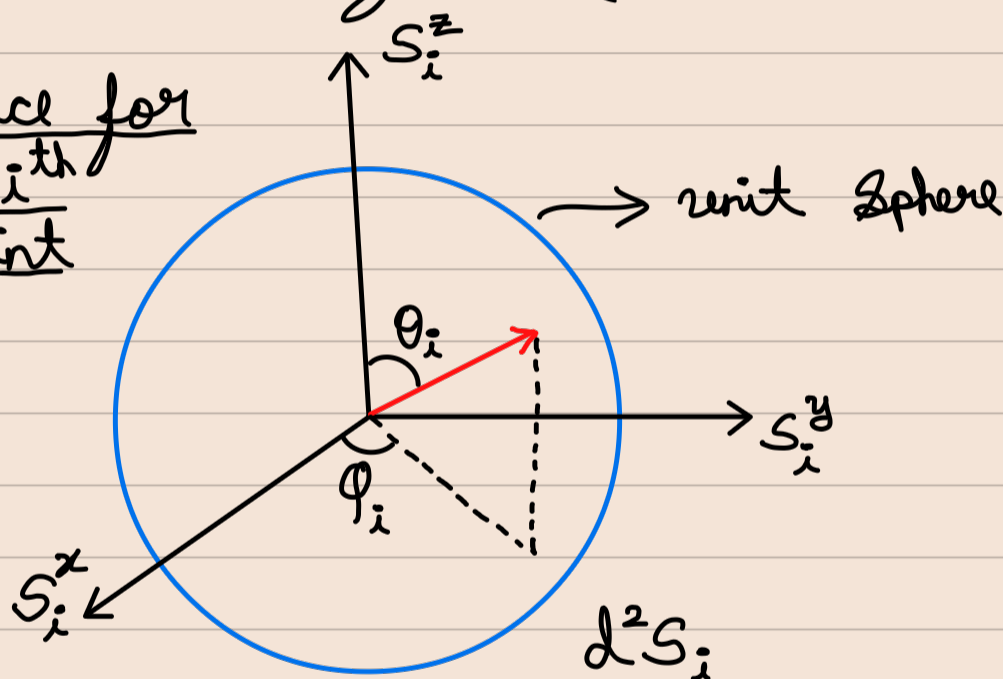
1D Classical Heisenberg Spins (Continuous Spins)

→ Spins are unit vectors $\Rightarrow |\vec{S}_i| = 1$

→ Periodic boundary condition

→ No external field (h)

Spin space for
spin at i^{th}
lattice point



$d^2 S_i = \sin(\theta_i) d\theta_i d\phi_i \Rightarrow$ area element for the surface of unit sphere
($d^2 S_i = d\Omega_i \Rightarrow$ solid angle element)

$\hat{S}_i = (\theta_i, \phi_i) \Rightarrow$ in 3D polar coordinates

$$\hat{S}_i = (\sin(\theta_i) \cos(\phi_i), \sin(\theta_i) \sin(\phi_i), \cos(\theta_i))$$

in 3D cartesian coordinates
→ It is not operator, it means unit vector.

The hamiltonian is given by,

$$\mathcal{H} = -J \sum_i \hat{S}_i \cdot \hat{S}_{i+1}$$

$\mathcal{Z} = \text{Trace}[e^{-\beta \mathcal{H}}]$, in the continuous spin limit, the summation over all possible spin orientation is written as integration.

$$\Rightarrow \mathcal{Z} = \int \frac{d^{2N} S_i}{(4\pi)^N} e^{K \hat{S}_1 \cdot \hat{S}_2} e^{K \hat{S}_2 \cdot \hat{S}_3} \dots e^{K \hat{S}_N \cdot \hat{S}_1}$$
$$\Rightarrow \mathcal{Z} = \int \dots \int_{D_1 D_2 \dots D_N} \prod_{i=1}^N \left[\left(\frac{d^2 S_i}{4\pi} \right) e^{K \hat{S}_i \cdot \hat{S}_{i+1}} \right] \quad (K = \beta J)$$

$D_i \Rightarrow$ domain of $\hat{S}_i$ which is the unit spin surface

$$\text{Let, } e^{K \hat{S}_i \cdot \hat{S}_{i+1}} = T(\hat{S}_i, \hat{S}_{i+1})$$

$T \Rightarrow$ infinite dimensional transfer matrix.

Let $\psi_k(\hat{S}_i)$ be the eigen function of 'T' matrix. Thus $\{\psi_k\}$ forms a complete orthonormal basis set.

$$\Rightarrow \int \frac{d^2 S_i}{4\pi} \psi_k^*(\hat{S}_i) \psi_{k'}(\hat{S}_i) = \delta_{kk'}$$

T can be written as an outer product:

$$T(\hat{S}_i, \hat{S}_{i+1}) = \sum_k \lambda_k \psi_k^*(\hat{S}_i) \psi_k(\hat{S}_{i+1})$$

$$\Rightarrow \int \frac{d^2 S_i}{4\pi} T(\hat{S}_{i+1}, \hat{S}_i) \psi_{k'}(\hat{S}_i)$$

$$= \int \frac{d^2 S_i}{4\pi} \left[\sum_k \lambda_k \psi_k^*(\hat{S}_i) \psi_k(\hat{S}_{i+1}) \right] \psi_{k'}(\hat{S}_i)$$

$$= \sum_k \lambda_k \psi_k(\hat{S}_{i+1}) \underbrace{\int \frac{d^2 S_i}{4\pi} \psi_k^*(\hat{S}_i) \psi_{k'}(\hat{S}_i)}_{\delta_{kk'}}$$

$$= \sum_k \lambda_k \psi_k(\hat{S}_{i+1}) \delta_{kk'} = \lambda_{k'} \psi_{k'}(\hat{S}_{i+1})$$

Thus the eigen value eqⁿ for ' T ' can be written as,

$$\int \frac{d^2 S_i}{4\pi} T(\hat{S}_i, \hat{S}_{i+1}) \psi_k(\hat{S}_i) = \lambda_k \psi_k(\hat{S}_{i+1})$$

Now

$$T(\hat{S}_1, \hat{S}_2) = e^{K \hat{S}_1 \cdot \hat{S}_2}$$

Let θ_{12} be the angle b/w $\hat{S}_1$ & $\hat{S}_2$

$$\Rightarrow T(\hat{S}_1, \hat{S}_2) = e^{K \cos(\theta_{12})}$$

Since $-1 \leq \cos(\theta_{12}) \leq +1$, we can expand

$e^{K \cos(\theta_{12})}$ in terms of Legendre polynomials of $\cos(\theta_{12})$, ' $P_l[\cos(\theta_{12})]$ ' as they form a complete set of orthogonal basis for any smooth function of $\cos(\theta_{12})$.

$$\Rightarrow e^{K \cos(\theta_{12})} = \sum_l a_l P_l[\cos(\theta_{12})]$$

To get ' a_l ' we will use the orthogonality of Legendre polynomials,

$$\int_0^\pi d\theta \sin(\theta) P_l[\cos(\theta)] P_{l'}[\cos(\theta)] = \frac{2 \delta_{ll'}}{2l+1}$$

$$\Rightarrow \int_0^\pi d\theta_{12} \sin(\theta_{12}) P_l[\cos(\theta_{12})] e^{K \cos(\theta_{12})}$$

$$= \sum_{l'} a_{l'} \int_0^\pi d\theta_{12} \sin(\theta_{12}) P_{l'}[\cos(\theta_{12})] P_l[\cos(\theta_{12})]$$

$$= \sum_{l'} a_{l'} \frac{2 \delta_{ll'}}{2l+1} = \frac{2a_l}{2l+1}$$

$$\Rightarrow a_l = \frac{2l+1}{2} \int_0^\pi d\theta_{12} \sin(\theta_{12}) e^{K \cos(\theta_{12})} P_l[\cos(\theta_{12})]$$

Let $u = \cos(\theta_{12})$

$$\Rightarrow a_l = \frac{2l+1}{2} \int_{-1}^{+1} du e^{Ku} P_l(u)$$

$$\bullet a_0 = \frac{1}{2} \int_{-1}^{+1} du e^{Ku} \quad (P_0(u) = 1)$$

$$\Rightarrow a_0 = \frac{\sinh(K)}{K}$$

$$\bullet a_1 = \frac{3}{2} \int_{-1}^{+1} du e^{Ku} u = 3 \frac{\partial a_0}{\partial K} \quad [P_1(u) = u]$$

$$\Rightarrow a_1 = 3 \left[\frac{\cosh(K)}{K} - \frac{\sinh(K)}{K^2} \right]$$

$$\begin{aligned}
 \bullet a_2 &= \frac{5}{2} \int_{-1}^{+1} dz e^{kz} \left(\frac{3z^2 - 1}{2} \right) \\
 &= \frac{15}{4} \int_{-1}^{+1} dz e^{kz} z^2 - \frac{5}{4} \int_{-1}^{+1} e^{kz} dz \\
 &= \frac{15}{2} \frac{\partial^2 a_0}{\partial k^2} - \frac{5}{2} a_0
 \end{aligned}$$

$$\begin{aligned}
 a_2 &= \frac{15}{2} \left[\frac{\sinh(k)}{k} - 2 \frac{\cosh(k)}{k^2} + 2 \frac{\sinh(k)}{k^3} \right] \\
 &\quad - \frac{5}{2} \left(\frac{\sinh(k)}{k} \right)
 \end{aligned}$$

$$a_2 = 15 \left[\frac{\sinh(k)}{k^3} - \frac{\cosh(k)}{k^2} + \frac{1}{3} \frac{\sinh(k)}{k} \right]$$

This way we can get all a_ℓ .

$$\text{For } e^{k \hat{S}_1 \cdot \hat{S}_2} = \sum_{\ell} a_{\ell} P_{\ell}[\hat{S}_1 \cdot \hat{S}_2]$$

we will use the spherical harmonics addition theorem,

$$P_{\ell}(\hat{S}_1 \cdot \hat{S}_2) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{+\ell} Y_{\ell m}^*(\hat{S}_1) Y_{\ell m}(\hat{S}_2)$$

$$\Rightarrow e^{K \hat{S}_1 \cdot \hat{S}_2} = \sum_{l=0}^{\infty} \frac{4\pi a_l}{2l+1} \sum_{m=-l}^l \gamma_{lm}^*(\hat{S}_1) \gamma_{lm}(\hat{S}_2)$$

$$e^{K \hat{S}_1 \cdot \hat{S}_2} = \sum_{l,m} \left[\frac{4\pi a_l}{2l+1} \right] \gamma_{lm}^*(\hat{S}_1) \gamma_{lm}(\hat{S}_2)$$

This looks exactly like the expansion of $T(\hat{S}_1, \hat{S}_2)$ where

$$T(\hat{S}_1 \cdot \hat{S}_2) = \sum_{\mathbf{k}} \lambda_{\mathbf{k}} \psi_{\mathbf{k}}^*(\hat{S}_1) \psi_{\mathbf{k}}(\hat{S}_2)$$

But we cannot just compare the terms directly to get $\lambda_{\mathbf{k}} \neq \psi_{\mathbf{k}}$.

This result should also be consistent with the eigen value eqⁿ for 'T'.

Consider the orthonormality of $\gamma_{lm}(\theta, \phi)$

$$\int_0^{\pi} d\theta \sin(\theta) \int_0^{2\pi} d\phi \gamma_{lm}^*(\theta, \phi) \gamma_{l'm'}(\theta, \phi) = \delta_{ll'} \delta_{mm'}$$

$$\Rightarrow \int \frac{d^2 S_i}{4\pi} \gamma_{lm}^*(\hat{S}_i) \gamma_{l'm'}(\hat{S}_i) = \frac{\delta_{ll'} \delta_{mm'}}{4\pi}$$

We use this orthogonality property to get eigen value eqⁿ for 'T'!

For $T(\hat{S}_1, \hat{S}_2) = e^{K\hat{S}_1 \cdot \hat{S}_2}$ we can write,

$$\int \frac{d^2 S_1}{4\pi} e^{K\hat{S}_1 \cdot \hat{S}_2} \gamma_{l'm'}(\hat{S}_1)$$

$$= \int \frac{d^2 S_1}{4\pi} \gamma_{l'm'}(\hat{S}_1) \sum_{l,m} \left[\frac{4\pi a_l}{2l+1} \right] \gamma_{lm}^*(\hat{S}_1) \gamma_{lm}(\hat{S}_2)$$

$$= \sum_{l,m} \frac{4\pi a_l}{2l+1} \gamma_{lm}(\hat{S}_2) \int \frac{d^2 S_1}{4\pi} \gamma_{lm}^*(\hat{S}_1) \gamma_{l'm'}(\hat{S}_1)$$

$$= \sum_{l,m} \frac{4\pi a_l}{2l+1} \gamma_{lm}(\hat{S}_2) \frac{\delta_{ll'} \delta_{mm'}}{4\pi} = \frac{a_{l'}}{2l'+1} \gamma_{l'm'}(\hat{S}_2)$$

$$\Rightarrow \int \frac{d^2 S_1}{4\pi} e^{K\hat{S}_1 \cdot \hat{S}_2} \gamma_{lm}(\hat{S}_1) = \frac{a_l}{2l+1} \gamma_{lm}(\hat{S}_2)$$

All these results can be written properly as,

$$\int \frac{d^2 S_i}{4\pi} \left[2\sqrt{\pi} \gamma_{lm}^*(\hat{S}_i) \right] \left[2\sqrt{\pi} \gamma_{l'm'}(\hat{S}_i) \right] = \delta_{ll'} \delta_{mm'}$$

$$e^{K\hat{S}_1 \cdot \hat{S}_2} = \sum_{l,m} \left[\frac{a_l}{2l+1} \right] \left[2\sqrt{\pi} \gamma_{lm}^*(\hat{S}_1) \right] \left[2\sqrt{\pi} \gamma_{lm}(\hat{S}_2) \right]$$

$$\int \frac{d^2 S_1}{4\pi} e^{K\hat{S}_1 \cdot \hat{S}_2} \left[2\sqrt{\pi} \gamma_{lm}(\hat{S}_1) \right] = \frac{a_l}{2l+1} \left[2\sqrt{\pi} \gamma_{lm}(\hat{S}_2) \right]$$

Thus we can identify the eigen functions of $T(\hat{S}_1, \hat{S}_2)$ as $\psi_l = 2\sqrt{\pi} Y_{l,m}$ and eigen values as $\lambda_l \equiv \frac{a_l}{2l+1}$.

Under the inner product defined as

$$\int \frac{d^2 \hat{S}_i}{4\pi} \psi_l^*(\hat{S}_i) \psi_l(\hat{S}_i) = \delta_{ll'}$$

Note that the eigen functions ψ_l are $2l+1$ fold degenerate.

Now the partition function can be calculated in terms of eigen values.

$$\begin{aligned} \Rightarrow Z &= \int \int \dots \int_{D_1 D_2 D_N} \prod_{i=1}^N \left[\left(\frac{d^2 S_i}{4\pi} \right) e^{K \hat{S}_i \cdot \hat{S}_{i+1}} \right] \\ &= \int \prod_{i=1}^N \left[\left(\frac{d^2 S_i}{4\pi} \right) \sum_{l_i, m_i} \lambda_{n_i} \psi_{n_i}^*(\hat{S}_i) \psi_{n_i}(\hat{S}_{i+1}) \right] \\ &= \int \frac{d^2 S_1}{4\pi} \sum_{l_1, m_1} \lambda_{l_1} \psi_{l_1}^*(\hat{S}_1) \psi_{l_1}(\hat{S}_2) \int \frac{d^2 S_2}{4\pi} \sum_{l_2, m_2} \lambda_{l_2} \psi_{l_2}^*(\hat{S}_2) \psi_{l_2}(\hat{S}_3) \\ &\quad \times \dots \int \frac{d^2 S_N}{4\pi} \sum_{l_N, m_N} \lambda_{l_N} \psi_{l_N}^*(\hat{S}_N) \psi_{l_N}(\hat{S}_1) \end{aligned}$$

$$= \sum_{\{\ell_i, m_i\}} \lambda_{\ell_1} \lambda_{\ell_2} \dots \lambda_{\ell_N} \int \frac{d^2 S_1}{4\pi} \psi_{\ell_1}^*(\hat{S}_1) \int \frac{d^2 S_2}{4\pi} \psi_{\ell_1}(\hat{S}_2) \psi_{\ell_2}^*(\hat{S}_2) \\ \times \int \frac{d^2 S_3}{4\pi} \psi_{\ell_2}(\hat{S}_3) \psi_{\ell_3}(\hat{S}_3) \dots \int \frac{d^2 S_N}{4\pi} \psi_{\ell_{N-1}}(\hat{S}_N) \psi_{\ell_N}^*(\hat{S}_N) \times \psi_{\ell_1}(\hat{S}_1)$$

we can use orthonormality of $\{\psi\}$ & simplify it to

$$\mathcal{Z} = \sum_{\{\ell_i\}} \lambda_{\ell_1} \lambda_{\ell_2} \dots \lambda_{\ell_N} \int \frac{d^2 S_1}{4\pi} \psi_{\ell_1}^*(\hat{S}_1) \delta_{\ell_1 \ell_2} \delta_{\ell_2 \ell_3} \\ \times \dots \times \delta_{\ell_{N-1} \ell_N} \psi_{\ell_N}(\hat{S}_1)$$

$$\Rightarrow \mathcal{Z} = \sum_{\ell_1, \ell_N} (\lambda_{\ell_1})^{N-1} \lambda_N \underbrace{\int \frac{d^2 S_1}{4\pi} \psi_{\ell_1}^*(\hat{S}_1) \psi_{\ell_N}(\hat{S}_1)}_{\delta_{\ell_1 \ell_N}}$$

$$\Rightarrow \mathcal{Z} = \sum_{\ell_1} (\lambda_{\ell_1})^N \Rightarrow \boxed{\mathcal{Z} = \sum_{\ell} (\lambda_{\ell})^N}$$

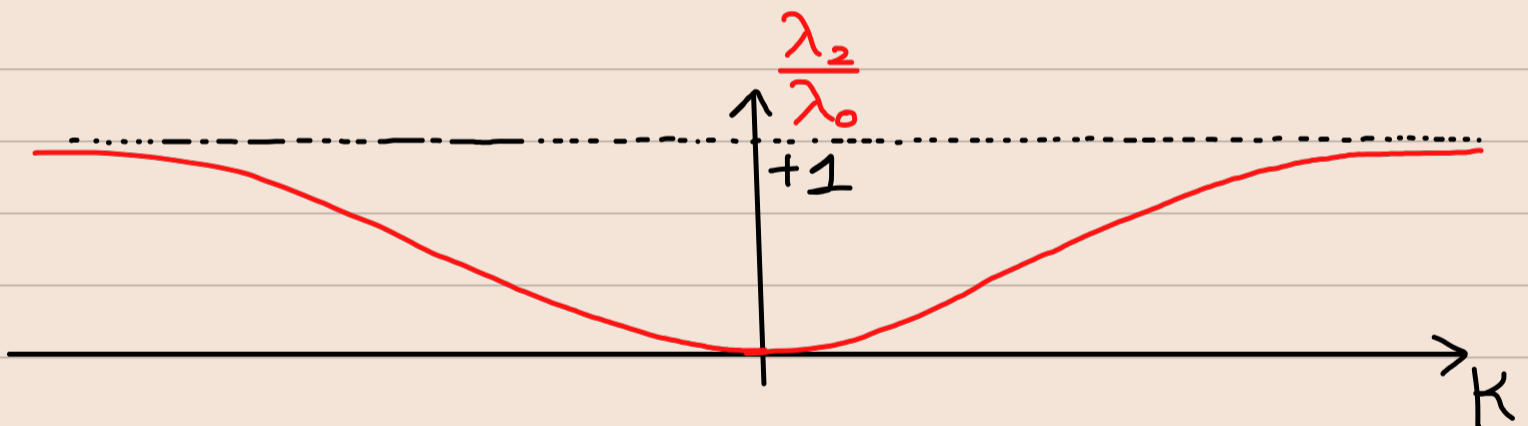
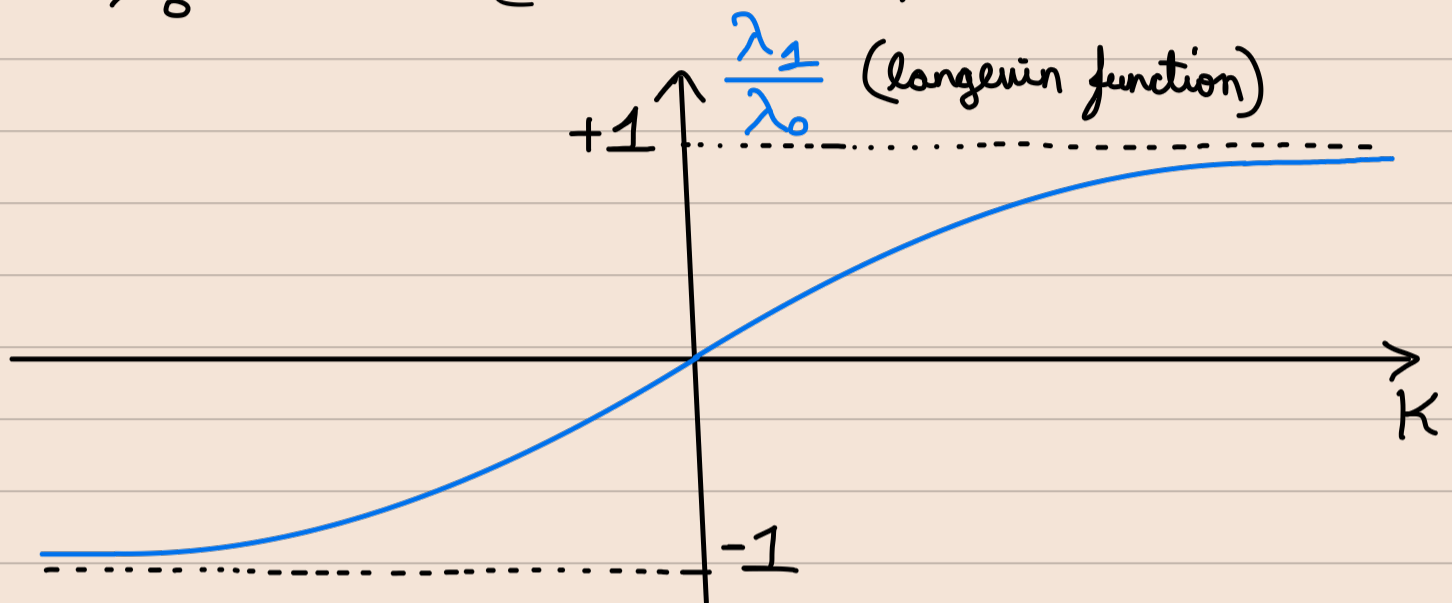
$$\lambda_0 = \frac{a_0}{2(0)+1} = \frac{\sinh(K)}{K}$$

$$\lambda_1 = \frac{a_1}{3} = \left[\frac{\cosh(K)}{K} - \frac{\sinh(K)}{K^2} \right]$$

$$\lambda_2 = \frac{a_2}{5} = 3 \left[\frac{\sinh(K)}{K^3} - \frac{\cosh(K)}{K^2} \right] + \frac{\sinh(K)}{K}$$

$$\frac{\lambda_1}{\lambda_0} = \coth(k) - \frac{1}{k} = \mathcal{L}(k) \quad (\text{Langevin Function})$$

$$\frac{\lambda_2}{\lambda_0} = 3 \left[\frac{1}{k^2} - \frac{\coth(k)}{k} \right] + 1$$



We can observe that $\lambda_0 > \lambda_l$ ($l \neq 0$)
 thus in thermodynamic limit ($N \rightarrow \infty$)

$$\mathcal{Z} = \lambda_0^N \left[1 + \sum_{l \neq 0} \underbrace{\left(\frac{\lambda_l}{\lambda_0} \right)^N}_{\text{tends to zero}} \right]$$

$$\Rightarrow \underline{Z \approx \lambda_0^N}$$

Thus in thermodynamic limit the partition function is given as,

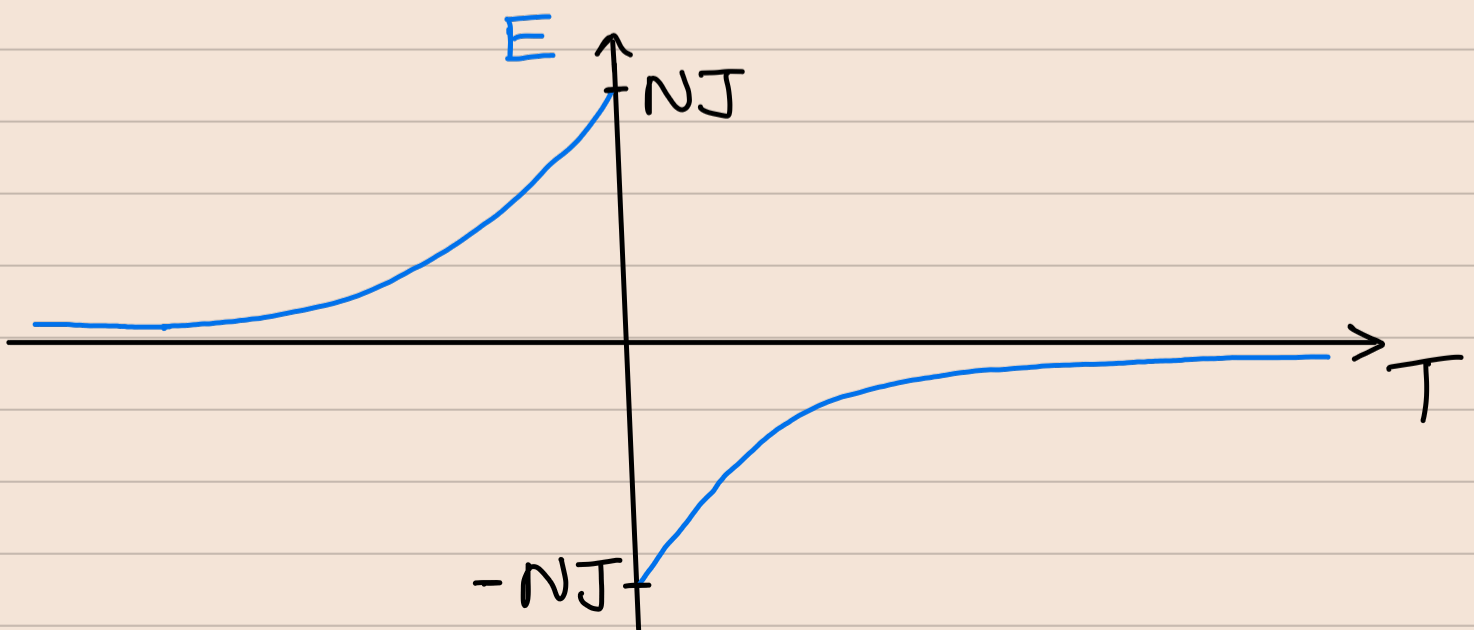
$$Z = \left[\frac{\sinh(\beta J)}{\beta J} \right]^N$$

$$E = - \frac{\partial}{\partial \beta} \ln(Z) = - \frac{\partial}{\partial \beta} \left(N \ln \left[\frac{\sinh(\beta J)}{\beta J} \right] \right)$$

$$E = -NJ \frac{\partial}{\partial K} \left(\ln \left[\frac{\sinh(K)}{K} \right] \right)$$

$$= -NJ \left(\frac{\cosh(K)}{\sinh(K)} - \frac{1}{K} \right)$$

$$E = -NJ \left[\coth(\beta J) - \frac{1}{\beta J} \right]$$

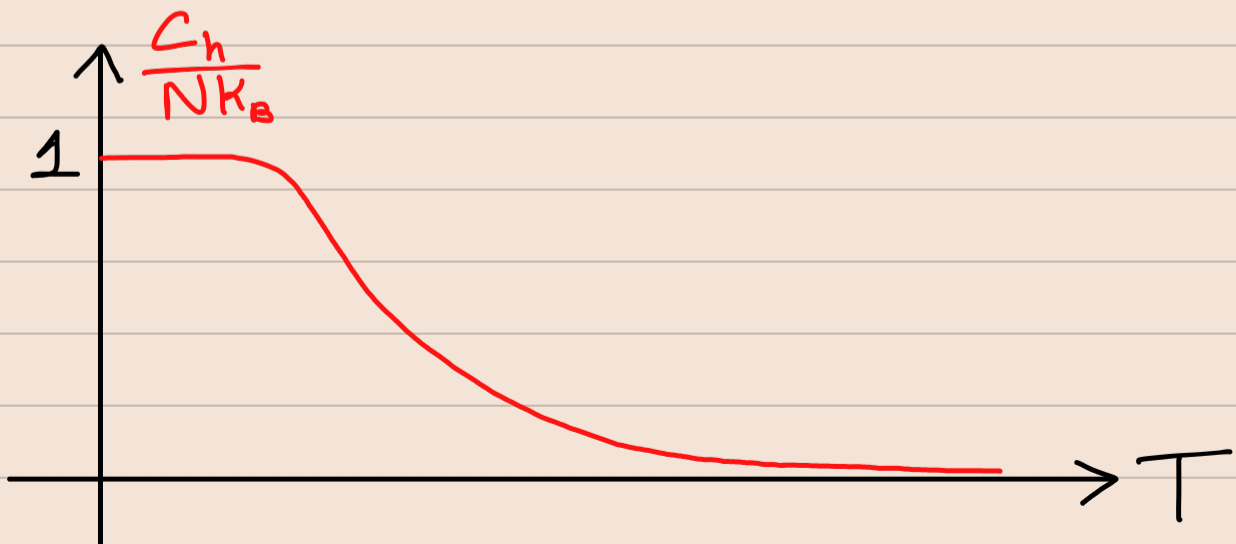


$$\begin{aligned}
C_h &= \left(\frac{\partial E}{\partial T} \right)_h = \left(\frac{\partial \beta}{\partial T} \right) \left(\frac{\partial E}{\partial \beta} \right)_h = \frac{-1}{k_B T^2} \frac{\partial E}{\partial \beta} \\
&= -k_B \beta^2 \frac{\partial}{\partial \beta} \left(-\frac{\partial \ln(Z)}{\partial \beta} \right) \\
&= k_B k^2 \left[\frac{\partial^2 \ln(\lambda_o^N)}{\partial k^2} \right] \\
&= N k_B \left(k^2 \frac{\partial^2 \ln(k)}{\partial k^2} \right)
\end{aligned}$$

$$\Rightarrow \boxed{\frac{C_h}{N k_B} = k^2 \frac{\partial^2 \ln(\lambda_o)}{\partial k^2}}$$

$$\frac{C_h}{N k_B} = k^2 \frac{\partial}{\partial k} \left(\coth(k) - \frac{1}{k} \right) = k^2 \left[-\operatorname{cosech}^2(k) + \frac{1}{k^2} \right]$$

$$\boxed{\frac{C_h}{N k_B} = 1 - (\beta J)^2 \operatorname{cosech}^2(\beta J)}$$



This model violates 3rd law of Thermodynamics

Correlation function for Classical Continuous Heisenberg Spins

$$\begin{aligned}\langle S_i^z S_{i+\gamma}^z \rangle &= \langle \gamma_{l_0}(\hat{S}_i) \gamma_{l_0}(\hat{S}_{i+\gamma}) \rangle \\&= \int \prod_{j=1}^N \frac{d^2 S_j}{4\pi} \gamma_{l_0}(\hat{S}_i) \gamma_{l_0}(\hat{S}_{i+\gamma}) T(\hat{S}_j, \hat{S}_{j+1}) \\&= \int \prod_{j=1}^N \left(\frac{d^2 S_j}{4\pi} \right) \gamma_{l_0}(\hat{S}_i) \gamma_{l_0}(\hat{S}_{i+\gamma}) \sum_{l_j} \lambda_{l_j} \psi(\hat{S}_j) \psi(\hat{S}_{j+1})\end{aligned}$$

After very complicated steps
we arrive at,

$$\langle S_i^z S_{i+\gamma}^z \rangle = \left(\frac{\lambda_1}{\lambda_0} \right)^\gamma = [L(BJ)]^\gamma$$

(Similar result as in 1D Ising model)

$$\text{where } L(BJ) = \coth(BJ) - \frac{1}{BJ}$$

$|L(BJ)| < 1$ for all finite value of BJ

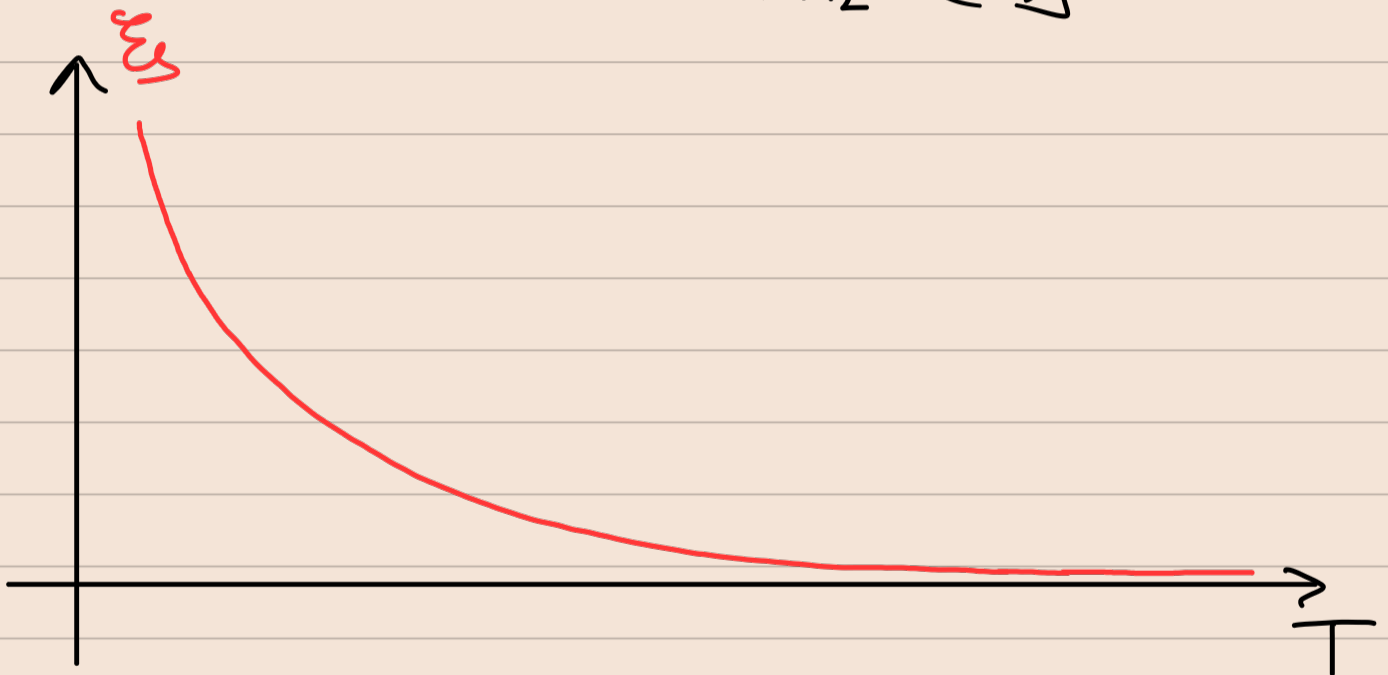
Thus $[L(BJ)]^\gamma$ decays exponentially
with γ .

$$\langle S_i^z S_{i+r}^z \rangle = [\mathcal{L}(\beta J)]^r = e^{\ln[\mathcal{L}(\beta J)]r}$$

$$= \exp \left[\frac{-r}{\left(\frac{-1}{\ln[\mathcal{L}(\beta J)]} \right)} \right] = \underline{\underline{e^{-r/\xi_g}}}$$

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

where $\xi_g = \frac{-1}{\ln[\mathcal{L}(\beta J)]}$



As $T \rightarrow 0$, the correlation length tends to infinity. Thus all spins align in same directions. Hence $T=0$ acts as the critical temperature.

The lowest energy state possible at $T=0$ is all spins pointing along same direction conventionally chosen to be z -direction.

The system goes to slightly higher energy when any one of the spins slightly deviate, by any non-zero infinitesimal angle.

Thus the excitation energy at $T=0$ for continuous spins is very small.

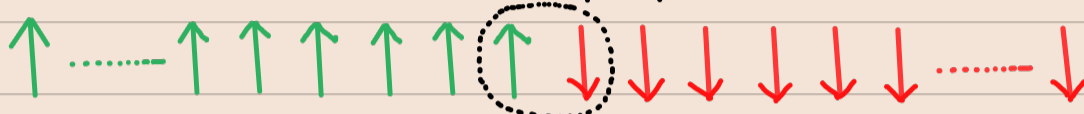
That is why the heat capacity of continuous classical Heisenberg spins even at $T=0$ is non-zero.

$$\underline{\underline{\lim_{T \rightarrow 0} C_h = N K_B}}}$$

Excitations of Ising model at $T=0$

At $T=0$, all the spins align together & $H_{\text{ising}} = -NJ$ at $T=0$

Ground State $\Leftarrow$ 

1st excited State $\Leftarrow$ 
 (non-periodic boundary) excitation energy = $2J$

The bloch wall can be in any position, with all degenerate energy. So, the 1st excited state is $N-1$ degenerate.

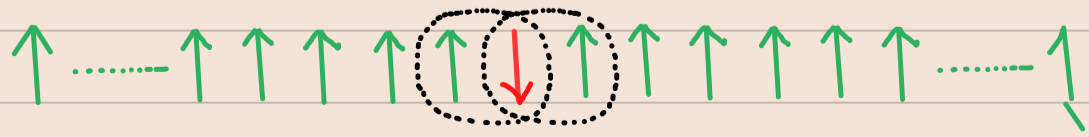
In thermodynamic limit, the degeneracy is approx. N .

$\Rightarrow$ entropy, $\underline{S_{1st\ ex.} \sim \ln(N)}$

The free energy is given by,

$$\underline{F_{1\ ex.} = E_{1\ ex.} - TS_{1\ ex.} \sim 2J - T \ln(N)}$$

Thus as $N \rightarrow \infty$, with $T \neq 0$, the free energy reduces, thus removing the ferromagnetic order.

2nd excited State $\Leftarrow$ 
 excitation energy = $4J$

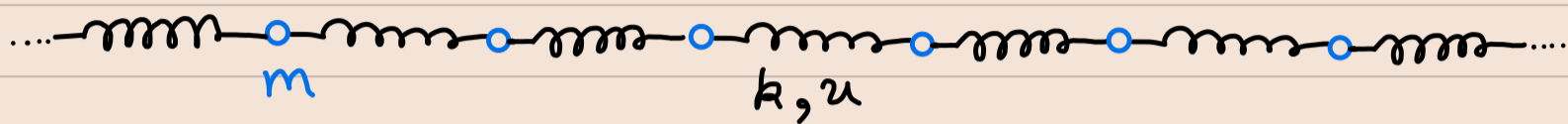
Note: The Ising hamiltonian has spin reversal symmetry i.e. when all spins are flipped, the hamiltonian remains invariant. But at $T=0$, in the ground state, all the spins orient to one particular direction. Thus the ground state has no spin reversal symmetry.

Thus when the hamiltonian has a particular symmetry & if the ground state doesn't obey that, it is called spontaneous symmetry breaking.

(Spin reversal = time reversal symmetry since the time reversal transformation of spin is just flipping of its sign.)

Anharmonic Oscillators

$$H = \sum_i \left[\frac{p_i^2}{2m} + \overbrace{\frac{k}{2} (x_{i+1} - x_i)^2 + \mathcal{U} (x_{i+1} - x_i)^4}^{V(x)} \right]$$



Here we consider a series of oscillators in a 1D chain. x_i 's are displacement of i^{th} oscillator from its mean position.

$k \Rightarrow$ Spring Constant, $u \Rightarrow$ Anharmonicity

$p_i \Rightarrow$ Momentum of i^{th} oscillator

$m \Rightarrow$ mass of oscillators

The canonical partition function is

$$Q = \frac{1}{N!} \int \frac{dp_1 dp_2 \dots dp_N dx_1 dx_2 \dots dx_N}{h^N} e^{-\beta H}$$

$$Q = \frac{1}{N!} \int \frac{d^N p d^N x}{h^N} e^{-\beta \sum_i \frac{p_i^2}{2m}} e^{-\beta V(x)}$$

$$Q = \frac{1}{N! h^N} \underbrace{\left[\int_{-\infty}^{\infty} dp e^{-\beta \frac{p^2}{2m}} \right]^N}_{\text{Gaussian integral}} \int d^N x e^{-\beta V(x)}$$

$$\int_{-\infty}^{\infty} dp e^{-\frac{p^2}{2mk_B T}} = \sqrt{2m\pi k_B T}$$

$$\Rightarrow Q = \frac{1}{N!} \underbrace{\left[\frac{\sqrt{2m\pi k_B T}}{h} \right]^N}_{\frac{1}{\Lambda_{th}^N}} \int d^N x e^{-\beta V(x)}$$

$$\Rightarrow Q = \frac{\int d^N x e^{-\beta V(x)}}{\Lambda_{th}^N N!}$$

$Z_{\text{config}} = \int d^N x e^{-\beta V(x)}$ is called the configurational integral. We can try to solve for Z_{config} by the transfer matrix method.

$$Z_{\text{config.}} = \int \prod_i (dx_i) e^{-\beta \left[\frac{K}{2} \sum_i (x_i - x_{i+1})^2 + \lambda \sum_i (x_i - x_{i+1})^4 \right]}$$

$$= \int \prod_i dx_i e^{-\beta \left[\frac{K}{2} (x_i - x_{i+1})^2 + \lambda (x_i - x_{i+1})^4 \right]}$$

Transfer Matrix $\leftarrow T(x_i, x_{i+1})$

$$\Rightarrow Z_{\text{config.}} = \int \prod_i dx_i T(x_i, x_{i+1})$$

The eigen function for transfer matrix can be found in the following way,

$$\int dx_i T(x_i, x_{i+1}) \psi(x_i) = \lambda \psi(x_{i+1})$$

Since $T(x_i, x_{i+1})$ is a function of $(x_i - x_{i+1})$ we can perform a fourier transform as eigen value eqⁿ of T with $e^{-iq(x_i)}$ as the eigen function.

$$\begin{aligned}
&\Rightarrow \int dx_i T(x_i, x_{i+1}) e^{-iqx_i} \\
&= \int dx_j e^{\left[-\frac{\beta k}{2} (x_j - x_{j+1})^2 - \beta u (x_j - x_{j+1})^4 \right]} e^{-iqx_j} \\
&\quad x_j - x_{j+1} = x \\
&\Rightarrow dx_j = dx
\end{aligned}$$

$$\begin{aligned}
&\Rightarrow \int dx_j T(x_j, x_{j+1}) e^{-iqx_j} \\
&= e^{-iqx_{j+1}} \underbrace{\int dx e^{-\beta \left[\frac{kx^2}{2} + ux^4 \right]}}_{\text{fourier transform of } e^{-\beta \left(\frac{kx^2}{2} + ux^4 \right)}} e^{-iqx} \\
&\quad \text{fourier transform of } e^{-\beta \left(\frac{kx^2}{2} + ux^4 \right)} \\
&\quad \quad \quad 'F(q)'
\end{aligned}$$

$$\Rightarrow \int dx_i T(x_j, x_{j+1}) e^{-iqx_j} = F(q) e^{-iqx_{j+1}}$$

Thus eigen function of $T(x_j, x_{j+1})$ is e^{-iqx_j} with eigen value as $F(q)$ which is fourier transform of $e^{-\beta \left(\frac{kx^2}{2} + ux^4 \right)}$.

$F(q)$ can be found numerically.

Mean Field Theory

Mean field theory is an approximate theory whose main idea is to replace the inter-particle interactions with respect to a particular body by the average effective interaction. This reduces the many-body problem to a self-consistent one body problem.

Note: In mean field approx. many interactions are replaced by one effective interaction, so if there are random interactions in original system, then they cancel out & hence mean field approx will be close to actual solution. This is true in the systems with higher spatial dimensions.

Thus for low dimensions this theory could fail badly & give wrong results.

Mean field Ising Model

Consider the Ising Hamiltonian for nearest neighbour interactions, in the presence of external magnetic field.

$$H_I = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

Here spins are arranged regularly in a d -dimensional lattice, with a total of ' N ' lattice points.

The average magnetization at a particular spin site ' i ' is

$$m = \langle S_i \rangle$$

Due to translational symmetry $\langle S_i \rangle = m$ for all values of ' i '.

Here ' m ' gives the information about the degree of order in the system. It characterizes the phase of the system. Hence ' m ' is called the "Order Parameter" of the system.

The deviation of a variable S_i from its mean value $\langle S_i \rangle$ is δS_i

$$\delta S_i = S_i - \langle S_i \rangle$$

$$\Rightarrow S_i S_j = [\delta S_i + \langle S_i \rangle][\delta S_j + \langle S_j \rangle]$$

$$= (\delta S_i \delta S_j) + \langle S_i \rangle \langle S_j \rangle + \delta S_i \langle S_j \rangle + \delta S_j \langle S_i \rangle$$

$$\Rightarrow S_i S_j = \delta S_i \delta S_j + m^2 + (\delta S_i + \delta S_j)m$$

$$\Rightarrow \mathcal{H} = -J \sum_{\langle i,j \rangle} [\delta S_i \delta S_j + (\delta S_i + \delta S_j)m + m^2]$$

$$- h \sum_i (\delta S_i + m)$$

Here $\delta S_i \neq \delta S_j$ are variables of Hamiltonian. 'm' is mean field parameter. The term $\delta S_i \delta S_j$ is a second order fluctuation term which can be neglected while summing over $\sum_{\langle i,j \rangle}$.

$$\Rightarrow \underbrace{\mathcal{H}}_{\text{M.F.}} = -J \sum_{\langle i,j \rangle} [(\delta S_i + \delta S_j)m + m^2]$$

$$- h \sum_i (\delta S_i + m)$$

mean field approximated hamiltonian

Now substitute back $2S_i = S_i - m$

$$\Rightarrow \mathcal{H}_{M.F.} = -J \sum_{\langle ij \rangle} \left((S_i - m) + (S_j - m) \right) m + m^2 - h \sum_i S_i$$
$$= -J \sum_{\langle ij \rangle} \left[(S_i + S_j) m - m^2 \right] - h \sum_i S_i$$

$$\mathcal{H}_{M.F.} = J \sum_{\langle ij \rangle} m^2 - Jm \sum_{\langle ij \rangle} (S_i + S_j) - h \sum_i S_i$$

Now,

→ to remove double counting

$$\sum_{\langle ij \rangle} = \frac{1}{2} \sum_i \sum_{j \in n(i)}$$

$n(i) = \{ \text{nearest neighbours of } i \}$

$$\sum_{j \in n(i)} 1 = z_i \quad \left(\text{coordination number of a spin in } i^{\text{th}} \text{ site} \right)$$

Coordination number is the number of immediate neighbours for each spin. For a perfect crystal lattice $z_i = z$ for all sites.

$z = 2$ for 1D chain

$z = 4$ for Square lattice

$z = 6$ for Simple cube

$z = 8$ for BCC

$z = 12$ for FCC

etc....

$$\Rightarrow \sum_{\langle ij \rangle} 1 = \frac{1}{2} \sum_i \sum_{j \in n(i)} 1 = \frac{3}{2} \underbrace{\sum_i 1}_N = \frac{N}{2} 3$$

total number of sites in lattice

$$\text{so } \sum_{\langle ij \rangle} m^2 = \frac{m^2 N}{2} 3$$

$$\sum_{\langle ij \rangle} S_i = \frac{1}{2} \sum_i S_i \sum_{j \in n(i)} 1 = \frac{3}{2} \sum_i S_i$$

$\downarrow$ equal

$$\& \sum_{\langle ij \rangle} S_j = \frac{1}{2} \sum_j S_j \sum_{i \in n(j)} 1 = \frac{3}{2} \sum_j S_j$$

$$\Rightarrow \mathcal{H}_{\text{M.F.}} = \frac{J m^2 N}{2} 3 - J m 3 \sum_i S_i - h \sum_i S_i$$

$$= \frac{J m^2 N}{2} 3 - (J m 3 + h) \sum_i S_i$$

denoting $h_{\text{eff}} = h + \underbrace{J m 3}_{\text{average magnetic energy due to interactions}}$

$$\Rightarrow \boxed{\mathcal{H}_{\text{M.F.}} = \frac{J m^2 N}{2} 3 - h_{\text{eff}} \sum_i S_i}$$

Thus we see that the mean field approximation has removed interactions where each spin ' S_i ' resides in a effective field " $h_{\text{eff}} = h + Jmz$ ".

The partition function for the mean field hamiltonian is given by,

$$Z = \sum_{\{S_i\}=\{\pm 1\}} e^{-\beta H_{\text{M.F.}}}$$

$$= \sum_{S_1, S_2, \dots, S_N} e^{-\beta \left[\frac{Jm^2 N z}{2} - h_{\text{eff}} \sum_i S_i \right]}$$

$$= e^{-\beta \frac{Jm^2 N z}{2}} \sum_{S_1, S_2, \dots, S_N} e^{-\beta h_{\text{eff}} (S_1 + S_2 + \dots + S_N)} \quad (S_i = \pm 1, -1)$$

$$= e^{-\beta \frac{Jm^2 N z}{2}} \left(e^{-\beta h_{\text{eff}}} + e^{\beta h_{\text{eff}}} \right)^N$$

$$\Rightarrow \boxed{Z = e^{-\beta \frac{Jm^2 N z}{2}} 2^N \cosh^N(\beta h_{\text{eff}})}$$

Consider,

$$\begin{aligned} M = N m &= \left\langle \sum_j S_j \right\rangle = \frac{\sum_{\{S_i\}} \left(\sum_j S_j \right) e^{-\beta \mathcal{H}}}{\mathcal{Z}} \\ &= \frac{\sum_{\{S_i\}} \left(\sum_j S_j \right) e^{\frac{-\beta J m^2 N_3}{2}} e^{\beta h_{\text{eff}} \sum_i S_i}}{\mathcal{Z}} \\ &= \frac{\sum_{\{S_i\}} \left(\sum_j S_j \right) e^{\frac{-\beta J m^2 N_3}{2}} e^{\beta (h + J m_3) \sum_i S_i}}{\mathcal{Z}} \\ &= \frac{1}{\mathcal{Z}} \left[\frac{\partial}{\partial h} \sum_{\{S_i\}} e^{\frac{-\beta J m^2 N_3}{2}} e^{\beta h_{\text{eff}} \sum_i S_i} \right]_{m, N, \beta} \\ &= \frac{1}{\mathcal{Z}} \left(\frac{\partial \mathcal{Z}}{\partial h} \right)_{m, N, \beta} \\ \Rightarrow M &= \left[\frac{\partial \log(\mathcal{Z})}{\partial h} \right]_{m, N, \beta} = N m \end{aligned}$$

$$\Rightarrow m = \frac{1}{N} \left(\frac{\partial}{\partial h} \log \left[e^{\frac{\beta J m^2 N z}{2}} 2^N \cosh^N(\beta h_{\text{eff}}) \right] \right)_{N, \beta, m}$$

$$m = \frac{1}{N} (N) \frac{\sinh(\beta h_{\text{eff}})}{\cosh(\beta h_{\text{eff}})}$$

$$\Rightarrow m = \tanh(\beta h_{\text{eff}})$$

But $h_{\text{eff}} = h + J m z$

$$\Rightarrow \boxed{m = \tanh[\beta h + \beta J z m]}$$

Thus we got a self consistent eqⁿ for $m(h, \beta)$.

For a simple case of $h=0$ we get:

$$m = \tanh(\beta J z m)$$

we can solve it graphically. We can perform Taylor expansion of $\tanh(\beta J z m)$

$$\tanh(\beta J_3 m) = \beta J_3 m - \frac{(\beta J_3 m)^3}{3} + \dots$$

$$\Rightarrow m = \beta J_3 m - \frac{(\beta J_3 m)^3}{3} + \dots$$

$$\Rightarrow m \left[1 - \beta J_3 + \frac{(\beta J_3)^3}{3} m^2 + O(m^4) \right] = 0$$

$m=0$ is one solⁿ. The other solⁿ is root of

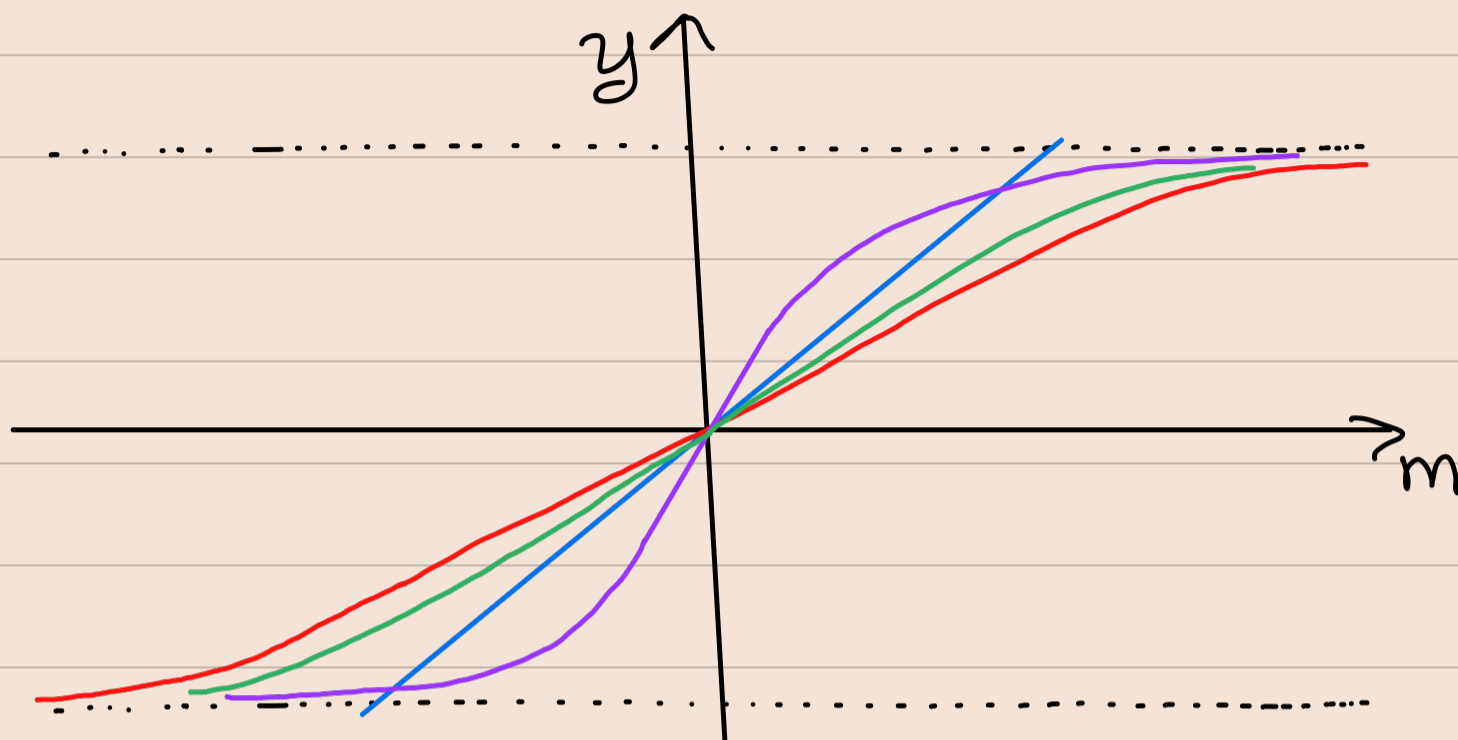
$$1 - \beta J_3 + \frac{(\beta J_3)^3}{3} m^2 = 0$$

$$\Rightarrow m^2 = \frac{3}{(\beta J_3)^3} (\beta J_3 - 1)$$

This solⁿ exists only if $\beta J_3 > 1$

Thus we have three solⁿ for $B > \frac{1}{J_3}$
& only one solⁿ for $B \leq \frac{1}{J_3}$.

$y = m$
 $\left. \begin{array}{l} \text{--- } \beta J_3 < 1 \\ \text{--- } \beta J_3 > 1 \\ \text{--- } \beta J_3 = 1 \end{array} \right\} y = \tanh(\beta J_3 m)$



Thus we can see that in the case of $h = 0$ (zero ext. field), the solution for 'm' depends on ' β '

• $\beta J_3 < 1$ or $T > \frac{J_3}{k_B}$

There is only one solⁿ $m = 0$ this implies that there is no magnetization at these temperatures. Here the entropy associated to random fluctuations will dominate over energetically preferred ordered state where all spins align.

- $\beta J_3 > 1$ or $T < \frac{J_3}{k_B}$

Here there are three solⁿ for magnetization.

One is $m = 0$ &

other is $m = \pm m_s \neq 0$. Thus there can be some non-zero "m" even in the absence of external "h".

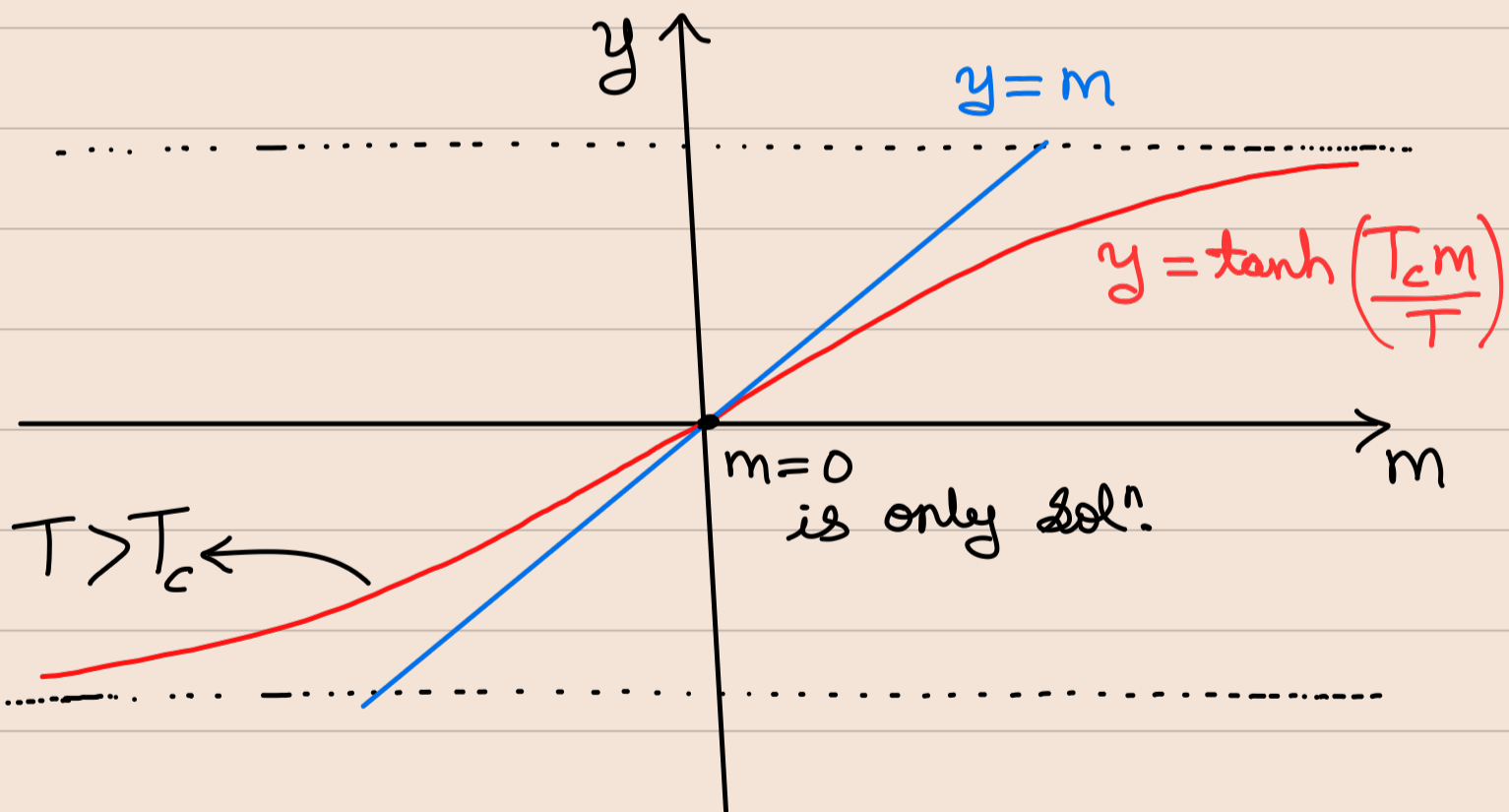
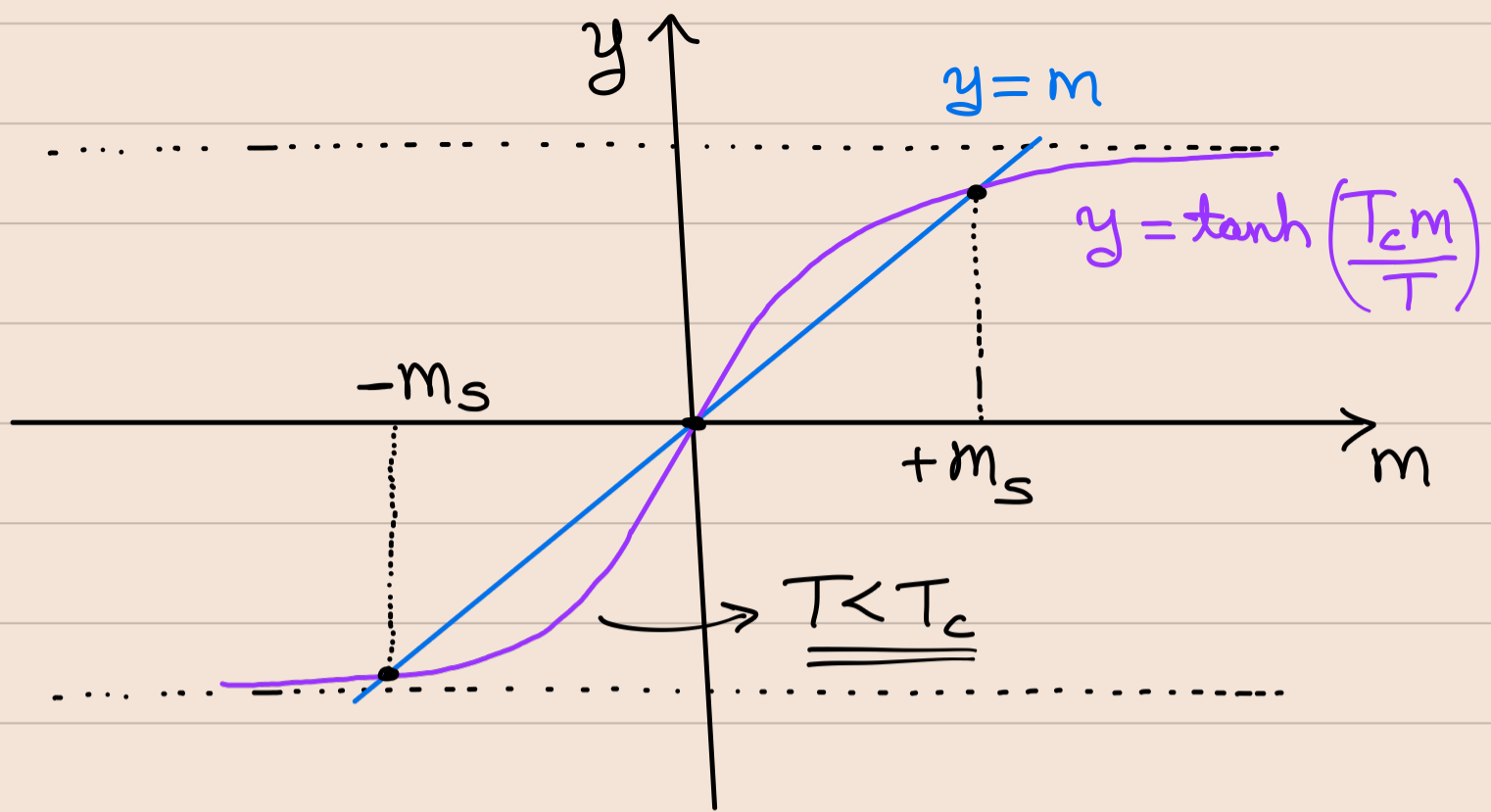
This is called Spontaneous magnetization or ferro-magnetic order which occurs as soon as T reduces below $\frac{J_3}{k_B}$ which acts as a

critical temperature for the system to change phase b/w random paramagnet & ferro-magnetic phase.

$$\Rightarrow T_c = \frac{J_3}{k_B}$$

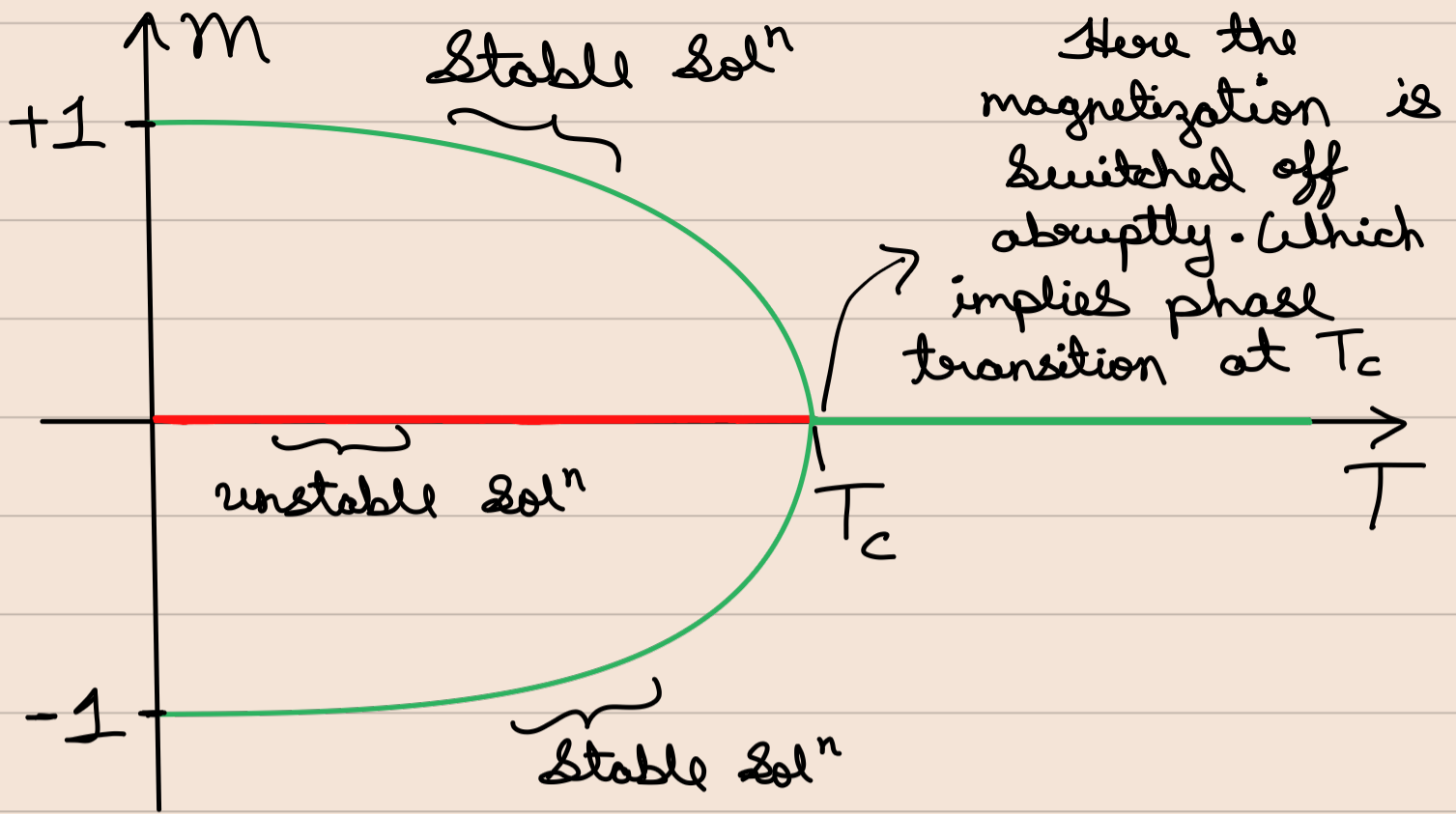
&

$$m = \tanh\left(\frac{T_c}{T} m\right)$$



We can solve for $m = m(T, h=0)$ using

$m = \tanh\left(\frac{T_c}{T} m\right)$ numerically & plot m vs T .



Critical exponent for phase Transitions

$$m = \tanh\left(\frac{T_c m}{T}\right) \rightarrow \text{Taylor Series}$$

$$m = \left[\frac{T_c}{T} m\right] - \frac{1}{3} \left(\frac{T_c}{T} m\right)^3 + O(m^5)$$

$$\Rightarrow m \left[\frac{T_c}{T} - \frac{1}{3} \left(\frac{T_c}{T}\right)^3 m^2 - 1 \right] \approx 0$$

So $m=0$ is trivial solution. But for spontaneous magnetization solution,

$$\left(\frac{T_c}{T} - 1\right) \approx \frac{1}{3} \left(\frac{T_c}{T}\right)^3 m_s^2$$

$$\Rightarrow m_s = \pm \sqrt{3} \left(\frac{T}{T_c} \right)^{3/2} \left[\frac{T_c}{T} - 1 \right]^{\frac{1}{2}}$$

(Spontaneous)

As $T \rightarrow T_c$ the order parameter approaches zero as follows,

$$m_s \propto \left[\frac{T_c}{T} - 1 \right]^{\frac{1}{2}}$$

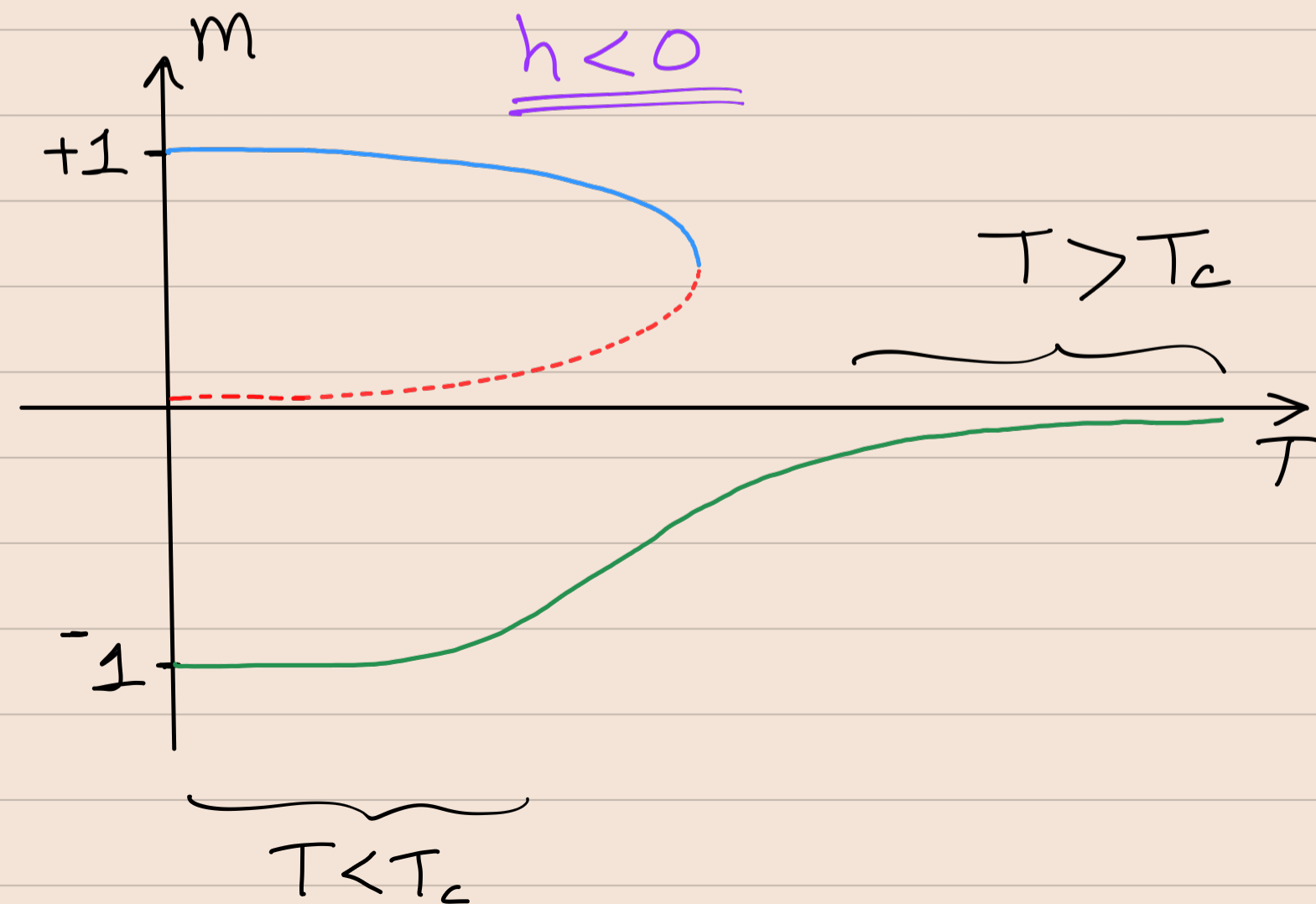
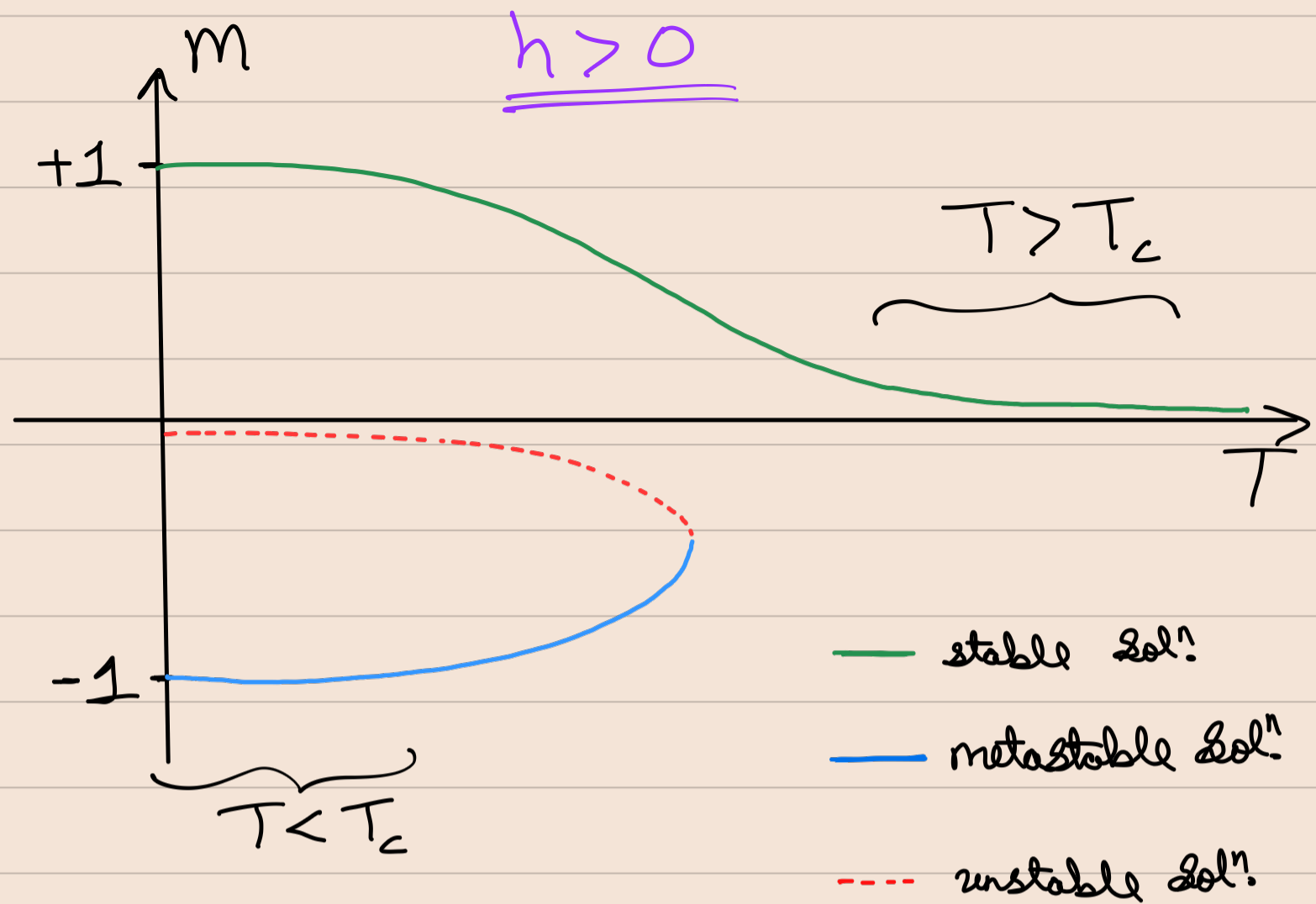
This exponent is called as a critical exponent denoted 'B'.

For $h \neq 0$

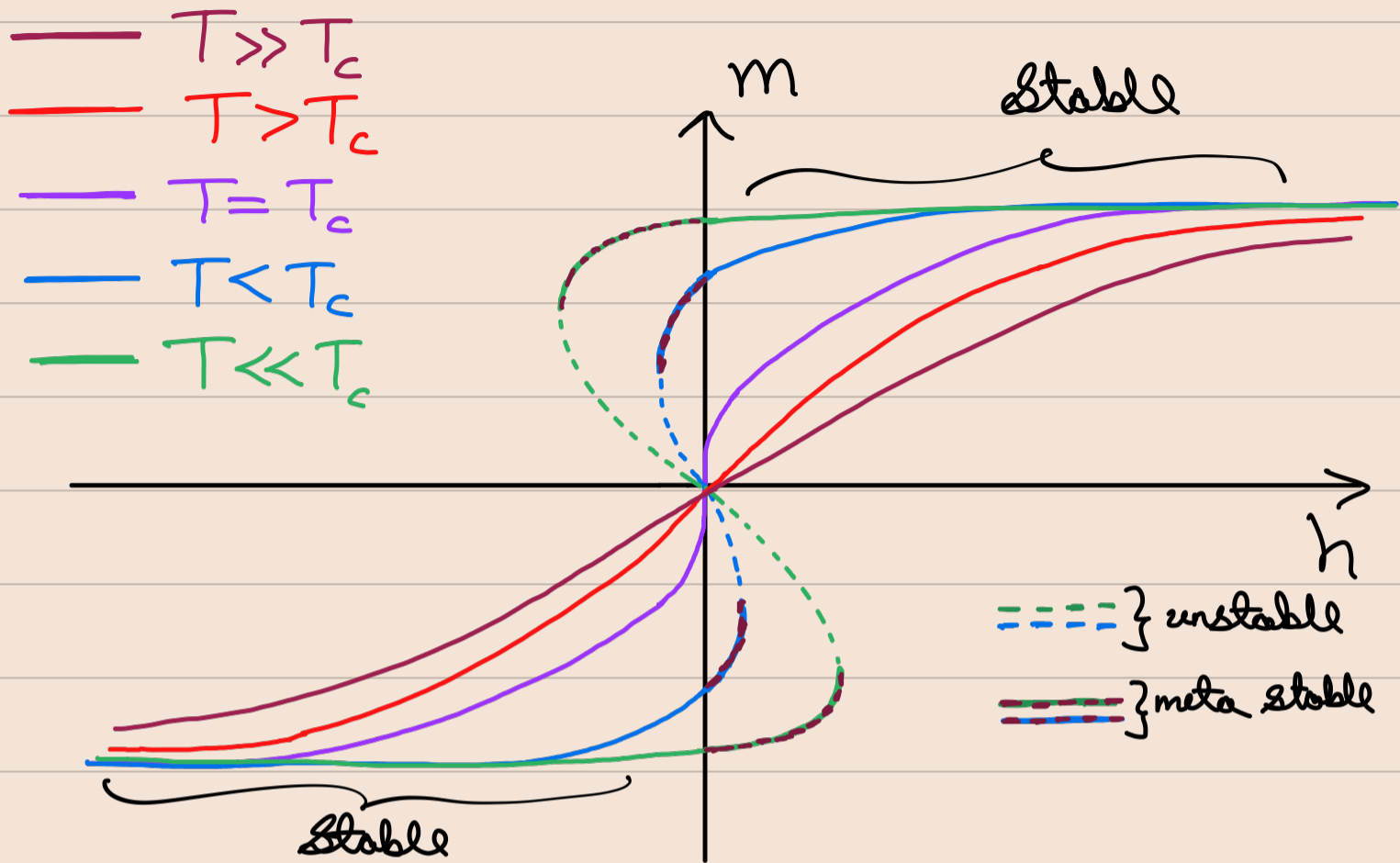
Here we have the equation for $m(h, T)$ as,

$$m = \tanh(Bh + \beta J_3 m)$$

Here the sign of 'h' will play an important role. This can be solved numerically.



magnetization vs magnetic field

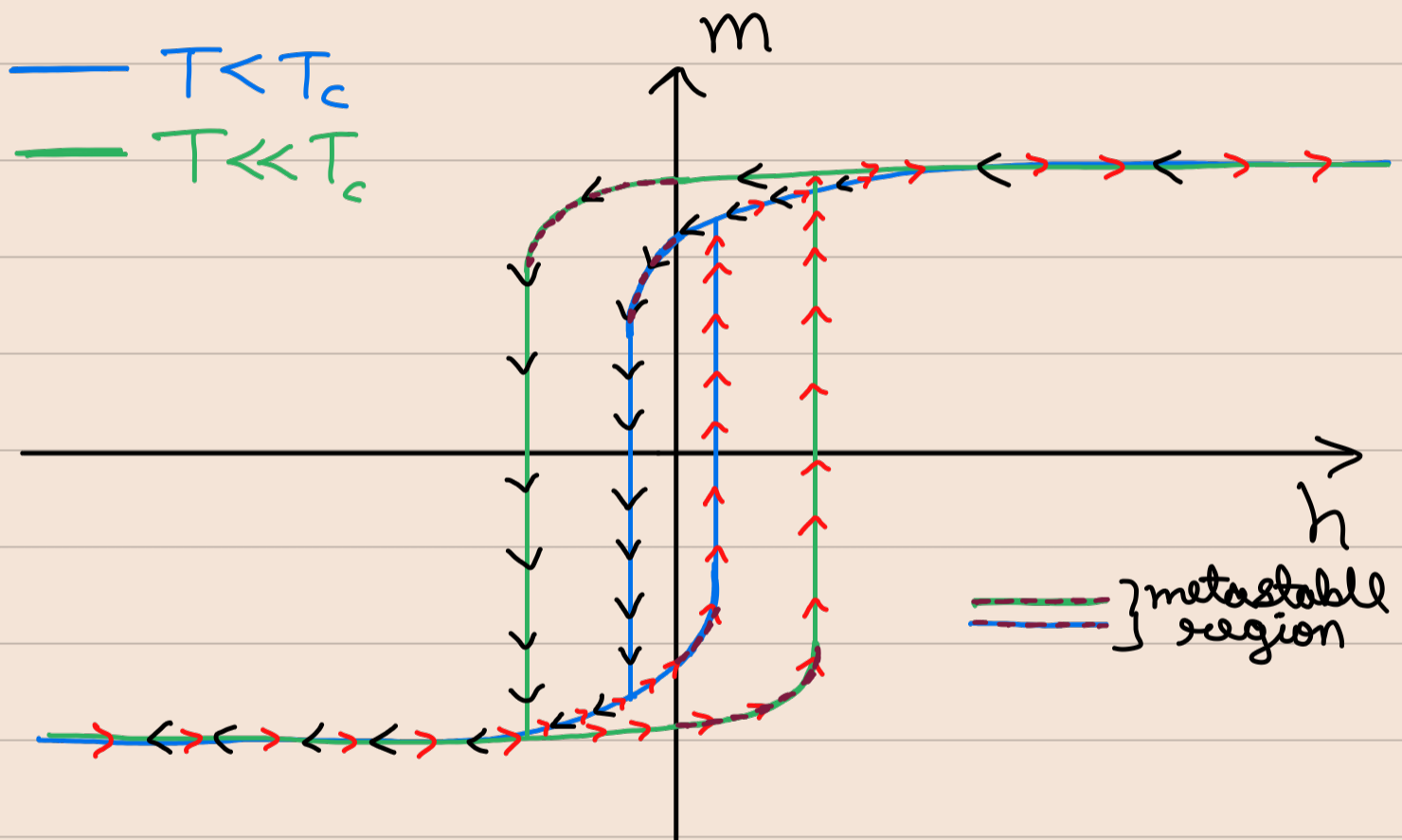


For a fixed temperature when we change magnetic field, we see that 'm' changes depending on 'T'.

For $T > T_c$: When h is changed from +ve to -ve, even the magnetization changes smoothly.

For $T = T_c$: When h is changed from +ve to -ve the 'm' changes smoothly, but near $h \sim 0$, the slope goes to ∞ .

For $T < T_c$: When h is changed from +ve to -ve there is a sudden jump of ' m ' from +ve to -ve in a discontinuous fashion. Also the system shows hysteresis and meta stability as shown below.



Magnetic Susceptibility

$$\chi_s = \left(\frac{\partial m}{\partial h} \right)_B = \frac{\partial}{\partial h} \left(\tanh \left[Bh + \frac{B}{B_c} m \right] \right)$$

$$\chi_s = \text{sech}^2 \left[Bh + \frac{B}{B_c} m \right] \left(B + \frac{B}{B_c} \chi_s \right)$$

$$\Rightarrow \frac{\chi_s}{\left(1 + \frac{\chi_s}{\beta_c}\right)} = \beta \operatorname{sech}^2\left(\beta h + \frac{\beta m}{\beta_c}\right)$$

$$= \beta \operatorname{sech}^2\left(\frac{\beta m}{\beta_c} + \beta h\right)$$

$$= \beta (1 - m^2)$$

$$\left[\text{used } \operatorname{sech}^2(x) = 1 - \tanh^2(x), \text{ where } m = \tanh\left(\frac{\beta m}{\beta_c} + \beta h\right) \right]$$

$$\Rightarrow \chi_s = \beta (1 - m^2) + \frac{\chi_s \beta (1 - m^2)}{\beta_c}$$

$$\chi_s \left[1 - \frac{\beta (1 - m^2)}{\beta_c} \right] = \beta (1 - m^2)$$

$$\chi_s = \frac{\beta (1 - m^2)}{\left[1 - \frac{\beta}{\beta_c} (1 - m^2) \right]}$$

In terms of $\beta = \frac{1}{k_B T}$ we get,

$$\chi_s = \frac{\frac{1}{k_B T} (1 - m^2)}{\left[1 - \frac{T_c}{T} (1 - m^2) \right]}$$

at $h=0, m=0$ $\chi_s = \frac{1}{\frac{k_B T}{(1 - \frac{T_c}{T})}}$

$$\Rightarrow \chi_s = \frac{1}{k_B} \frac{1}{T - T_c}$$

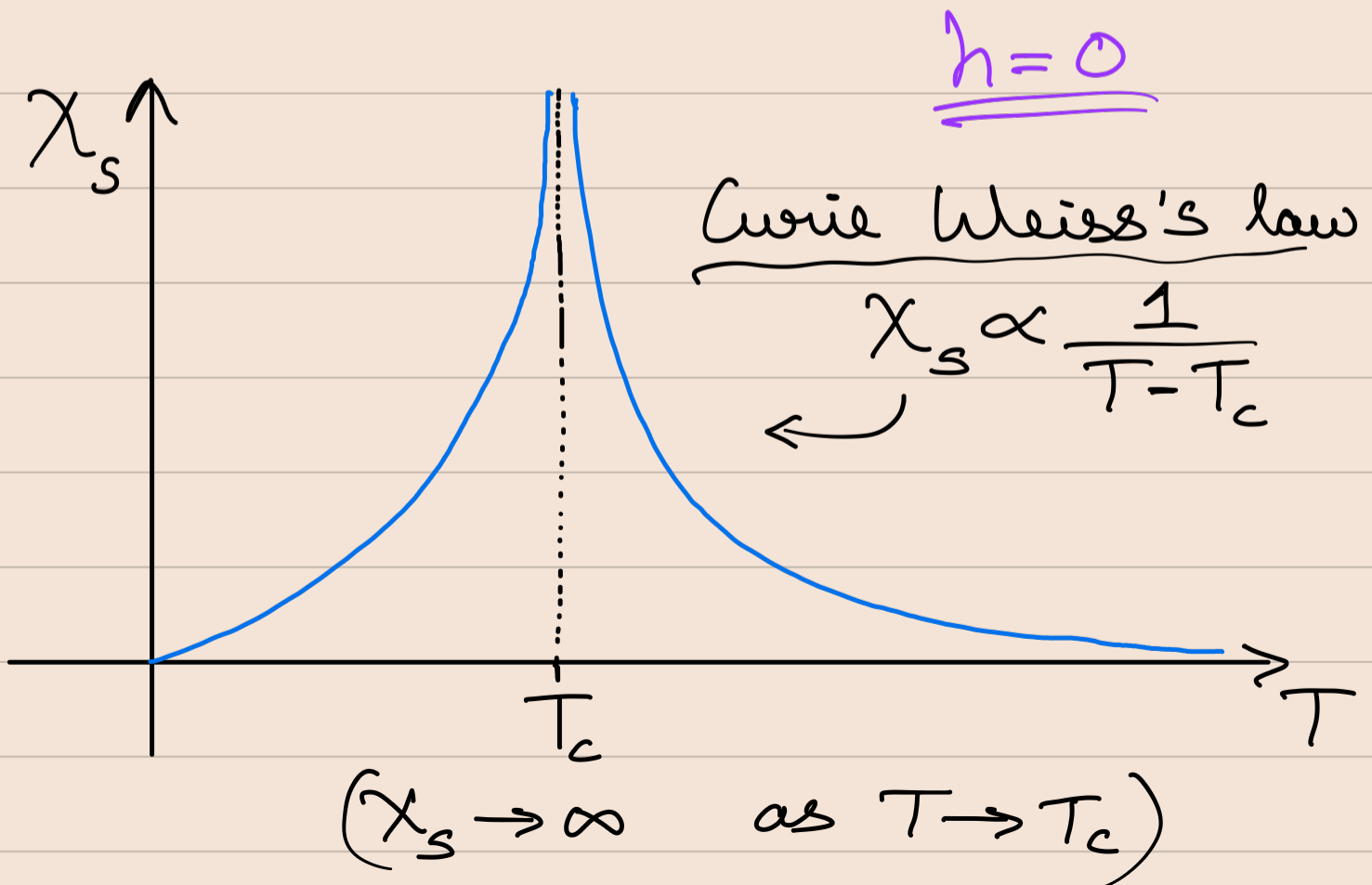
This is Curie-Weiss's law.

In S.I we get $\chi_s = \frac{\mu_B^2}{k_B (T - T_c)}$

or $\chi_m = N \chi_s \Rightarrow$

$$\chi_m = \frac{N \mu_B^2}{k_B (T - T_c)}$$

$\mu_B \Rightarrow$ Bohr Magneton



Curie - Weiss's law: It states that
for $T > T_c$, $\chi_s \propto \frac{1}{T - T_c}$

