

10/02/25

Lecture 10

Consider the below result,

$$\Gamma(\vec{q}) = \frac{\partial \vec{m}_{\vec{q}}}{\partial \tilde{h}(\vec{q})} = \frac{B(1-m^2)}{[1 - J(\vec{q}) B(1-m^2)]}$$

For $\vec{q}=0$ the above eqⁿ reduces to

$$\frac{\partial \vec{m}_{\vec{q}=0}}{\partial \tilde{h}_{(\vec{q}=0)}} = \frac{B(1-m^2)}{1 - J(\vec{q}=0) B(1-m^2)}$$

$$\partial \vec{m}_{\vec{q}=0} = \sum_i \partial m_i = \partial M$$

& $\partial \tilde{h}_{\vec{q}=0} = \sum_i \partial h_i$. If ∂h_i is same on all the sites, i.e. uniform variation, then $\partial h_i \rightarrow \partial h$. So we get,

$$\partial \tilde{h}_{\vec{q}=0} = \partial h \sum_i (1) = N \partial h //$$

$$\& J(\vec{q}=0) = \sum_i J_{ij} = J_j = J //$$

$$\Rightarrow \frac{\partial M}{N \partial h} = \Gamma(\vec{q}=0) = \frac{B(1-m^2)}{1 - Bg(1-m^2)}$$

using $m = \frac{M}{N}$ & $\frac{\partial m}{\partial h} \sim \frac{\partial m}{\partial h} = \chi_s$

we get the usual result of,

$$\chi_s = \frac{B(1-m^2)}{1 - Bg(1-m^2)} \Rightarrow \text{Susceptibility per spin.}$$

Here $g = k_B T_c$ $T_c \Rightarrow$ critical temperature

Thus $\Gamma(\vec{q}=0) = \chi_s$. Hence we can tell $\Gamma(\vec{q})$ is like susceptibility.

Now we wish to find the inverse fourier transform of $\Gamma(\vec{q})$ where $\Gamma(\vec{q}) = \frac{\partial \tilde{m}_{\vec{q}}}{\partial h_{\vec{q}}}$ is the fourier transform of the correlation functions.

Consider a function $Q(\vec{r})$ whose fourier transform is $\Gamma(\vec{q})$. Then,

$$\Gamma(\vec{q}) = \sum_{\vec{r}} Q(\vec{r}) e^{i\vec{q} \cdot \vec{r}}$$

Now we established previously that $\Gamma(\vec{q}=0)$ gives χ_s , which implies

$$\Gamma(\vec{q}=0) = \sum_{\vec{r}} Q(\vec{r}) e^{i\vec{q} \cdot \vec{r}} \Big|_{\vec{q}=0}$$

$$\Rightarrow \chi_s = \sum_{\vec{r}} Q(\vec{r})$$

But we know that sum of all pair correlation function is related to the susceptibility per spin by

$$\chi_s = \beta \sum_{\vec{r}} G(\vec{r})$$

$$\Rightarrow Q(\vec{r}) = \beta G(\vec{r})$$

$$\Rightarrow \Gamma(\vec{q}) = \beta \sum_{\vec{r}} G(\vec{r}) e^{i\vec{q} \cdot \vec{r}}$$

$$\Rightarrow G(\vec{r}) = \frac{1}{BN} \sum_{\vec{q}} \Gamma(\vec{q}) e^{-i\vec{q} \cdot \vec{r}}$$

We can get $G(\vec{r}) \Rightarrow$ Pair correlation function by inverse fourier transform of $\Gamma(\vec{q})$, where,

$$\Gamma(\vec{q}) = \frac{B(1-m^2)}{1 - g(\vec{q}) B(1-m^2)}$$

We need to know the form of $g(\vec{q})$ to find $G(\vec{r})$.

$$g(\vec{q}) = \sum_{\vec{r}} J(\vec{r}) e^{i\vec{q} \cdot \vec{r}}$$

$$= \sum_{\vec{r}} J(\vec{r}) \left[1 + i(\vec{q} \cdot \vec{r}) - \frac{(\vec{q} \cdot \vec{r})^2}{2!} - \dots \right]$$

$$g(\vec{q}) = \sum_{\vec{r}} J(\vec{r}) + i \sum_{\vec{r}} (\vec{q} \cdot \vec{r}) J(\vec{r}) - \sum_{\vec{r}} \frac{J(\vec{r})(\vec{q} \cdot \vec{r})^2}{2!} - \dots$$

If there is inversion Symmetry:

i.e. if the lattice is such that if all $\vec{r} \rightarrow -\vec{r}$, still, it is invariant, then it has inversion symmetry. Then all the odd powers of $(\vec{q} \cdot \vec{r})$ vanish,

$$\sum_{\vec{r}} (\vec{q} \cdot \vec{r}) \xrightarrow{\vec{r} \rightarrow -\vec{r}} \sum_{(-\vec{r})} [\vec{q} \cdot (-\vec{r})] = - \sum_{\vec{r}} (\vec{q} \cdot \vec{r})$$

equal to its -ve

$$\Rightarrow \sum_{\vec{r}} (\vec{q} \cdot \vec{r}) = 0. \text{ Similarly for all}$$

odd powers of $(\vec{q} \cdot \vec{r})$ the sum vanishes.

$$\Rightarrow f(\vec{q}) = \sum_{\vec{r}} J(\vec{r}) - \sum_{\vec{r}} \frac{J(\vec{r})(\vec{q} \cdot \vec{r})^2}{2!} + \sum_{\vec{r}} \frac{J(\vec{r})(\vec{q} \cdot \vec{r})^4}{4!} \dots$$

$$J(\vec{q}=0) = \sum_{\vec{r}} J(\vec{r}) \left(e^{-i\vec{q} \cdot \vec{r}} \right)_{\vec{q}=0} = \sum_{\vec{r}} J(\vec{r})$$

$$\Rightarrow f(\vec{q}) = f(0) - \sum_{\vec{r}} \frac{J(\vec{r})(\vec{q} \cdot \vec{r})^2}{2!} + O(q^4)$$

In long wavelength limit, $q \sim$ very small.

We can actually show that for cubic lattices in d -dim with only nearest neighbour interactions,

$$J(\vec{q}) = \sum_{\vec{r}} J(\vec{r}) e^{i\vec{q} \cdot \vec{r}}$$

$$\vec{r} = \{ \pm a\hat{x}_1, \pm a\hat{x}_2, \pm a\hat{x}_3, \dots, \pm a\hat{x}_d \}$$

$a \Rightarrow$ lattice constant.

& $J(\vec{r}) = J \Rightarrow$ same for neighbouring sites

$$\Rightarrow J(\vec{q}) = J \left[(e^{-iq_1 a} + e^{iq_1 a}) + (e^{-iq_2 a} + e^{iq_2 a}) \right. \\ \left. + (e^{-iq_3 a} + e^{iq_3 a}) + \dots + (e^{-iq_d a} + e^{iq_d a}) \right]$$

$$J(\vec{q}) = 2J \left[\cos(q_1 a) + \cos(q_2 a) + \cos(q_3 a) + \dots + \cos(q_d a) \right]$$

In long wavelength limit, we get,

$$J(\vec{q}) = 2J \left[d - \frac{a^2}{2} (q_1^2 + q_2^2 + q_3^2 + \dots + q_d^2) + O(q^4) \right]$$

$$J(\vec{q}) = 2dJ \left[1 - \frac{a^2 q^2}{2d} + O(q^4) \right]$$

Now $2d \Rightarrow$ Coordination number (3)
of d-dim. cubic lattice

$$\Rightarrow f(\vec{q}) = 3J \left[1 - \frac{a^2 q^2}{3} + O(q^4) \right]$$

where $f(0) = 3J$

$$\Rightarrow f(\vec{q}) = \underbrace{f(0)}_{3J} \left[1 - \frac{a^2 q^2}{3} + O(q^4) \right]$$

For d-dim cubic lattice

$$\text{Then, } f(\vec{q}) = f(0) - \sum_{\vec{s}} \frac{J(\vec{s})(\vec{q} \cdot \vec{s})^2}{2!} + O(q^4)$$

can be written as follows:

$$\underbrace{f(\vec{q})}_{\text{for general lattice}} = f(0) \left[1 - \underbrace{\alpha q^2}_{\text{can be neglected}} + O(q^4) \right]$$

$\left(\alpha = \frac{a^2}{2d} \Rightarrow \text{d-dim. cubic lattice} \right)$

$\alpha \Rightarrow$ depends on structure of lattice.
 $(\alpha > 0)$

Thus for long wavelength limit, we can write $g(\vec{q})$ as

$g(\vec{q}) = g(0)[1 - \alpha q^2]$, we can put this value of $g(\vec{q})$ in the expression of $\Gamma(\vec{q})$.

$$\Rightarrow \Gamma(\vec{q}) = \frac{\beta(1-m^2)}{1 - g(0)[1 - \alpha q^2] \beta(1-m^2)}$$

$$\Rightarrow \Gamma(\vec{q}) = \frac{\beta(1-m^2)}{1 - \beta g(0)(1-m^2) + \beta g(0)\alpha q^2(1-m^2)}$$

$$= \frac{\beta}{\left(\frac{1}{1-m^2}\right) - \beta g(0) + \beta g(0)\alpha q^2}$$

$$\Gamma(\vec{q}) = \frac{\cancel{\beta}}{\cancel{\beta g(0)\alpha} \left[\frac{\frac{1}{1-m^2} - \beta g(0)}{\beta g(0)\alpha} + q^2 \right]}$$

Use
$$K^2 = \left[\frac{\frac{1}{1-m^2} - \beta g(0)}{\beta g(0) \alpha} \right]$$

$$\Rightarrow \Gamma(\vec{q}) = \frac{1}{g(0) \alpha [K^2 + q^2]}$$
 → (in long wave limit)

Now put this in,
$$G(\vec{r}) = \frac{1}{N \beta} \sum_{\vec{q}} \Gamma(\vec{q}) e^{-i \vec{q} \cdot \vec{r}}$$

$$\Rightarrow G(\vec{r}) = \frac{1}{N \beta} \sum_{\vec{q}} \frac{e^{-i \vec{q} \cdot \vec{r}}}{g(0) \alpha [K^2 + q^2]}$$

$$G(\vec{r}) = \frac{1}{\beta g(0) \alpha} \left(\frac{1}{N} \sum_{\vec{q}} \frac{e^{-i \vec{q} \cdot \vec{r}}}{[K^2 + q^2]} \right)$$

For long wavelength behaviour $\vec{q}$ is very small. So the summation becomes a Riemann integral. & the ' $\vec{q}$ ' varies in entire ' q ' space.

for $\vec{q} \rightarrow 0$ $\frac{1}{N} \sum_{\vec{q}} \rightarrow \int \frac{d^d q}{(2\pi)^d}$
 q -space.

$$\Rightarrow G(\vec{r}) = \frac{1}{\beta g(0) \alpha} \int \frac{d^d q}{(2\pi)^d} \left[\frac{e^{-i\vec{q} \cdot \vec{r}}}{(k^2 + q^2)} \right]$$

$G(\vec{r})$ in 3D

$$G(\vec{r}) = \frac{1}{\beta g(0) \alpha} \frac{1}{(2\pi)^3} \underbrace{\int_0^{2\pi} d\phi}_0 \underbrace{\int_0^\infty dq q^2}_0 \underbrace{\int_0^\pi d\theta \sin(\theta)}_0 \frac{e^{-i\vec{q} \cdot \vec{r}}}{(k^2 + q^2)}$$

(we chose $\vec{r}$ along ' q_z ' axis)

$$= \frac{2\pi}{\beta g(0) \alpha (2\pi)^3} \underbrace{\int_0^\infty dq q^2 \int_0^\pi d\theta \sin(\theta) \frac{e^{-iqr \cos(\theta)}}{(k^2 + q^2)}}_0$$

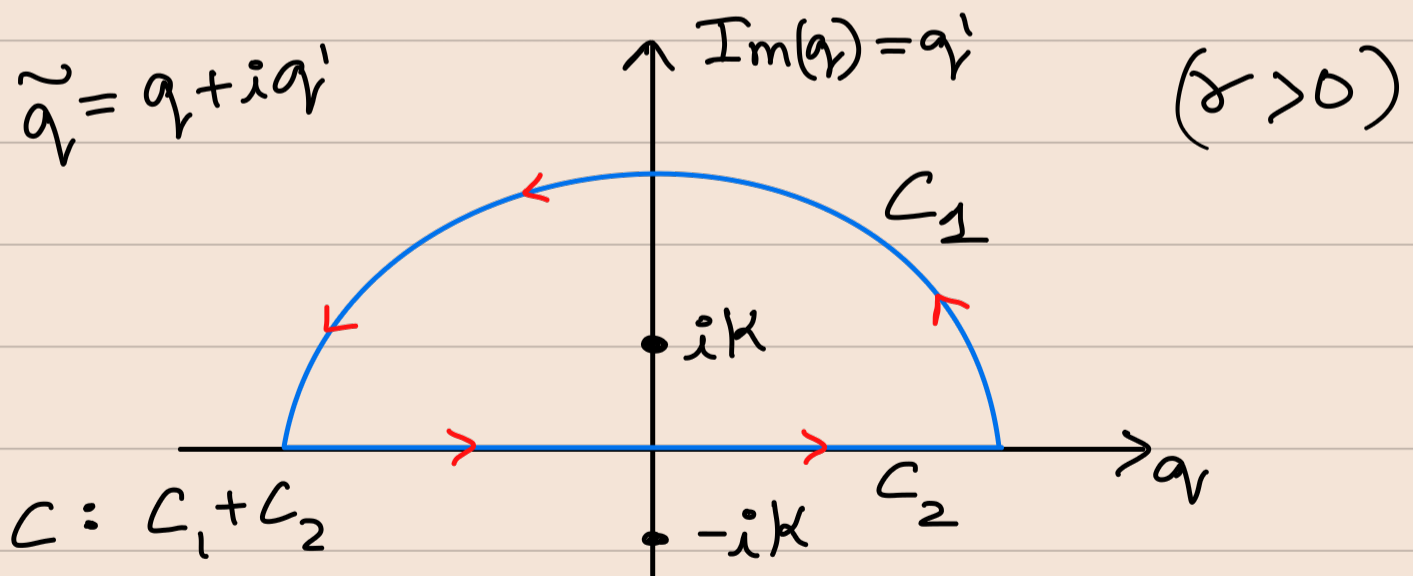
Substitute $x = \cos(\theta)$

$$\Rightarrow G(\vec{r}) = \frac{2\pi}{\beta g(0) \alpha (2\pi)^3} \int_0^\infty \frac{dq q^2}{(k^2 + q^2)} \left[\frac{e^{-iqr} - e^{iqr}}{(-iqr)} \right]$$

$$G(\vec{r}) = \frac{2\pi}{\beta g(0) \alpha (2\pi)^3 (i\gamma)} \int_0^{\infty} dq \left(\frac{q}{k^2 + q^2} \right) \underbrace{(e^{iq\gamma} - e^{-iq\gamma})}_{\text{Put } q \rightarrow -q}$$

$$= \frac{2\pi}{\beta g(0) \alpha (2\pi)^3 (i\gamma)} \underbrace{\left[\int_{-\infty}^{\infty} dq \frac{q}{(k^2 + q^2)} e^{iq\gamma} \right]}_I$$

$$I = \int_{-\infty}^{\infty} dq \frac{q e^{iq\gamma}}{(k^2 + q^2)} \quad (\text{go to complex plane})$$



The integrand along C_1 curve vanishes by Jordan's lemma as $(\gamma > 0)$.

$$\Rightarrow \oint_C \frac{\tilde{q} e^{i\tilde{q}\vec{r}\cdot\vec{\tau}}}{(k^2 + \tilde{q}^2)} d\tilde{q} = \underbrace{\int_{-\infty}^{\infty} \frac{q e^{iq\tau} dq}{(k^2 + q^2)}}_I + \underbrace{\int_{C_1} \frac{\tilde{q} e^{i\tilde{q}\tau}}{(k^2 + \tilde{q}^2)} d\tilde{q}}_{\text{Zero.}}$$

(Jordan's lemma)

$$I = \oint_C \frac{\tilde{q} e^{i\tilde{q}\tau}}{k^2 + \tilde{q}^2} d\tilde{q} \Rightarrow \text{Only } \tilde{q} = ik \text{ Pole will contribute.}$$

$$I = 2\pi i \lim_{q \rightarrow ik} \underbrace{\left[\frac{\tilde{q} e^{i\tilde{q}\tau} (\cancel{q - ik})}{(\tilde{q} + ik)(\cancel{\tilde{q} - ik})} \right]}_{\text{Residue}}$$

$$I = 2\pi i \frac{(ik) e^{-k\tau}}{(2ik)} = \underline{\underline{\pi i e^{-k\tau}}}$$

$$\Rightarrow G(\vec{r}) = \frac{2\pi}{\beta g(0) \alpha (2\pi)^3} (\pi i e^{-k\tau})$$

$$G(\vec{r}) = \left(\frac{1}{\beta g(0) \alpha} \right) \frac{e^{-k\tau}}{4\pi\tau}$$

We define correlation length (ξ) as

$$\xi = \frac{1}{k} \Rightarrow G(\vec{r}) = \left(\frac{1}{\beta g(0) \alpha} \right) \frac{e^{-r/\xi}}{4\pi r}$$

$$\Rightarrow \xi = \left(\frac{\beta g(0) \alpha}{\frac{1}{1-m^2} - \beta g(0)} \right)^{\frac{1}{2}}$$

$$\Rightarrow \xi = \left(\frac{\beta g(0) \alpha (1-m^2)}{1 - \beta g(0) (1-m^2)} \right)^{\frac{1}{2}}$$

When $h=0$ for $T > T_c \Rightarrow m=0$

$$\text{Here } \xi = \sqrt{\frac{\beta g(0) \alpha}{1 - \beta g(0)}} = \sqrt{\frac{T_c \alpha}{(T - T_c)}}$$

$$\left(\beta g(0) = \frac{T_c}{T} \right)$$

$$\Rightarrow \xi = \sqrt{\frac{T_c \alpha}{T - T_c}} \Rightarrow \underline{\underline{\xi \propto (T - T_c)^{-\frac{1}{2}}}}$$

$$\text{At } T = T_c, \quad \epsilon_s \rightarrow \infty$$

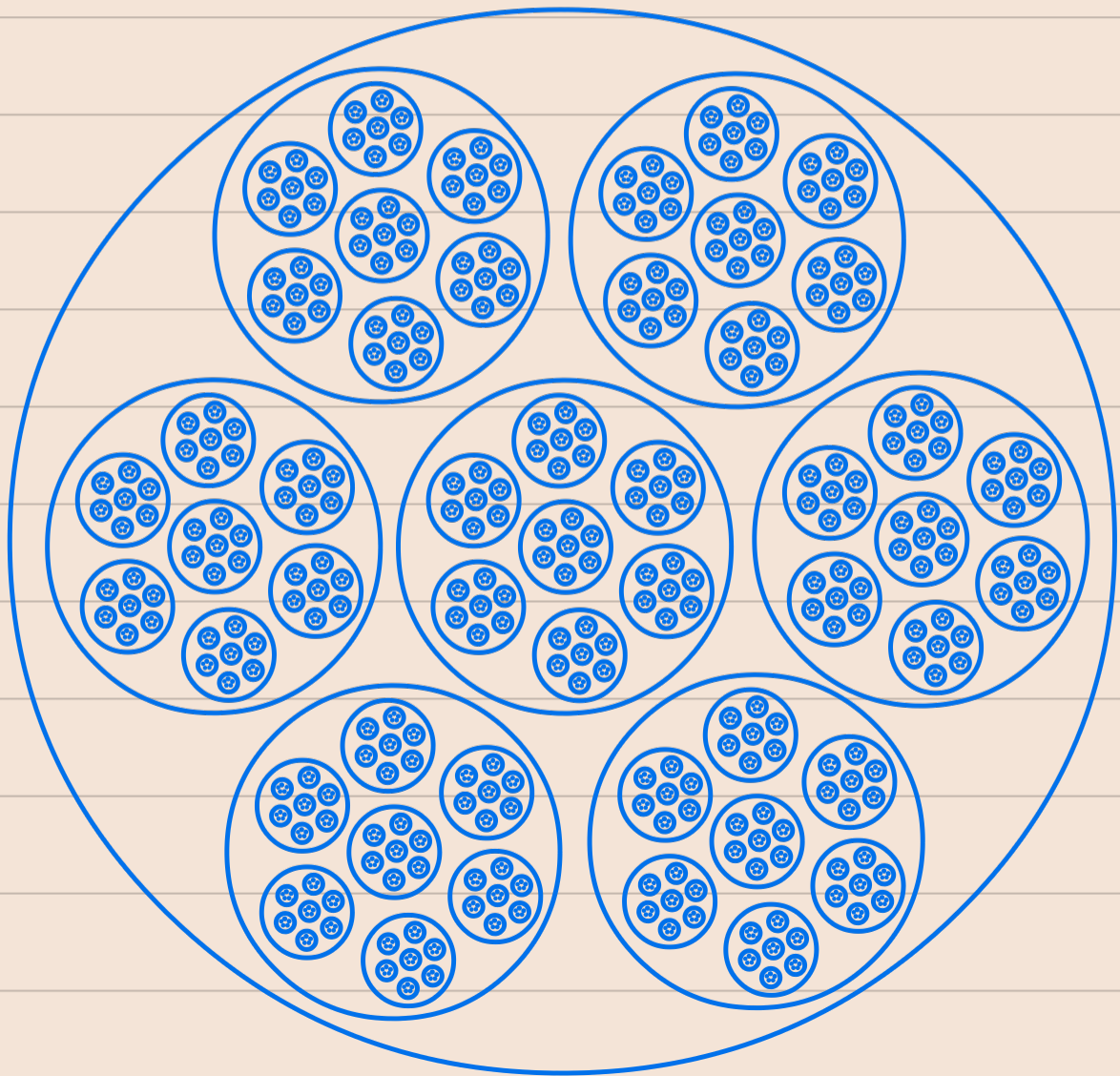
$$\Rightarrow \frac{1}{\epsilon_s} \rightarrow 0.$$

$$\Rightarrow G(r) \propto \frac{1}{r} \quad \text{at } T = T_c$$

Thus at the critical temperature, the correlation function is long range & doesn't decay exponentially with the distance. Hence there can be long range ordered structure formation at the critical temperature & can lead to Fractal structure formation.

Eg: In liquid-gas phase transition, at critical point the matter is like a fractal of droplets inside bubbles inside droplets inside bubbles, and so on... (like a cloud).

Fractal like structure of a liquid - vapour is shown below. The geometric order repeats infinitely when zoomed (theoretically).



Behaviour of Thermodynamic quantities near the Critical Temperature T_c

We denote the relative temperature shift from ' T_c ' by $t = \frac{T - T_c}{T_c}$.

& check how various thermodynamic quantities are related to ' t ' near the Critical temperature.

Magnetization order parameter (m)

In mean field theory ' m ' is given by the self consistent eqⁿ.
($h=0$)

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

$$m = \frac{T_c m}{T} - \frac{1}{3} \left(\frac{T_c m}{T}\right)^3 + \frac{2}{15} \left(\frac{T_c m}{T}\right)^5 + \dots$$

neglect higher order terms

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

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

When $T > T_c$ the only allowed solution with $h=0$ is $m=0$. But when $T < T_c$ i.e. $t < 0$, we get non-zero spontaneous magnetization (m_s) given by,

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

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

$$\Rightarrow m_s^2 \frac{T_c^2}{3T^2} = \frac{T_c - T}{T_c}$$

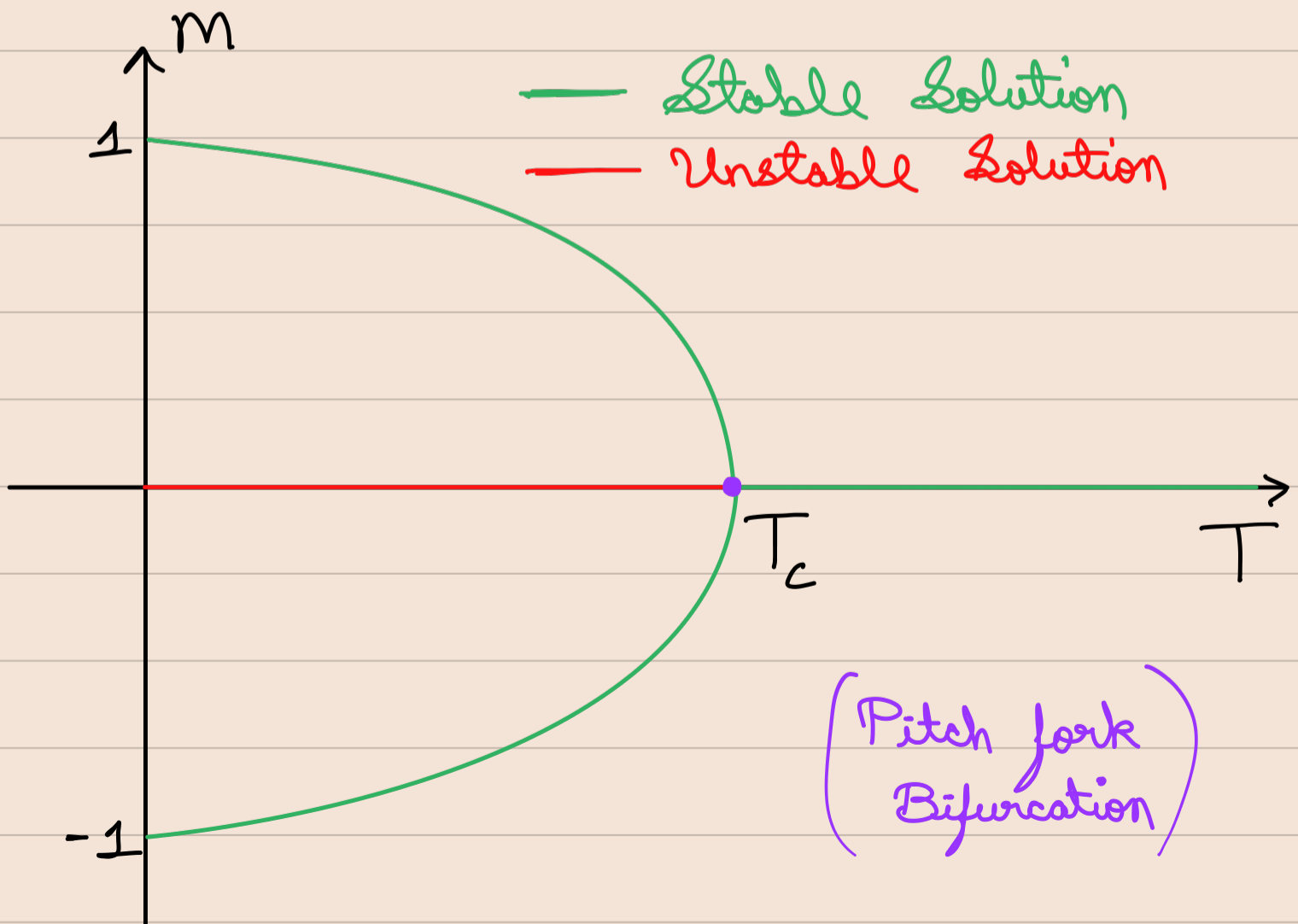
$$\Rightarrow m_s^2 = 3 \frac{T^2}{T_c^2} \left(\frac{T_c - T}{T_c} \right)$$

using $t = \frac{T - T_c}{T_c} \Rightarrow$ Scaled relative temperature

$$\begin{aligned}
 \Rightarrow m_s^2 &= 3(t+1)^2(-t) \\
 &= -3t(t+1)^2 \\
 &= -3t(1+2t+t^2) \\
 \Rightarrow m_s^2 &= -3t - 6t^2 - 3t^3
 \end{aligned}$$

$\Rightarrow$ For $t \rightarrow 0^-$ i.e. near the critical point from the left of T_c we get

$$m_s^2 \propto -t \Rightarrow m_s \propto \sqrt{\frac{T_c - T}{T_c}}$$



Variation of magnetization 'm' with 'h' at specific values of 'T'

$$m = \tanh(\beta H) \quad H = g m + h$$

$$\Rightarrow m = \tanh(\beta g m + \beta h)$$

$$m = \tanh\left[\frac{T_c m + h/k_B}{T}\right]$$

$$\underline{\text{At } T = T_c} \quad m = \tanh\left(m + \frac{h}{k_B T_c}\right)$$

expanding this w.r.t 'h' we get,

$$m = m + \frac{h}{k_B T_c} - \frac{1}{3} \left(m + \frac{h}{k_B T_c}\right)^3 + \dots$$

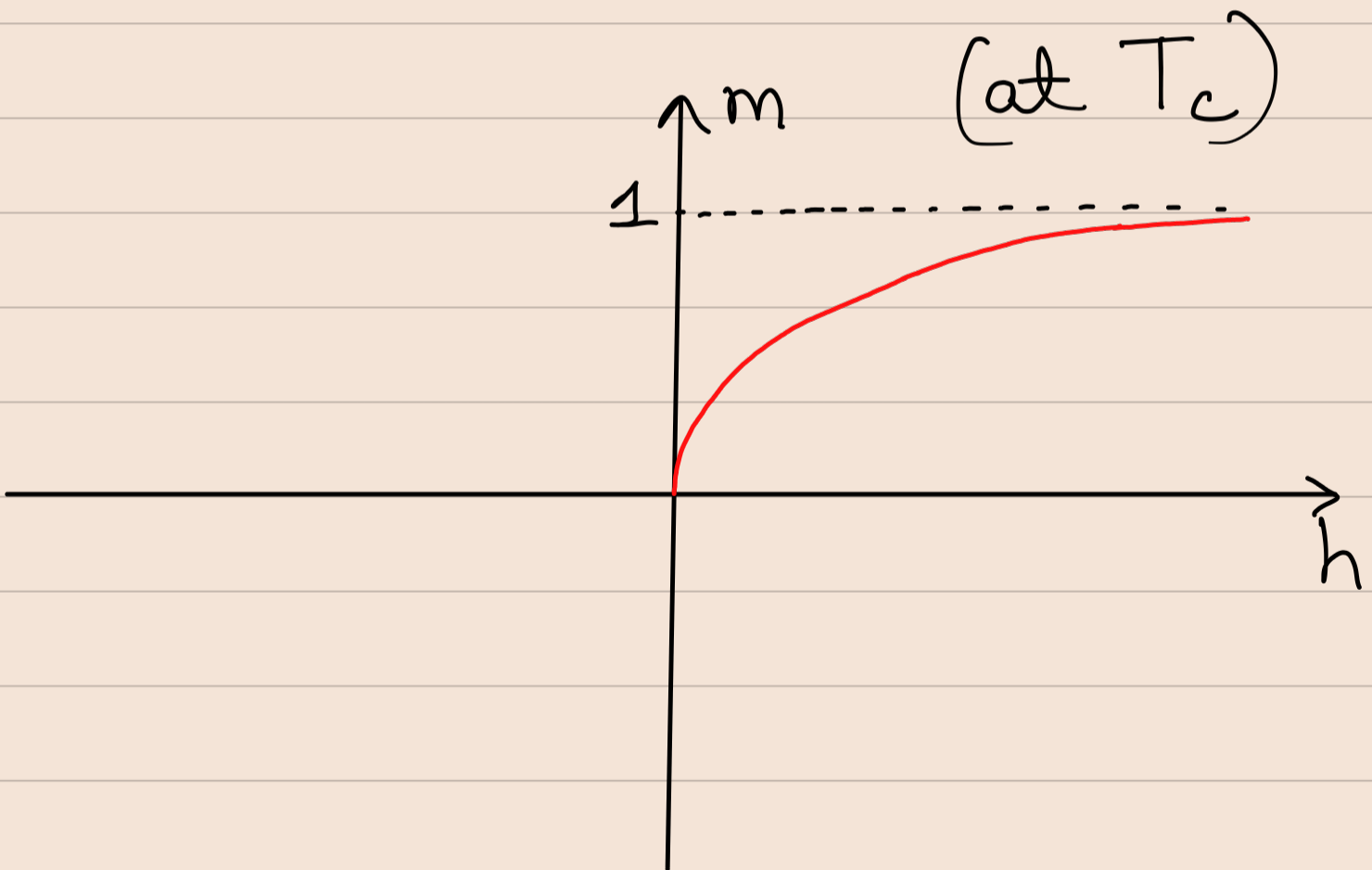
$$\Rightarrow \frac{1}{3} \left(m + \frac{h}{k_B T_c}\right)^3 = \frac{h}{k_B T_c}$$

$$\Rightarrow \left(m + \frac{h}{k_B T_c}\right) = \left(\frac{3h}{k_B T_c}\right)^{1/3}$$

$$m = \left(\frac{3h}{k_B T_c} \right)^{1/3} - \frac{h}{k_B T_c}$$

For $h \rightarrow 0$ only 1st term dominates. Thus near $h \sim 0$, at $T = T_c$

$$\underline{\underline{m \propto h^{1/3}}}$$



Energy (H)

The mean field partition function is given by $Z = 2^N \cosh(BH)^N$, $H \Rightarrow$ effective field ($H = gm + h$)

The average Energy (Enthalpy) is given by

$$E = - \frac{\partial \ln(Z)}{\partial \beta} = -NH \tanh(BH)$$
$$= -NHm \quad (m = \tanh(BH))$$

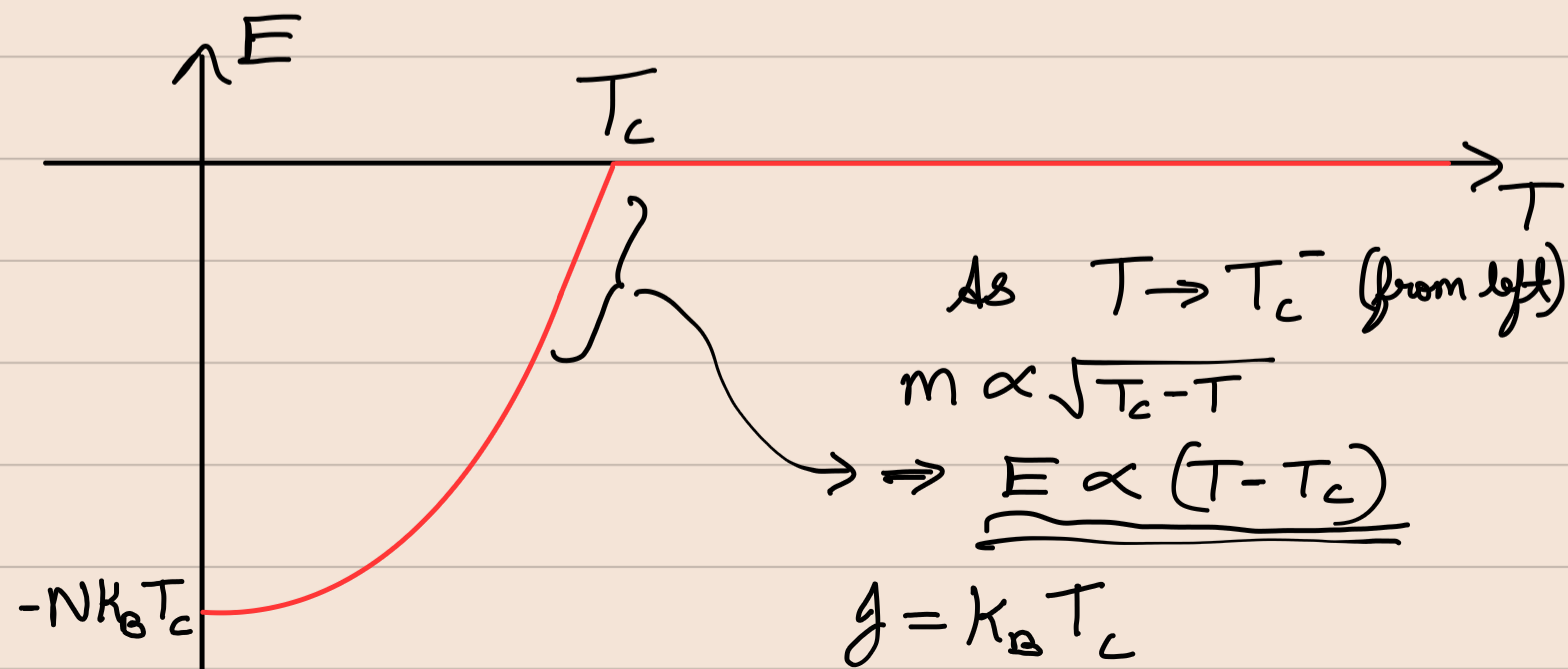
$$\Rightarrow E = -N(gm + h)m$$

In the case $h=0$

- For $T > T_c$, $m=0 \Rightarrow E=0$

- For $T < T_c$, $m \rightarrow m_s$

$$\Rightarrow E = -Ngm_s^2$$



Specific heat (C_h)

C_h is related to the second derivative of free energy function since it can be written as,

$$C_h = \frac{k_B}{N} \beta^2 \frac{\partial^2}{\partial \beta^2} \ln(Z)$$

In mean field theory $Z = 2^N \cosh(\beta H)^N$
(where $H = h + g m$)

$$\Rightarrow \ln(Z) = N \ln(2) + N \cosh(\beta H)$$

$$\Rightarrow \left(\frac{\partial \ln(Z)}{\partial \beta} \right)_{h,m,N} = N H \tanh(\beta H)$$

$$\Rightarrow \left[\frac{\partial^2 \ln(Z)}{\partial \beta^2} \right]_{h,m,N} = N H^2 \operatorname{sech}^2(\beta H)$$

$$m = \tanh(\beta H)$$

$$\Rightarrow C_h = k_B \beta^2 H^2 \operatorname{sech}^2(\beta H) = k_B (\beta H)^2 (1 - m^2)$$

$$\Rightarrow C_h = k_B (\beta h + \beta g m)^2 (1 - m^2)$$

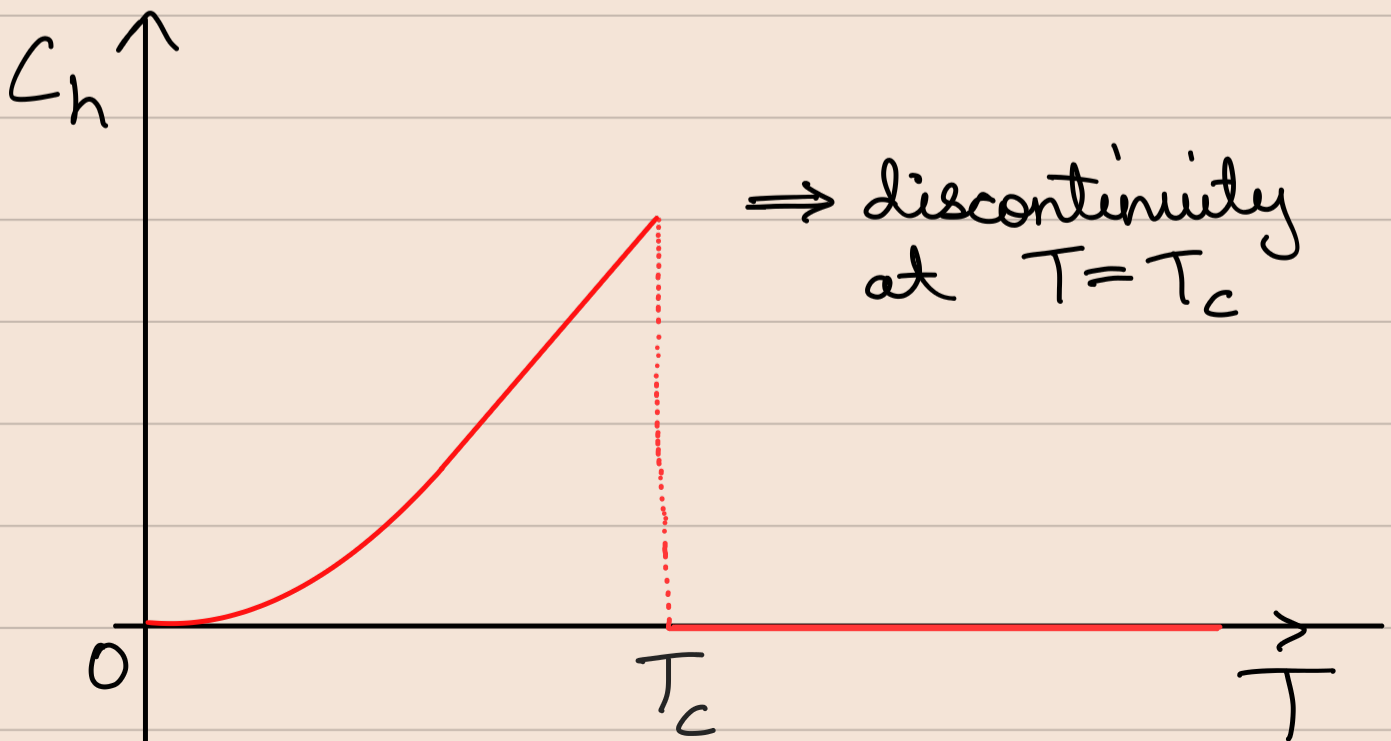
when $h=0$, & using $\beta g = \frac{T_c}{T}$, we get,

$$\Rightarrow C_h = k_B \left(\frac{T_c m}{T} \right)^2 (1 - m^2) \quad \left(t = \frac{T - T_c}{T_c} \right)$$

$$\Rightarrow C_h = k_B \left[\frac{T_c m}{T_c (1+t)} \right]^2 (1 - m^2)$$

- When $T > T_c$, $m = 0 \Rightarrow C_h = 0$
- When $T < T_c$, $m \rightarrow m_3 \propto \sqrt{-3t}$
 $\Rightarrow C_h \propto \frac{(-3t)(1+3t)}{(1+t)^2}$
 $\Rightarrow C_h \propto \frac{-3t(1+3t)}{(1+t)^2} = -3t - 3t^2 + 9t^3 + \dots$

$$\Rightarrow \underline{\underline{C_h \propto -t}} \quad (\text{for } \underline{\underline{t \rightarrow 0^-}})$$



Susceptibility (χ)

$$\chi = \left(\frac{\partial m}{\partial h} \right)_\beta \Rightarrow \text{Susceptibility per spin particle}$$

we had already calculated this in mean field theory. It is given by,

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

When $h = 0$

- For $T > T_c$, $m = 0$

$$\Rightarrow \chi \propto \frac{1}{T - T_c} \quad (T > T_c)$$

- For $T < T_c \rightarrow m \rightarrow m_s \neq 0$.

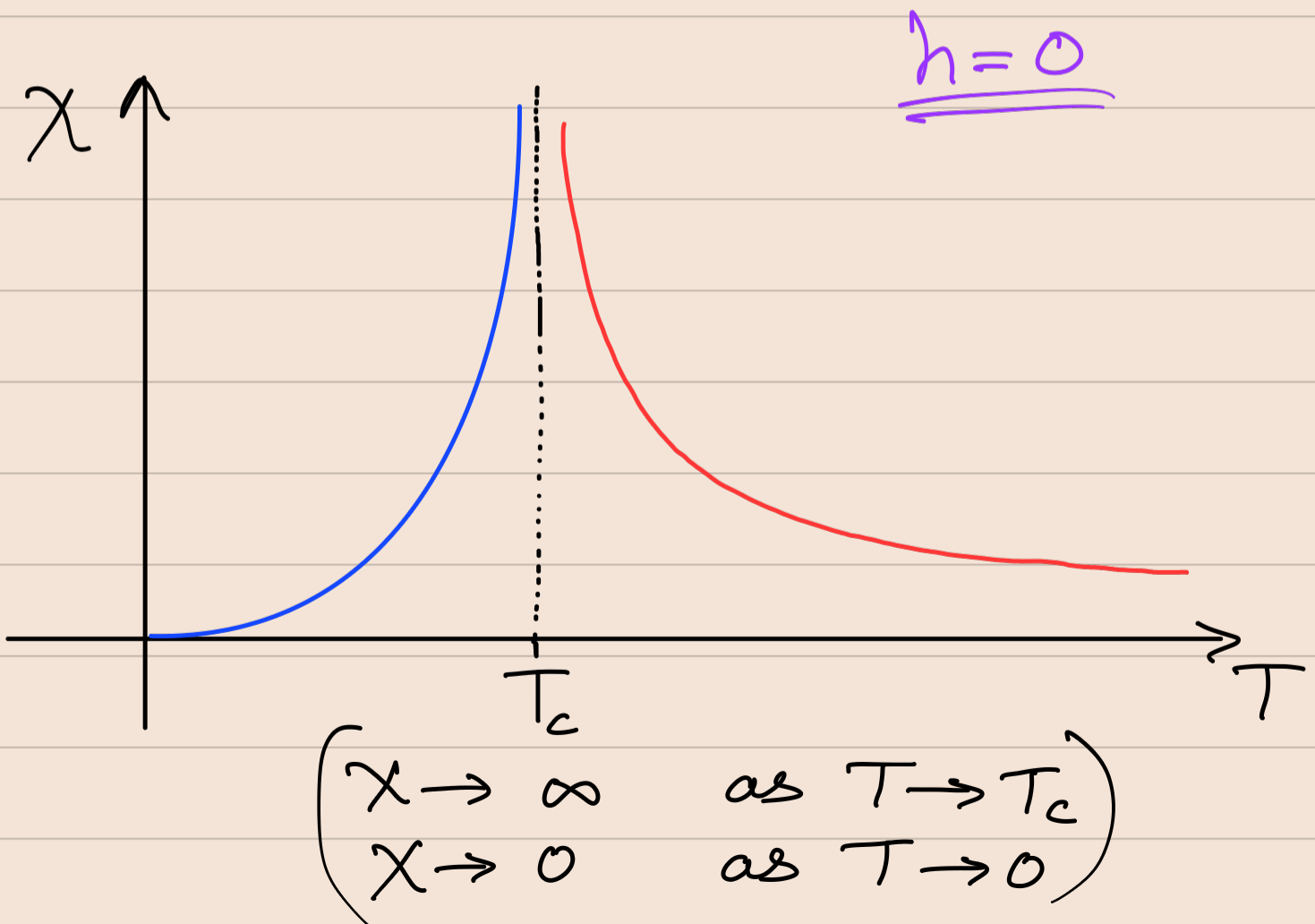
$$\Rightarrow \chi = \frac{(1 - m_s^2)}{k_B [T - T_c (1 - m_s^2)]}$$

But as $T \rightarrow T_c^-$, $m_s \propto \sqrt{T_c - T}$

$$\Rightarrow \chi \propto \frac{(1+t)}{T - T_c (1+t)} \Rightarrow \text{tends to '}\infty\text{' rapidly as } T \rightarrow T_c^-$$

$$\Rightarrow \chi \propto \frac{1}{|T - T_c|} \text{ (approximately)}$$

$$\Rightarrow \chi \propto \frac{-1}{|t|} \Rightarrow \chi \propto |T_c - T|^{-1}$$



Correlation length

$$\xi_s = \left(\frac{\beta g \alpha (1-m^2)}{1 - \beta g (1-m^2)} \right)^{\frac{1}{2}}$$

(according to
Onstein
Zernike
Theory)

When $h=0$

- For $T > T_c$, $m=0$

$$\Rightarrow \xi_s = \sqrt{\frac{\beta g \alpha}{1 - \beta g}}$$

$$\underline{\underline{\beta g = \frac{T_c}{T}}}$$

$$\Rightarrow \xi_s = \sqrt{\frac{\alpha T_c}{(T - T_c)}}$$

$$\Rightarrow \underline{\xi_s} \propto (T - T_c)^{-1/2} \quad \text{for } \underline{\underline{T > T_c}}$$

For $T < T_c$ $m \rightarrow m_s \neq 0$.

$$\Rightarrow \xi_s = \left(\frac{T_c \alpha (1-m_s^2)}{T - T_c (1-m_s^2)} \right)^{\frac{1}{2}}$$

$(T \rightarrow T_c^-)$

$$\xi_g = \sqrt{\frac{\alpha (1+t)}{(t+1) - (1+t)}} \rightarrow 0$$

$(t \rightarrow 0^-)$

But a higher order expansion of ' m_s '
gives $\xi_g \propto \sqrt{T - T_c}$

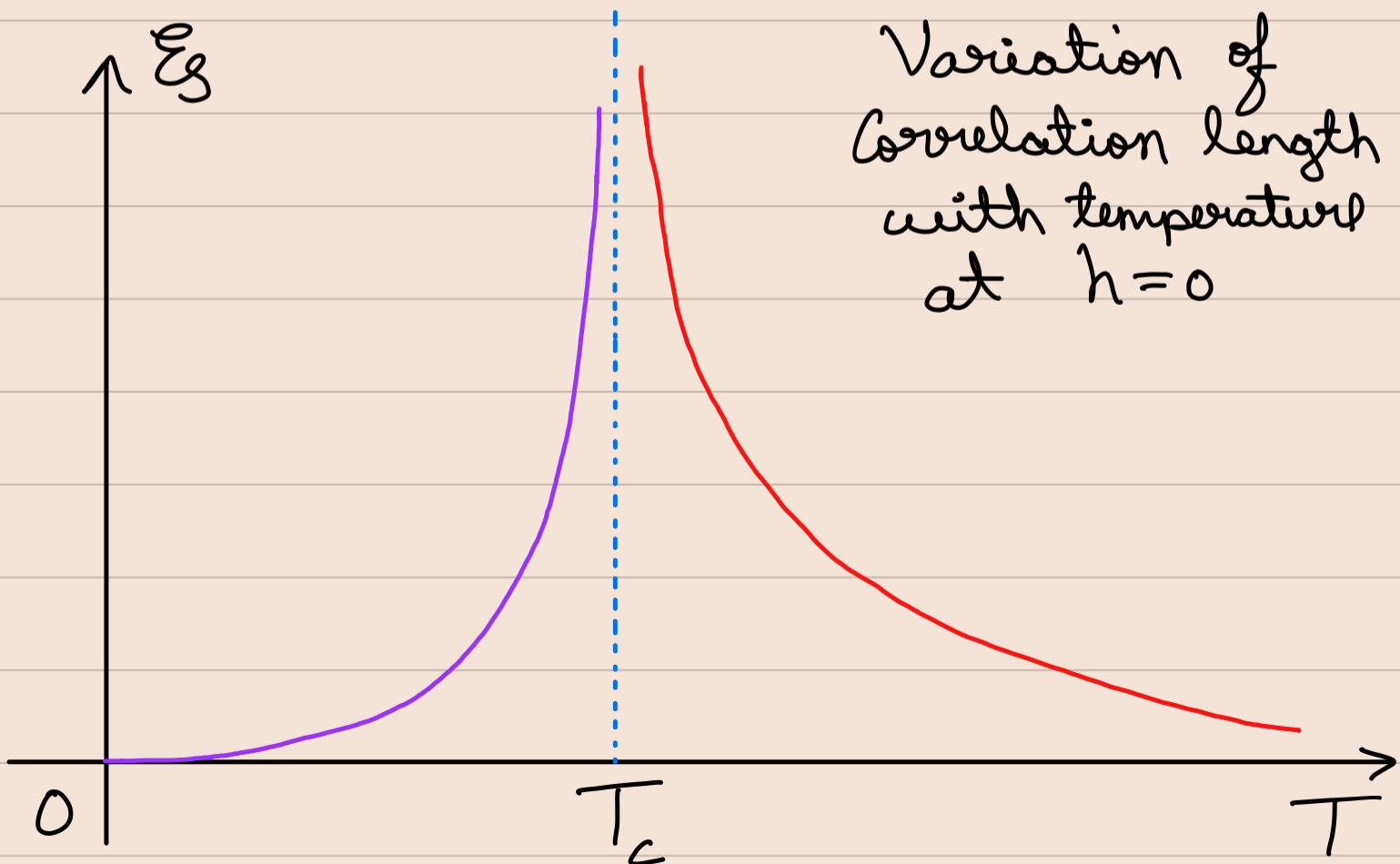
Note: $m_s \propto (-3t - 6t^2 - 3t^3)$

$$\Rightarrow \xi_g = \left[\frac{T_c \alpha (1+3t)}{T_c (t+1) - T_c (1+3t)} \right]^{\frac{1}{2}}$$

$(t \rightarrow 0^-)$

$$\Rightarrow \xi_g \propto \sqrt{\frac{-1}{t}} = (-t)^{-1/2}$$

$(t \rightarrow 0^-)$



Landau Theory of Phase Transitions

From the mean field theory with site dependent magnetization ' m_i ' as the variational parameters we get free energy function in the form,

$$\Phi = -\frac{1}{2} \sum_{i,j} J_{ij} m_i m_j - \sum_i h_i m_i + \frac{1}{B} \sum_i \left[\frac{1+m_i}{2} \ln \left(\frac{1+m_i}{2} \right) + \frac{1-m_i}{2} \ln \left(\frac{1-m_i}{2} \right) \right]$$

In Landau theory we expand this in powers of ' m_i ' & keep the terms until 4-th power of ' m_i '.

$$\text{Now } (m_i - m_j)^2 = m_i^2 + m_j^2 - 2m_i m_j$$

$$\Rightarrow m_i m_j = \frac{m_i^2 + m_j^2 - (m_i - m_j)^2}{2}$$

& we shall keep $h_i \rightarrow h$ (uniform)

We need to now expand the below term

$$\sum_i \left[\frac{1+m_i}{2} \ln\left(\frac{1+m_i}{2}\right) + \frac{1-m_i}{2} \ln\left(\frac{1-m_i}{2}\right) \right]$$

$$= \sum_i \left[\left(\frac{1+m_i}{2}\right) \ln(1+m_i) - \left(\frac{1+m_i}{2}\right) \ln(2) \right. \\ \left. + \left(\frac{1-m_i}{2}\right) \ln(1-m_i) - \left(\frac{1-m_i}{2}\right) \ln(2) \right]$$

$$= \sum_i \left[\frac{(1+m_i)}{2} \left[m_i - \frac{m_i^2}{2} + \frac{m_i^3}{3} - \frac{m_i^4}{4} \right] \right. \\ \left. - \frac{(1-m_i)}{2} \left[m_i + \frac{m_i^2}{2} + \frac{m_i^3}{3} + \frac{m_i^4}{4} \right] - \ln(2) \right]$$

$$= \sum_i \frac{1}{2} \left[\cancel{m_i} - \frac{m_i^2}{2} + \cancel{\frac{m_i^3}{3}} - \frac{m_i^4}{4} + m_i^2 - \cancel{\frac{m_i^3}{2}} + \frac{m_i^4}{3} \right. \\ \left. - \cancel{m_i} - \frac{m_i^2}{2} - \cancel{\frac{m_i^3}{3}} - \frac{m_i^4}{4} + m_i^2 + \cancel{\frac{m_i^3}{2}} + \frac{m_i^4}{3} \right. \\ \left. - 2\ln(2) \right]$$

$$= \sum_i \left[-\frac{m_i^2}{2} + m_i^2 - \frac{m_i^4}{4} + \frac{m_i^4}{3} - \ln(2) \right]$$

$$= \sum_i \frac{m_i^2}{2} + \sum_i \frac{m_i^4}{12} - \sum_i \ln(2)$$

Thus $\Phi(\{m_i\})$ approximately can be written as,

$$\Phi \approx -\frac{1}{2} \sum_{i,j} J_{ij} \left[\frac{m_i^2 + m_j^2 - (m_i - m_j)^2}{2} \right] - h \sum_i m_i + \frac{1}{\beta} \left[\sum_i \left(\frac{m_i^2}{2} \right) + \sum_i \frac{m_i^4}{12} - \sum_i \ln(2) \right]$$

$$= -\frac{1}{4} \sum_{i,j} J_{ij} m_i^2 - \frac{1}{4} \sum_{i,j} J_{ij} m_j^2 + \frac{1}{4} \sum_{i,j} J_{ij} (m_i - m_j)^2 - h \sum_i m_i + \frac{1}{2\beta} \sum_i m_i^2 + \frac{1}{12\beta} \sum_i m_i^4 - \frac{1}{\beta} \sum_i \ln(2)$$

$$= -\frac{1}{2} \sum_{i,j} J_{ij} m_i^2 + \frac{1}{2\beta} \sum_i m_i^2 - h \sum_i m_i + \frac{1}{4} \sum_{i,j} J_{ij} (m_i - m_j)^2 + \frac{1}{12\beta} \sum_i m_i^4 - \frac{1}{\beta} \sum_i \ln(2)$$

$$\left(\text{use } \sum_{i,j} J_{ij} m_i^2 = \sum_i m_i^2 \underbrace{\sum_j J_{ij}}_{g(0)} = g(0) \sum_i m_i^2 \right)$$

$$\Rightarrow \Phi \approx \frac{1}{2} \left[\frac{1}{\beta} - g(0) \right] \sum_i m_i^2 - h \sum_i m_i$$

$$+ \frac{1}{4} \sum_{i,j} J_{ij} (m_i - m_j)^2 + \frac{1}{12\beta} \sum_i m_i^4 - \underbrace{\frac{1}{\beta} \sum_i \ln(2)}_{\text{independent of } m_i}$$

We can neglect terms independent of ' m_i ' whenever needed as it won't affect the variational free energy function.

Now we can go to the continuum limit where the lattice sites can be so close that $m_i \rightarrow m(\vec{r})$ where $\vec{r}$ is any arbitrary position.

Then we can define free energy $\Phi[m(\vec{r})]$ as a functional, $\Phi = \int (dx)^d \phi[m(\vec{r})]$

$$\Phi[m(\vec{r})] = \int (dx)^d \left[\phi_0 - h m(\vec{r}) + a [m(\vec{r})]^2 + c [\vec{\nabla} m(\vec{r})]^2 + b [m(\vec{r})]^4 \right]$$

(Summation became integration)

Free energy function

$\Rightarrow \varphi[m(\vec{r})]$ is the free energy per unit d -dimensional volume.

$$\varphi[m(\vec{r})] = \varphi_0 - hm(\vec{r}) + a[m(\vec{r})]^2 + c[\nabla m(\vec{r})]^2 + b[m(\vec{r})]^4$$

Here $m(\vec{r})$ is the magnetization defined on the bulk of the d -dim spin system which is a variational parameter & those values of $m = m^*$ are chosen by the system for which φ has a global minima at $m = m^*$.

- $\varphi_0 = -k_B T \ln(2) \Rightarrow \text{const w.r.t 'm'}$

- $a = \frac{1}{2} \left[\frac{1}{\beta} - g(0) \right] = \frac{k_B}{2} (T - T_c) \propto (T - T_c)$

$a > 0$ when $T > T_c$ & $a < 0$ when $T < T_c$

- $b = \frac{k_B T}{12} \Rightarrow b \propto T \Rightarrow b$ is always +ve

- $h \Rightarrow$ external magnetic field (+ve or -ve)

- $c \Rightarrow$ Related to the inhomogeneity of system.

$\vec{\nabla}m$ is got by the term $\sum_{i,j} J_{ij} (m_i - m_j)^2$

If $m_i = m_j$ everywhere then this will obviously reduce the free energy & also matches with the previous mean field theory.

If $\vec{\nabla}m = 0$, then, we get the free energy function to be,

$$\varphi = \varphi_0 - hm + am^2 + bm^4$$

This is the ansatz for ' φ ' which was proposed by Landau for his theory of phase transitions which can mimic many critical properties of spin systems.

From here φ_0 term is neglected as it won't affect the outcomes at critical phenomena.

In the absence of External field ($h=0$)

$$\varphi = am^2 + bm^4 \Rightarrow \frac{\partial \varphi}{\partial m} = 2am + 4bm^3$$

$$\text{now } \left. \frac{\partial \varphi}{\partial m} \right|_{m=m_*} = 0 \quad (m_* \Rightarrow \text{solution})$$

$$\Rightarrow 2am_* + 4bm_*^3 = 0$$

$$\Rightarrow 2m_*[a + 2bm_*^2] = 0$$

$$\Rightarrow m_* = 0 \quad \text{or} \quad m_* = \pm \sqrt{\frac{-a}{2b}}$$

1) when $a < 0$ i.e. when $T < T_c$,
' m ' has three solutions:

- $m_* = 0$ is unstable as $\left. \frac{\partial^2 \varphi}{\partial m^2} \right|_{m=0} = 2a < 0$

$\Rightarrow \varphi$ has a local maxima at $m=0$.

- $m_* = \pm \sqrt{\frac{-a}{2b}}$ is a stable 2-fold

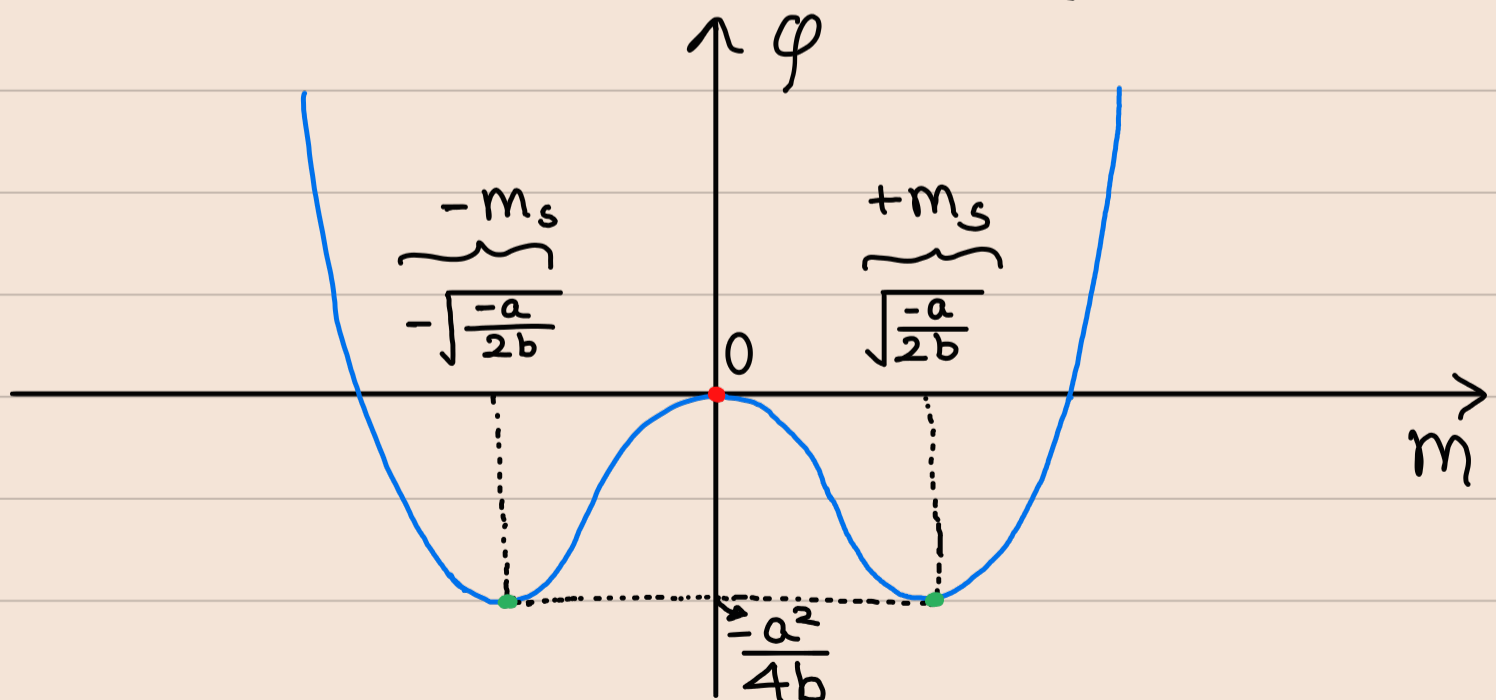
degenerate solⁿ as φ has two global minima at these values of ' m '.

$$\left. \frac{\partial^2 \varphi}{\partial m^2} \right|_{m = \pm \sqrt{\frac{-a}{2b}}} = 2a + 12b \left(\frac{-a}{2b} \right) = 2a - 6a = -4a$$

Thus when $a < 0$ $\left. \frac{\partial^2 \varphi}{\partial m^2} \right|_{m = \pm \sqrt{\frac{-a}{2b}}} > 0$

Hence φ has a minima at these values of 'm'. And $\varphi_{\min} = a \left(\frac{-a}{2b} \right) + b \left(\frac{-a}{2b} \right)^2$

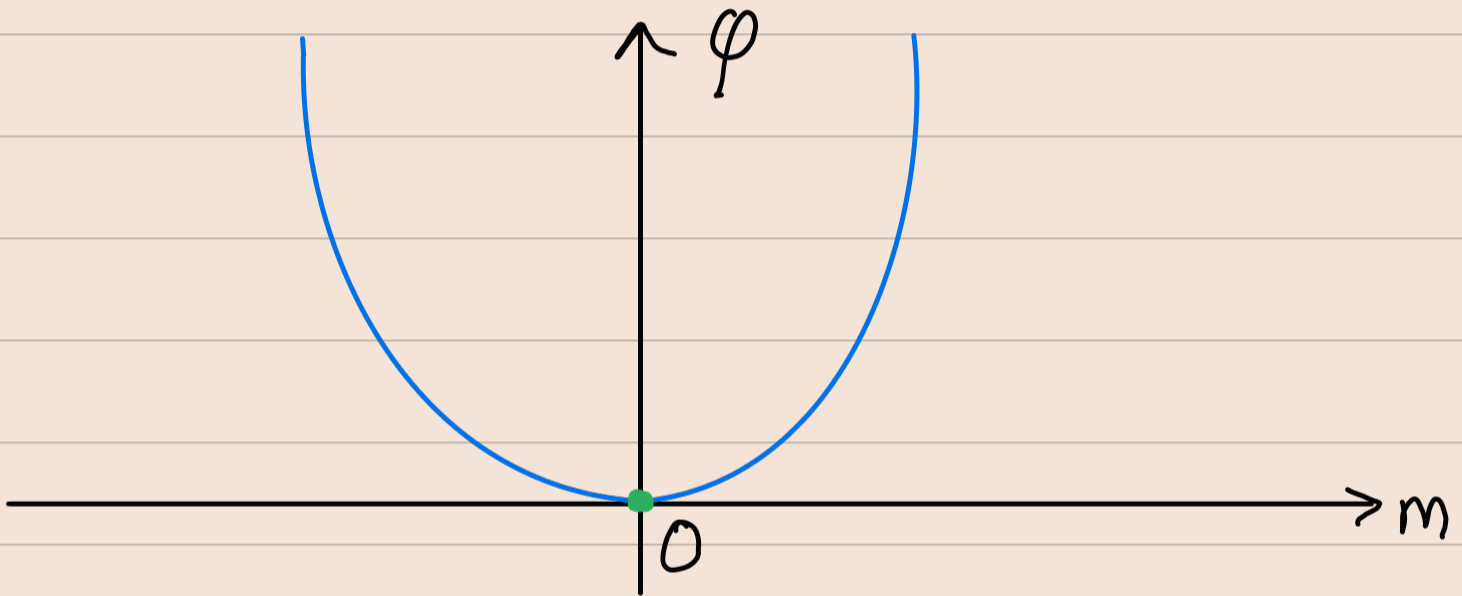
$$\varphi_{\min} = \frac{-a^2}{2b} + \frac{a^2}{4b} = \underline{\underline{\frac{-a^2}{4b}}}$$



The non-zero value of m_x even at $h=0$ is Spontaneous magnetization (m_s)

2) when $a > 0$ i.e. when $T > T_c$,
 $m_* = 0$ is the only solⁿ, since,
 $m_* = \pm \sqrt{\frac{-a}{2b}}$ is imaginary.

Also $\left. \frac{\partial^2 \varphi}{\partial m^2} \right|_{m=0} = 2a > 0$, hence it is a
 minima at $m=0$.
 So $m=0$ is stable solⁿ when $T > T_c$.



Variation of $\varphi_{\min}$ with a ($h=0$)

$\varphi_{\min} \Rightarrow$ actual attainable free energy

$F = \varphi_{\min} \Rightarrow$ analogous to free energy
 got by evaluating $\sum_{\nu} e^{-\beta \langle \nu | \hat{H} | \nu \rangle}$. This
 is the free energy attained by the
 system at any temperature.

$$\Rightarrow F = \begin{cases} \frac{-a^2}{4b}, & a < 0 \\ 0, & a > 0. \end{cases} \quad (b \propto T)$$

$$F \propto -\frac{(T-T_c)^2}{T} \quad (a < 0)$$

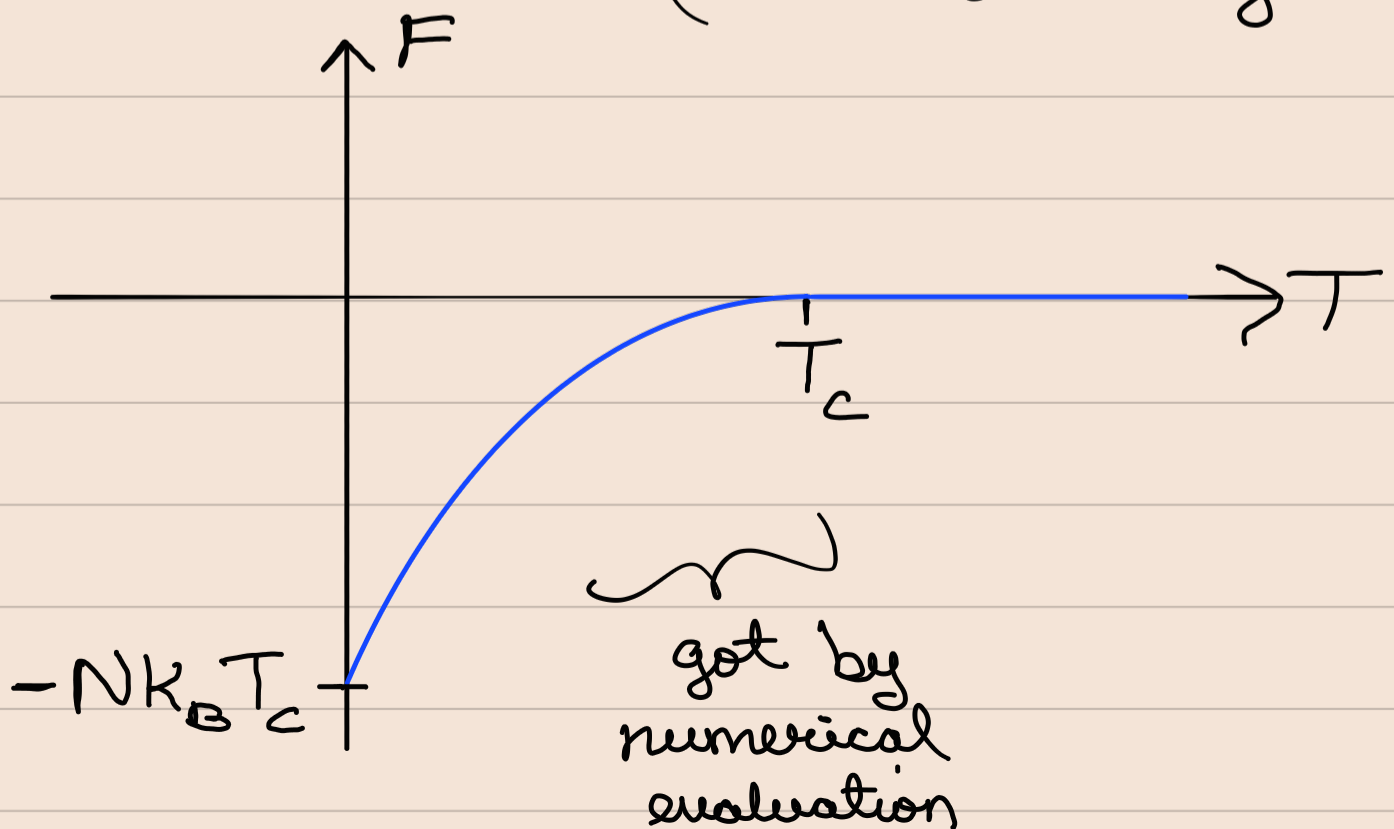
$$\Rightarrow F \propto -\frac{(t T_c)^2}{T_c(t+1)} \quad \left(t = \frac{T-T_c}{T_c}\right)$$

$$\Rightarrow F \propto -\frac{t^2}{t+1} = t^2 \underbrace{(1 - t + t^2 + \dots)}_{\text{neglect}}$$

$$\Rightarrow \text{As } T \rightarrow T_c, \quad \underline{\underline{F \propto -t^2}}$$

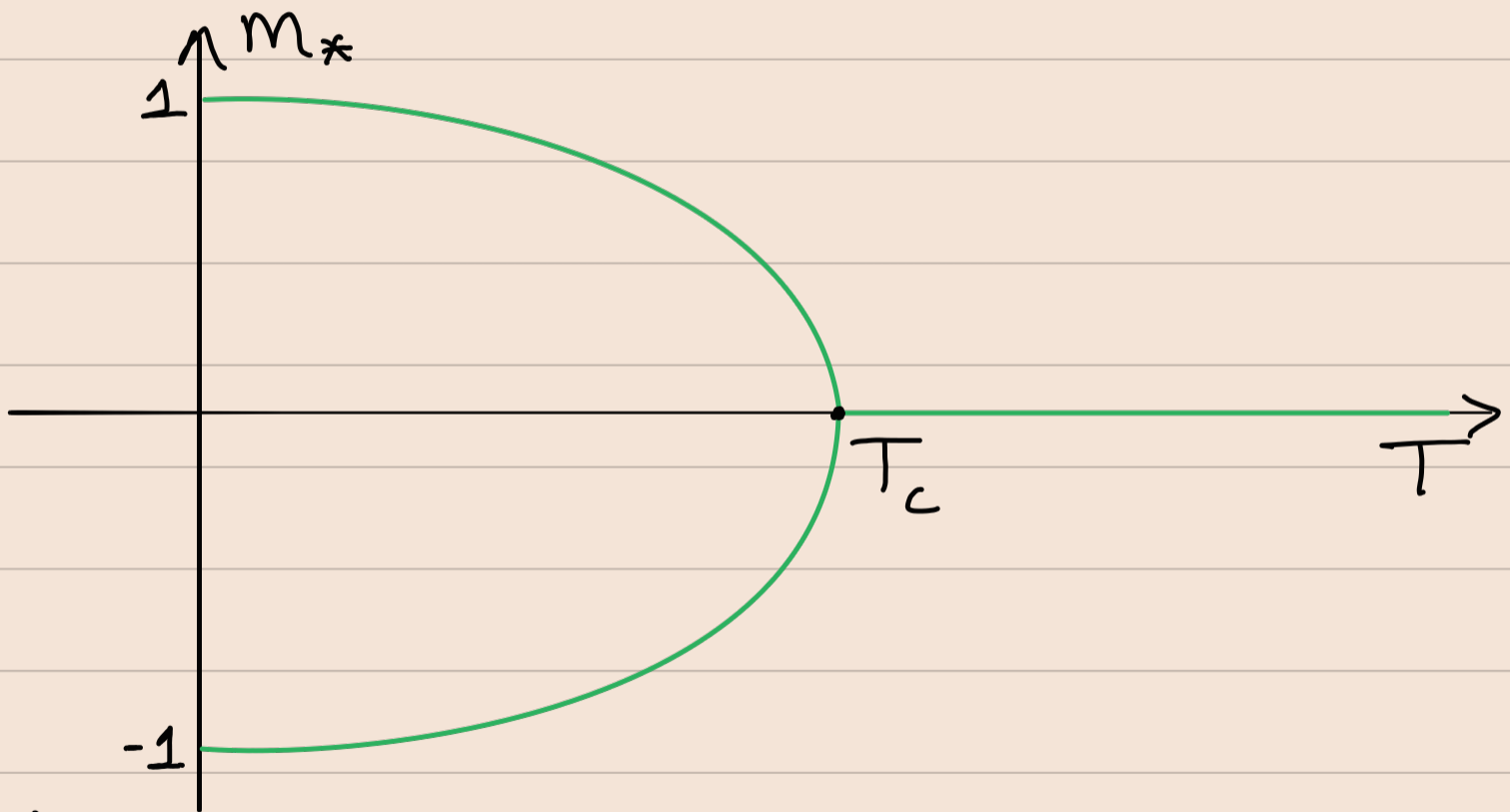
(near critical temp.)

(Here φ_0 is neglected)



Variation of m^* with T ($h=0$)

- when $a < 0$ i.e. when $T < T_c$,
 $m_* = \pm \sqrt{\frac{-a}{2b}}$ is a stable Sol^n
 $\Rightarrow m_* \propto \sqrt{T_c - T}$ (as $T \rightarrow T_c^-$)
- when $a > 0$ i.e. when $T > T_c$,
 $m_* = 0$ is the only Sol^n .



Observe that m_* which is related to the 1st derivative of ' φ ' is continuous at T_c but not differentiable at ' T_c '. The slope of $m_*(T) \rightarrow \infty$ as $T \rightarrow T_c$.

Susceptibility as $h \rightarrow 0$

$$\varphi = -hm + am^2 + bm^4$$

$$\Rightarrow \left. \frac{\partial \varphi}{\partial m} \right|_{m_*} = -h + 2am_* + 4bm_*^3 = 0$$

$$\Rightarrow 2m_* [a + 2bm_*^2] = h$$

Differentiating the above eqⁿ w.r.t 'h'
we get,

$$-1 + 2a \frac{\partial m_*}{\partial h} + 12bm_*^2 \frac{\partial m_*}{\partial h} = 0$$

$$\text{But } \frac{\partial m_*}{\partial h} = \chi \quad \left(\begin{array}{l} \text{Susceptibility per} \\ \text{Spin} \end{array} \right)$$

$$\Rightarrow 2a\chi + 12bm_*^2\chi = 1$$

$$\Rightarrow 2\chi (a + 6bm_*^2) = 1$$

$$\Rightarrow \chi = \frac{1}{2(a + 6bm_*^2)}$$

Now when $h \rightarrow 0$ we know
that $m_* \rightarrow \begin{cases} 0, & \text{if } a > 0 \\ \pm \sqrt{\frac{-a}{2b}}, & \text{if } a < 0 \end{cases}$

$$\Rightarrow \lim_{h \rightarrow 0} \chi = \begin{cases} \frac{1}{2a}, & \text{if } a > 0 \\ \frac{1}{2a+12b\left(\frac{-a}{2b}\right)}, & \text{if } a < 0 \end{cases}$$

$$\Rightarrow \lim_{h \rightarrow 0} \chi = \begin{cases} \frac{1}{2a}, & \text{if } a > 0 \\ -\frac{1}{4a}, & \text{if } a < 0 \end{cases}$$



Since χ is related to the 2nd derivative of Φ & since it blows up (or has a discontinuity at T_c) but the 1st derivative (m^*) is continuous at T_c , we can say that London mean field theory predicts a 2nd order phase Transition.

In the presence of External field ($h \neq 0$)

Here $\varphi = -hm + am^2 + bm^4$. The presence of odd power makes ' φ ' asymmetric about origin. The roots of $\frac{\partial \varphi}{\partial m} \Big|_{m_*}$ gives the stable/unstable solⁿ for magnetization.

$$\Rightarrow \frac{\partial \varphi}{\partial m} \Big|_{m_*} = -h + 2am_* + 4bm_*^3 = 0$$

$$\Rightarrow \underline{4bm_*^3 + 2am_* = h}$$

We can analyze the behaviour in the presence of ' h ' graphically.

The point of intersection b/w the two curves $y(m_*) = h$

$$\& y(m_*) = 4bm_*^3 + 2am_*$$

gives the points of extrema of ' φ '.
The curve $y(m_*) = h$ is just a straight horizontal line.

The cubic term $y(m_*) = 4bm_*^3 + 2am_*$ is a bit complicated since it can have local maxima/minima/saddle depending on the sign of 'a'.

Now the critical points of $y(m_*) = 4bm_*^3 + 2am_*$ is given by

$$\frac{\partial y(m_*)}{\partial m_*} = 0 \Rightarrow 12bm_*^2 + 2a = 0$$
$$\Rightarrow m_* = \pm \sqrt{\frac{-a}{6b}}$$

only when $a \leq 0$ there is an extrema.

$$y\left[\pm \sqrt{\frac{-a}{6b}}\right] = \pm 4b\left(\frac{-a}{6b}\right)^{3/2} \pm 2a\left(\frac{-a}{6b}\right)^{1/2}$$

$$= \pm 2\sqrt{\frac{-a}{6b}} \left[2b\left(\frac{-a}{6b}\right) + a \right] = \pm 2\sqrt{\frac{-a}{6b}} \left(\frac{2a}{3} \right)$$

$$\Rightarrow y_{\text{extrema}} = \pm \frac{4}{3} a \sqrt{\frac{-a}{6b}}$$

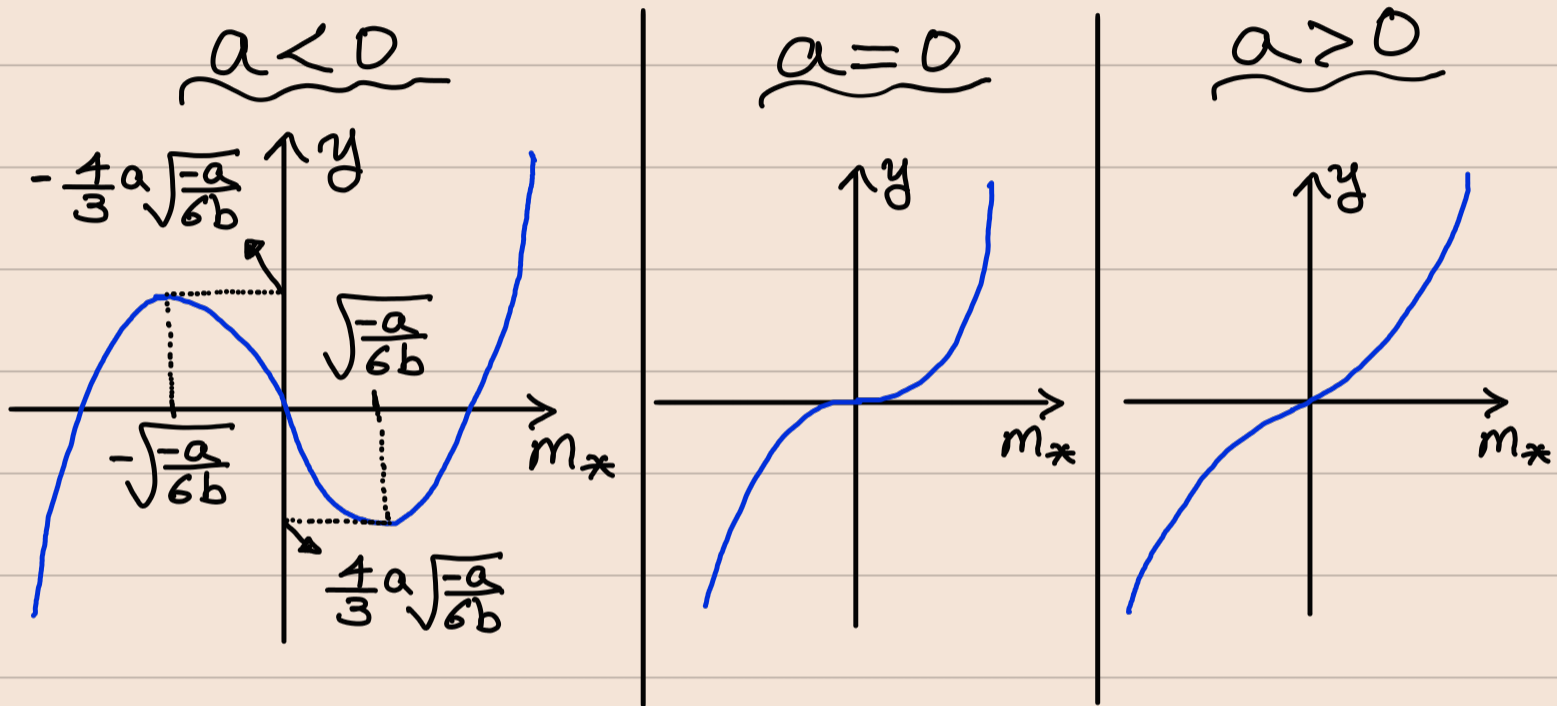
$$\text{If } a < 0, \quad m_* = -\sqrt{\frac{-a}{6b}} \Rightarrow \text{maxima}$$

$$\& \quad m_* = \sqrt{\frac{-a}{6b}} \Rightarrow \text{minima}$$

$$\text{If } a = 0 \Rightarrow m_* = 0 \Rightarrow \text{saddle point}$$

But when $a > 0$, $y(m_*) = 4bm_*^3 + 2am_*$ is monotonically increasing function.

Thus we get three scenarios for $y(m_*) = 4bm_*^3 + 2am_*$

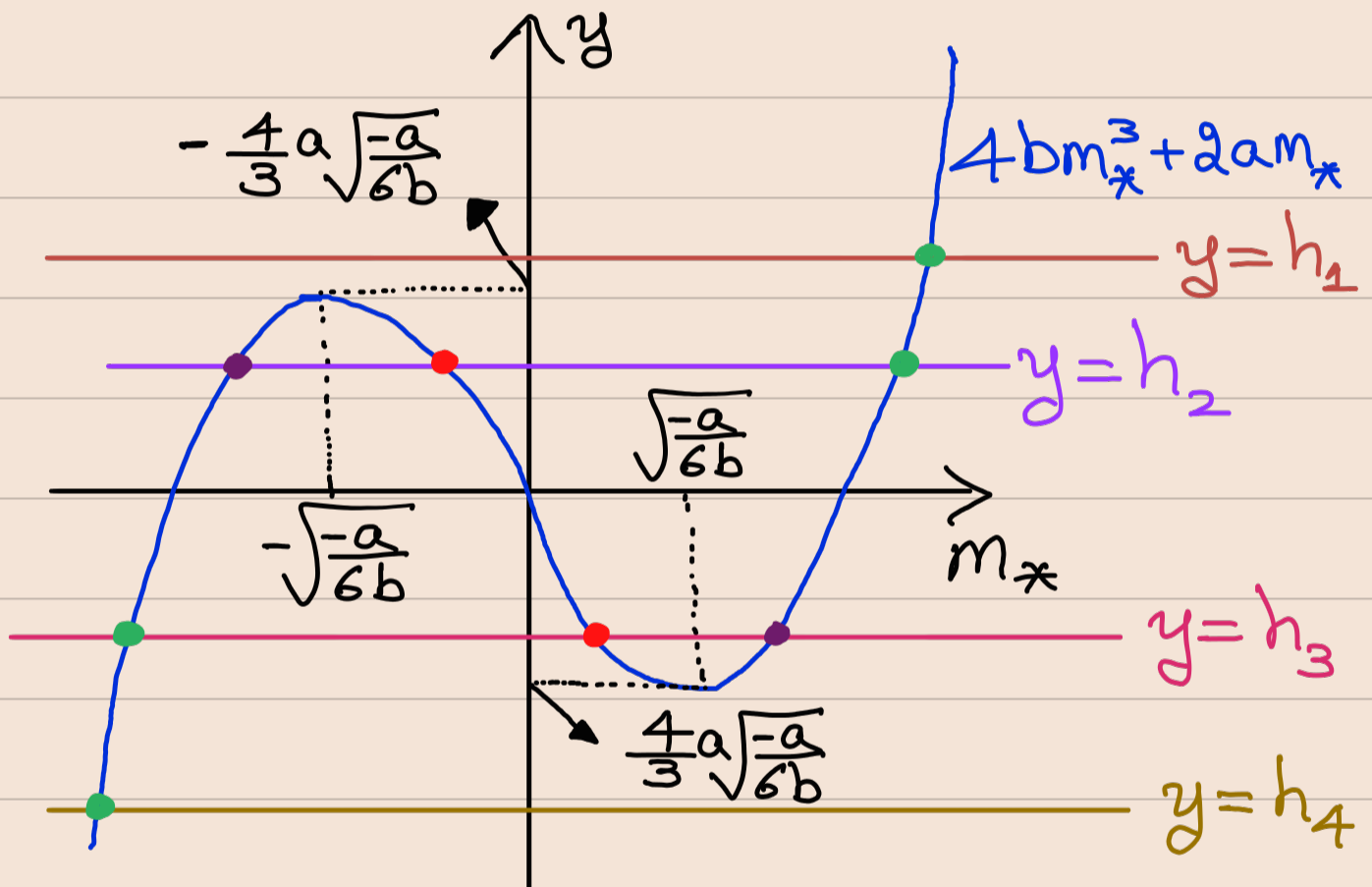


Now consider the roots of:

$$\left. \frac{\partial \phi}{\partial m} \right|_{m_*} = -h + 2am_* + 4bm_*^3 = 0$$

When $a \geq 0$ there is only one solⁿ for ' m_* ' which is a function of ' h ' & ' T '.

But when $a < 0$, the curves for intersection $y(m_*) = h$ & $y(m_*) = 4bm_*^3 + 2am_*$ have either three or one intersection points depending on the value of 'h'



- Unstable points
- Meta stable points
- Stable points

$$\frac{4}{3}a\sqrt{\frac{-a}{6b}} < h_2, h_3 < -\frac{4}{3}a\sqrt{\frac{-a}{6b}}$$

$$h_1 > -\frac{4}{3}a\sqrt{\frac{-a}{6b}} \quad \& \quad h_4 < \frac{4}{3}a\sqrt{\frac{-a}{6b}}$$

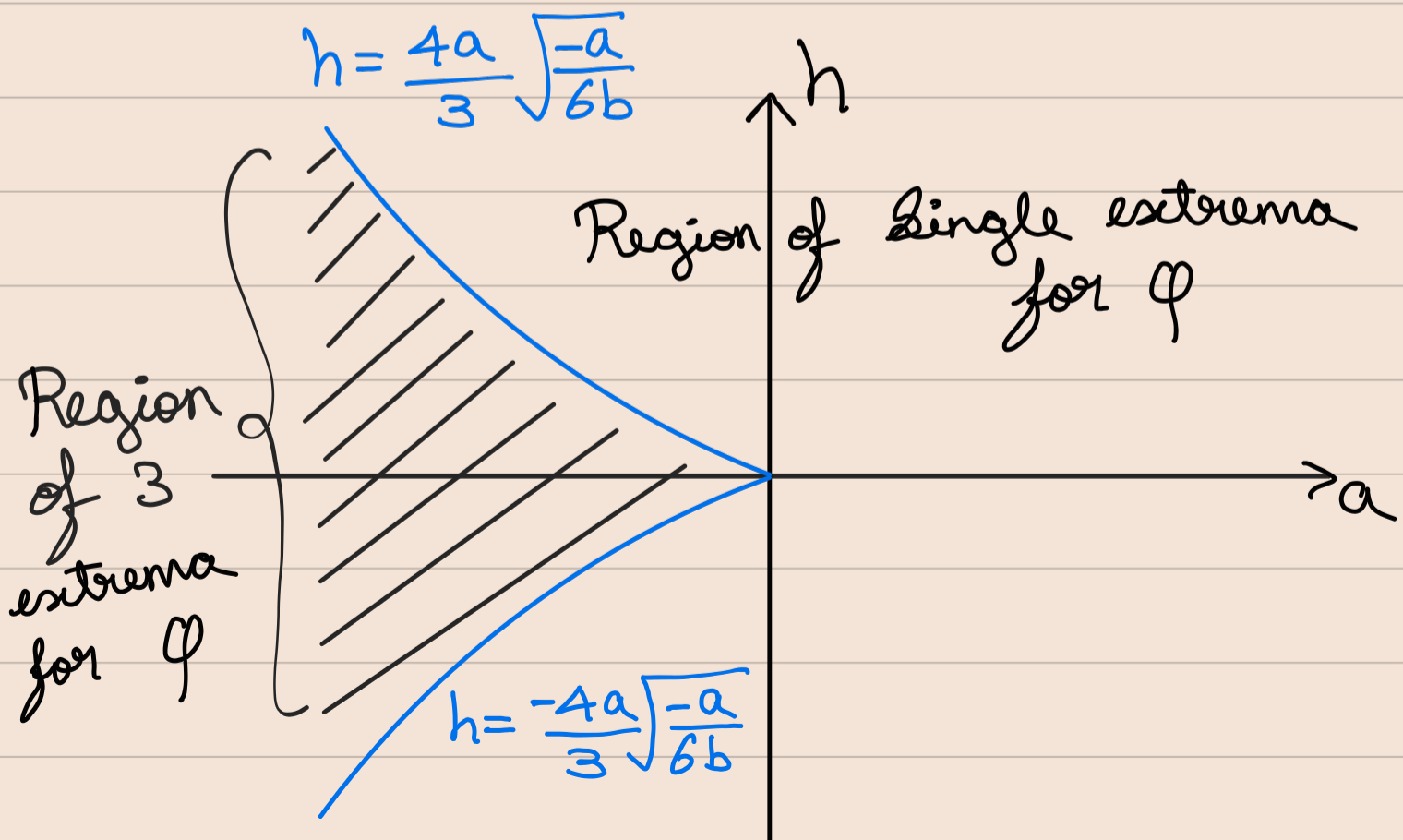
Thus if $-\frac{4a}{3}\sqrt{\frac{-a}{6b}} < h < \frac{4a}{3}\sqrt{\frac{-a}{6b}}$

$h_c = -\frac{4a}{3}\sqrt{\frac{-a}{6b}} \Rightarrow$ coercive magnetic field

then there are three intersection point $\neq$ hence three extremas for

$$\varphi = -hm + am^2 + bm^4$$

One is a stable global minima, one is a meta stable local minima $\neq$ lastly one is an unstable maxima.

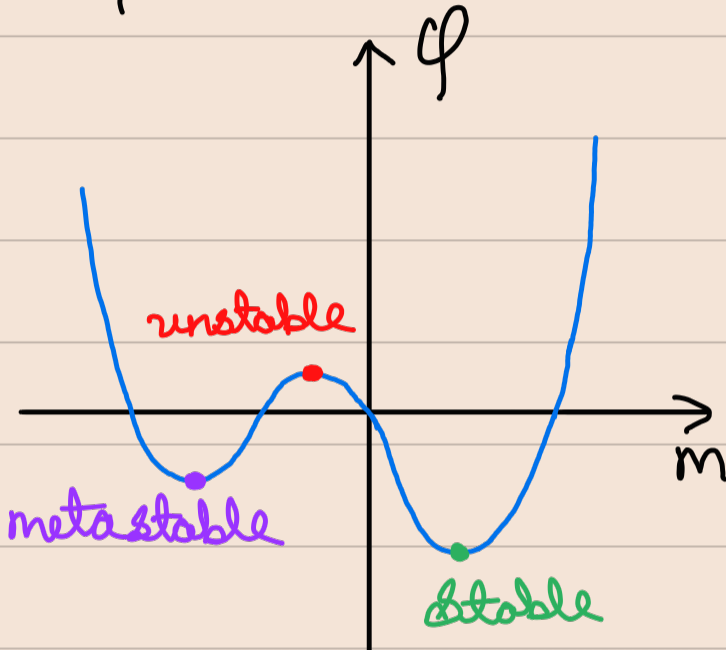


If $a < 0$ ($T < T_c$), then in presence of 'h'

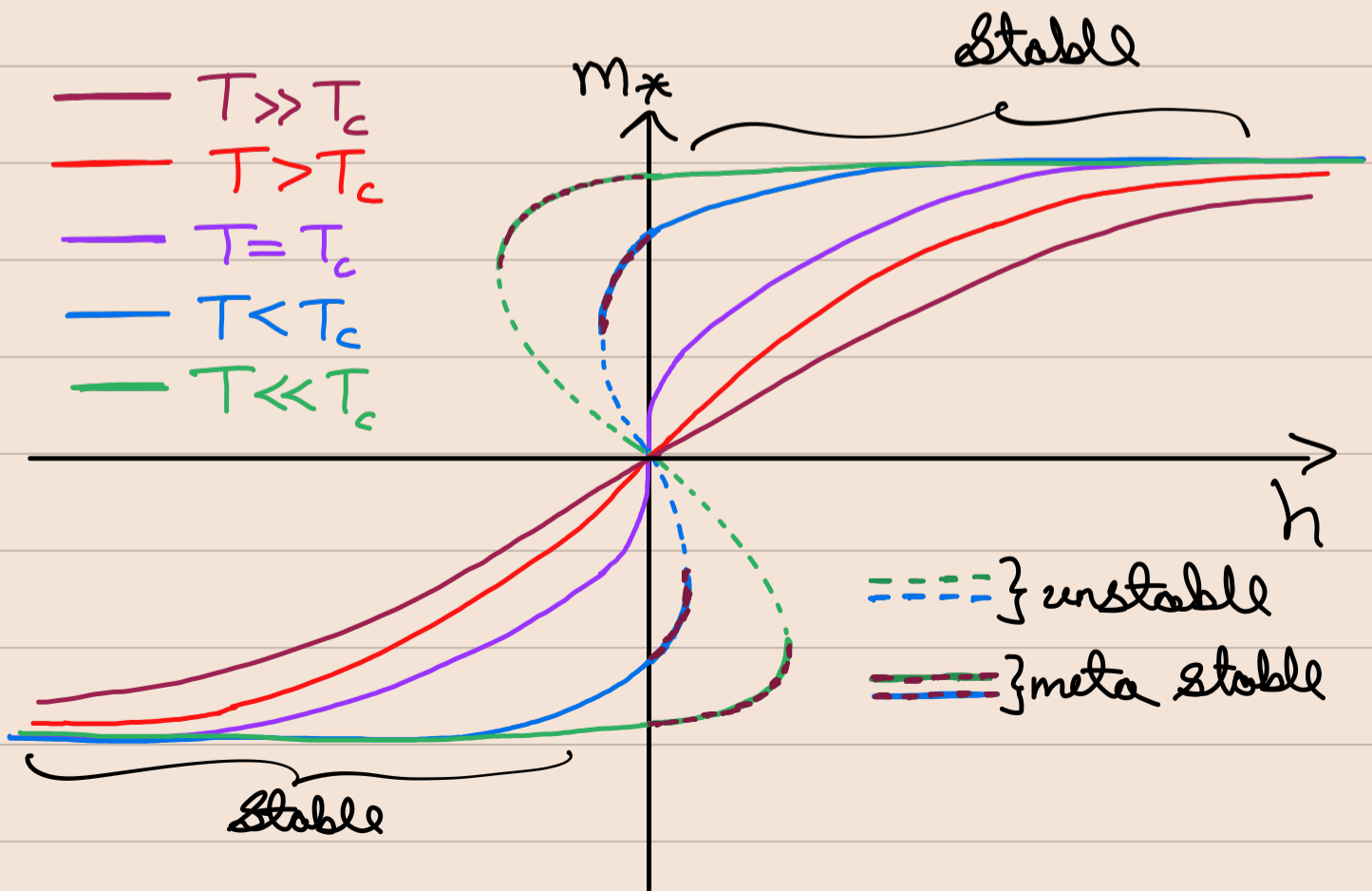
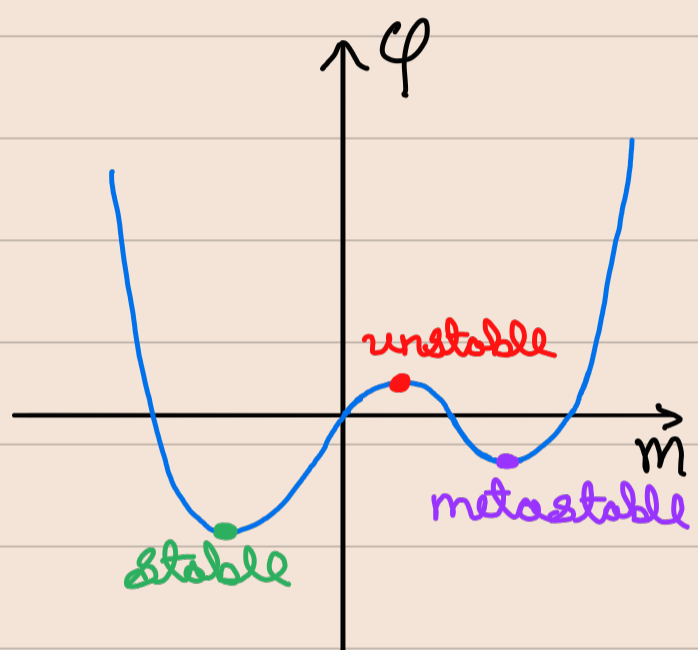
such that $\frac{4a\sqrt{-a}}{3\sqrt{6b}} < h < -\frac{4a\sqrt{-a}}{3\sqrt{6b}}$

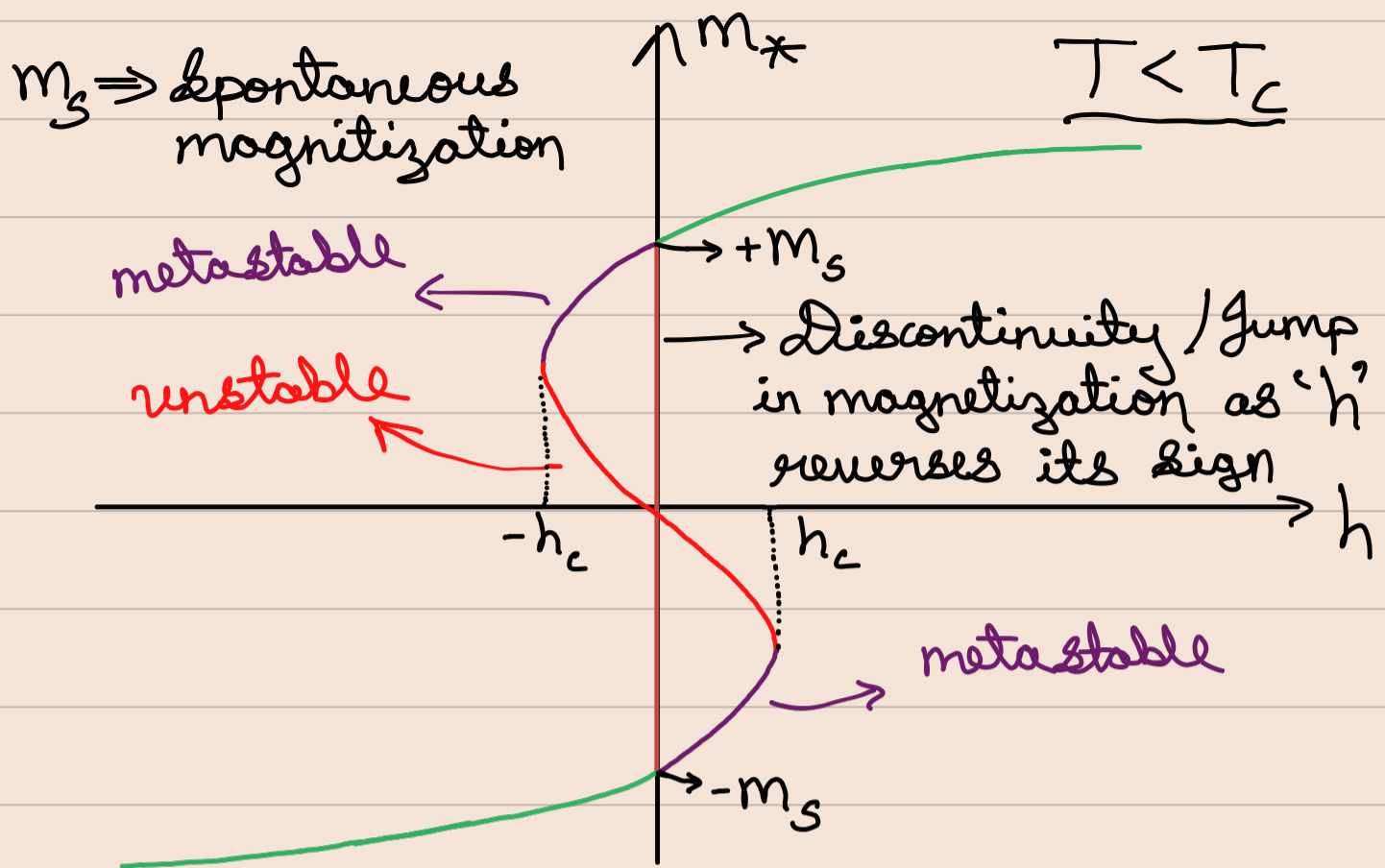
φ is an asymmetric double well.

$$0 < h < -\frac{4a\sqrt{-a}}{3\sqrt{6b}}$$



$$\frac{4a\sqrt{-a}}{3\sqrt{6b}} < h < 0$$





When $a = 0$ i.e. at $T = T_c$

$$\varphi = -hm + bm^4$$

$$\Rightarrow \left. \frac{\partial \varphi}{\partial m} \right|_{m_*} = -h + 4bm_*^3$$

Stable solⁿ when $m_* = \left(\frac{h}{4b} \right)^{\frac{1}{3}}$

$$\Rightarrow \underline{m_* \propto h^{1/3}} \quad (\text{at } T_c) \quad (b \propto T_c)$$