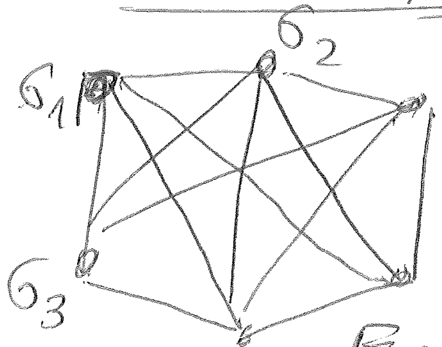
Lecture 10 (1)

Ising model. Mean-field theory of ~~continuous phase transitions~~



We consider all-to-all interaction.
(Comlete graph)

Energy is a sum of spin pairs

$$E = -J\sigma_1\sigma_2 - J\sigma_1\sigma_3 - J\sigma_1\sigma_4 - \dots$$
$$- J\sigma_2\sigma_3 - J\sigma_2\sigma_4 - \dots \Rightarrow$$

Energy is

$$E = -\frac{1}{2}J\sum_{j\neq i}\sigma_i\sigma_j - H\sum_{i=1}^{n}\sigma_i$$

Rescaling

$$J \to \frac{J}{N} \qquad \vec{\sigma} = (\sigma_1\sigma_2\dots\sigma_N)$$

Energy equals

$$E(\vec{\sigma}) = -\frac{J}{2N}\sum_{j\neq i}\sigma_i\sigma_j - H\sum_{i=1}\sigma_i$$

Partition function

$$Z = \sum_{\{\vec{\sigma}\}} e^{-\beta E(\vec{\sigma})}$$

We can write

$$\sum_{j\neq i}\sigma_i\sigma_j = \left(\sum_i\sigma_i\right)\left(\sum_j\sigma_j\right) - \sum_{ij}\sigma_i\sigma_j\delta_{i,j}$$

$$= \left(\sum_i\sigma_i\right)^2 - \sum_{i=1}^{N}\sigma_i^2 = \left(\sum_i\sigma_i\right)^2 - N$$

Thus, the energy is

$$E(\sigma) = -\frac{J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2 + \frac{J}{2} - H\sum_i \sigma_i$$

We use so-called the Hubbard-Stratonovich transformation:

$$e^{+\frac{A^2}{2}} = \int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\, e^{-\frac{x^2}{2}+xA}$$

In order to prove this equality, we can rewrite

$$-\frac{x^2}{2} + xA = -\frac{(x-A)^2}{2} + \frac{A^2}{2}$$

The integral takes a form

$$\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\, e^{-\frac{x^2}{2}+xA} = \int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\, e^{-\frac{(x-A)^2}{2}+\frac{A^2}{2}}$$

$$= e^{\frac{A^2}{2}}\underbrace{\int_{-\infty}^{\infty}\frac{dy}{\sqrt{2\pi}}\, e^{-\frac{y^2}{2}}}_{=1} = e^{A^2/2}$$

Partition function is

$+\beta H\sum_{i=1}^{N}\sigma_i$

$$Z=\sum_{\vec{\sigma}}{}' e^{-\beta E(\sigma)}=\sum_{\vec{\sigma}}{}' e^{+\frac{\beta J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2-\frac{\beta J}{2}}$$

We introduce

$$A^2\equiv\frac{\beta J}{N}\left(\sum_{i=1}^{N}\sigma_i\right)^2\Rightarrow A=\sqrt{\frac{\beta J}{N}}\left(\sum_{i=1}^{N}\sigma_i\right)$$

Using the Hubbard-Stratonovich transformation, we get

$$Z=\sum_{\vec{\sigma}}{}'\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\,e^{-\frac{x^2}{2}+Ax+\beta H\sum\sigma_i}$$

$+\beta H\sum\sigma_i-\beta J/2$

$$=\sum_{\{\sigma\}}\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}\exp\left[-\frac{x^2}{2}+x\sqrt{\frac{\beta J}{N}}\left(\sum_{i=1}^{N}\sigma_i\right)\right]$$

Replacement. We use a new variable

$$x=m\sqrt{N\beta J}$$

Then

$$Z=\sum_{\{\sigma\}}{}'\int_{-\infty}^{\infty}\frac{dm}{\sqrt{2\pi}}\sqrt{N\beta J}\,\exp\left[-\frac{m^2N\beta J}{2}+\beta J\,m\sum_{i=1}^{N}\sigma_i\right]$$

$+\beta H\sum\sigma_i$
$-\beta J/2$

Summation over spins states ($\sigma_i = \pm 1$) ④

$$\sum_{\{\sigma_1\sigma_2\ldots\sigma_N\}} e^{-(m\beta J+\beta H)\sum_{i=1}^{N}\sigma_i} = \prod_{i=1}^{N}\sum_{\sigma_i=\pm 1} e^{-(m\beta J+\beta H)\sigma_i} =$$

$$= \prod_{i=1}^{N} 2\cosh(m\beta J+\beta H) = \left[2\cosh(m\beta J+\beta H)\right]^N$$

we get

$$Z = \int_{-\infty}^{\infty}\frac{dm}{\sqrt{2\pi/N\beta J}}\exp\left\{-\frac{1}{2}N\beta J m^2\right\}\times$$

$$\times\left[2\cosh(m\beta J+\beta H)\right]^N$$

The partition function takes a form

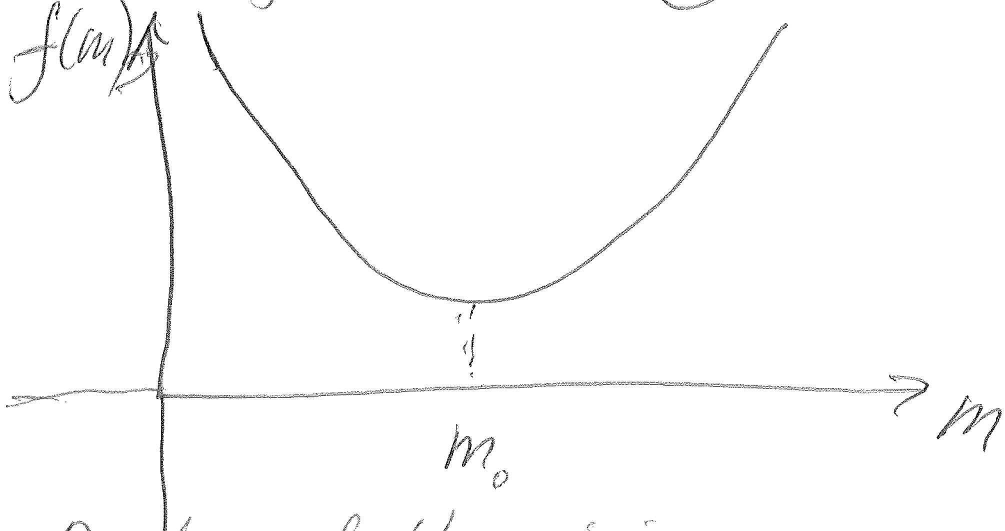
$$\boxed{Z = \int_{-\infty}^{\infty} dm\sqrt{\frac{N\beta J}{2\pi}}\exp\left\{-\frac{1}{2}N\beta J m^2 + N\ln 2\mathrm{ch}(m\beta J+\beta H)\right\}}$$

~~Free energy $f(m)$ per spin is~~

$$\boxed{f = +\frac{1}{2}J m^2 - T\ln\left[2\mathrm{ch}(\beta J m+\beta H)\right]}$$

$$\boxed{Z = \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty} dm\,\cancel{\exp[-\beta N f(m)]}\ \exp[-\beta N f(m)]}$$

Plot $f(m)$ versus m



Position of the minimum is given by an equation

$$f'(m_0) = 0$$

We obtain

$$f'(m) = \cancel{\beta} J m - \frac{\cancel{T}\cancel{2}\, sh(\beta J m + \beta h)\cancel{\beta} J}{\cancel{2} ch(\beta J m + \beta H)} = 0$$

$$= J m - J\, th(\beta J m + \beta H)$$

Therefore

$$\Rightarrow \boxed{m = th(\beta J m + \beta H)}$$

This equation determines the position of the minimum of $f(m)$

In zero magnetic field, we have

$$\begin{cases} m = th\, \beta J m \\ f(m) = \frac{1}{2} J m^2 - T \ln\left[2 ch(\beta J m)\right] \end{cases}$$

Let us solve the equation for m.

<u>Graphic method.</u>

$$m = \tanh \beta J m$$

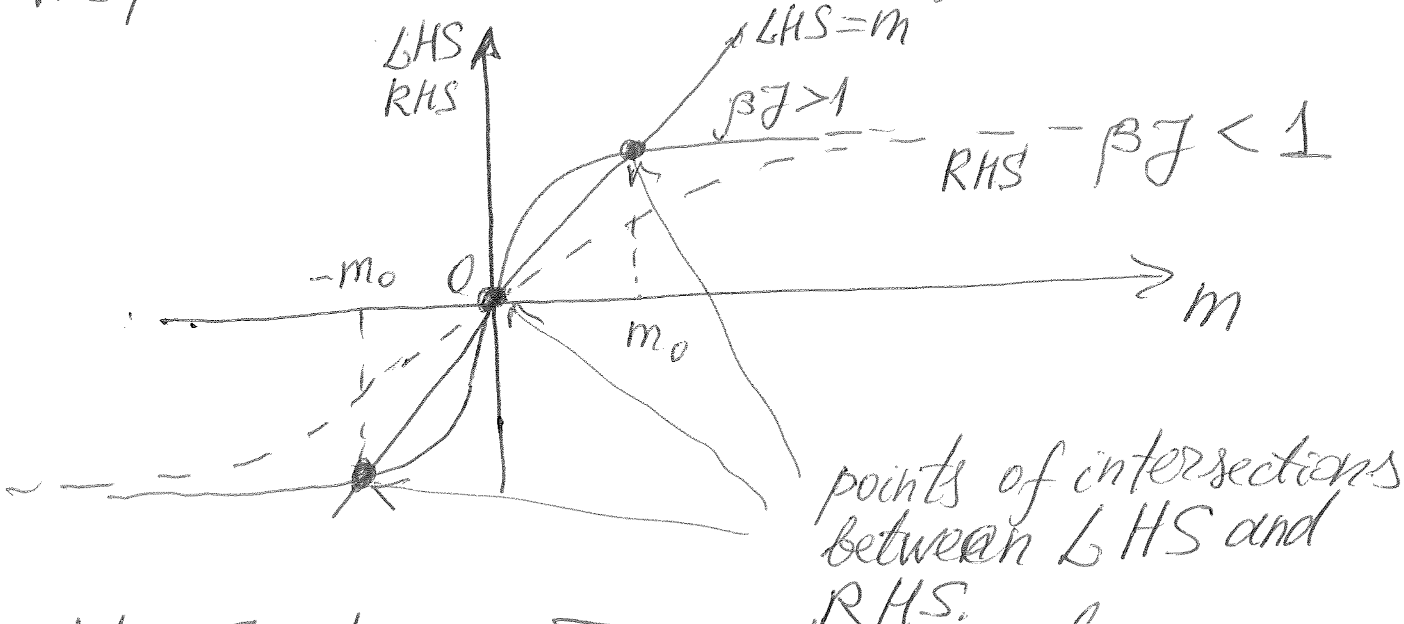
Left-hand side

$$LHS = m$$

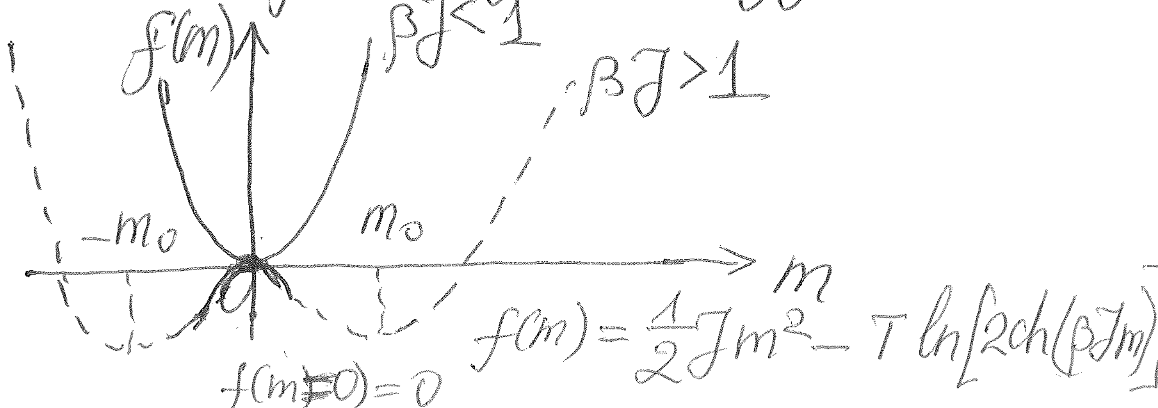
Right-hand side

$$RHS = \tanh \beta J m \approx \beta J m + O(m^3)$$

We plot LHS and RHS as function of m.



At $\beta J < 1$, i.e. $T > J$, there is only one solution, namely, $m = 0$.
At $\beta J > 1$, i.e at $T < J$, there are three solutions: $m = 0$, $m = \pm m_0$
These solutions correspond to minima and maximum of the $f(m)$



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In the thermodynamic limit $N \to \infty$,
Free energy $\mathcal{F}$ is equal to

$$\mathcal{F} = -T \ln Z \approx f(m_0)$$

This follows from

$$Z \approx \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} dm\, e^{-TNf(m)}$$

we use so-called

Saddle-point method:

~~Teylor expansion near~~ minimum

$$f(m) = f(m_0) + \underbrace{f'(m_0)}_{=0}(m - m_0) + \frac{1}{2} f''(m - m_0)^2$$

we have

$$Z = \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} dm\, \exp\left\{ -\beta N f(m_0) - \frac{1}{2}\beta N f''(m_0)(m - m_0)^2 \right\}$$

$$= e^{-\beta N f(m_0)} \sqrt{\frac{N\beta J}{2\pi}} \underbrace{\int_{-\infty}^{\infty} e^{-\frac{1}{2}\beta N f''(m - m_0)^2} dm}_{= \sqrt{\frac{2\pi}{\beta N f''(m_0)}}}$$

the Gaussian integral

$$= e^{-\beta N f(m_0)} \sqrt{\frac{\cancel{N\beta} J}{\cancel{2\pi}}} \cdot \sqrt{\frac{\cancel{2\pi}}{\cancel{\beta N} f''(m_0)}}$$

Thus

$$Z = \sqrt{\frac{J}{f''(m_0)}} \exp\left(-\beta N f(m_0)\right)$$

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Free-energy is

$$\mathcal{F} = -\frac{T}{N} \ln Z = -\frac{T}{N}\left\{-\beta N f(m_0) + \ln\sqrt{\frac{J}{f''(m_0)}}\right\}$$

$$= f(m_0) - \underbrace{\frac{T}{N} \ln\sqrt{\frac{J}{f''(m_0)}}}_{\to 0,\ N\to\infty}$$

Thus we obtain

$$\boxed{\mathcal{F} \underset{N\to\infty}{=} f(m_0)} \qquad \mathcal{F} = N f(m_0, T, H)$$

$$\frac{\partial \mathcal{F}}{\partial m} = 0$$

Free energy

$$f(m) = \frac{1}{2} J m^2 - T \ln[2 ch(\beta J m + \beta H)]$$

Minimum energy

Magnetic moment of a spin:

$$f'(m) = 0 \Rightarrow m = th[\beta m] + \beta H]$$

Critical temperature $T_c = J$

Susceptibility is determined by an equation

$$\chi = \frac{dm}{dH} = \frac{1}{ch^2[\beta m] + \beta H]}\left[\beta J \frac{dm}{dH} + \beta\right]$$

$$\frac{dm}{dH}\left(1 - \frac{\beta J}{ch^2[\beta m] + \beta H)}\right) = \frac{\beta}{ch^2[?}$$

Physical meaning of m

magnetic moment

Thermodynamic relationship between magnetization m and the free energy f

$$m = -\frac{df}{dH}$$

We use our result. In our case, this derivative is

$$\frac{df}{dH} = \frac{\partial f}{\partial m}\overset{=0 \text{ (because we stay in minimum)}}{} \frac{dm}{dH} + \frac{\partial f}{\partial H} =$$

$$= -T\,\frac{\beta\, sh(\beta J m + \beta H)}{ch(\beta J m + \beta H)} = -th(\beta J m + \beta H) = -m$$

because

$$m = th(\beta J m + \beta H)$$

Thus, m has a meaning of the magnetization

Susceptibility is

$$\chi \equiv \frac{dm}{dH} = \frac{d}{dH}\,th(\beta J m + \beta H) =$$

$$= \frac{1}{ch^2(\beta J m + \beta H)}\left(\beta J \frac{dm}{dH} + \beta\right)$$

$\cancel{\frac{dm}{dH}\ \chi = \frac{\dots}{ch^2()}\beta J \chi +}$

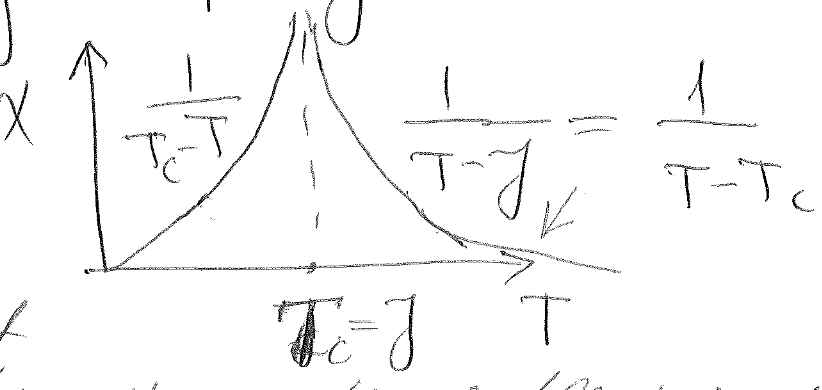
$$\chi = \frac{\beta J}{ch^2()}\chi + \frac{\beta}{ch^2()}$$

$$\chi = \frac{\beta}{ch^2()\left(1 - \frac{\beta J}{ch^2()}\right)} =$$ we get

$$1 = \frac{\beta}{ch^2() - \beta J} \Rightarrow \boxed{\chi = \frac{\beta}{ch^2(\beta J m + \beta H) - \beta J}}$$

Consider $H = 0$ and $T > T_c$. Then $m = 0$
Susceptibility is

$$\chi = \frac{\beta}{1 - \beta J} = \frac{1}{T - J}, \quad T < T_c$$



One can see that $\chi(T)$ diverges at the critical temperature $T_c = J$

Solution at $T < T_c$

$$m = \tanh \beta J m$$

we use the Taylor expansion

$$\text{th}\, x = x - \frac{1}{3} x^3 + O(x^5)$$

Indeed

$$\frac{d\,\text{th}\, x}{dx} = \frac{1}{\text{ch}^2 x}\Big|_{x=0} = 1$$

$$\frac{d^2}{dx^2}\text{th}\, x = -\frac{2\,\text{sh}\, x}{\text{ch}^3 x}\Big|_{x=0} = 0$$

$$\frac{d^3\,\text{th}\, x}{dx^3} = -\frac{2}{\text{ch}^2 x} + \frac{6\,\text{sh}^3 x}{\text{ch}^4 x}\Big|_{x=0} = -2$$

$$\text{th}\, x = x + \frac{1}{3!}(-2)x^3 = x - \frac{1}{3}x^3$$

Our equation takes a form,

$$\Rightarrow m = \beta J m - \frac{1}{3}(\beta J)^3 m^3 + O(m^5)$$

Therefore,

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

we get

$$m^2 = \frac{\beta J - 1}{\frac{1}{3}(\beta J)^3} = \frac{J - T}{\frac{1}{3}\beta^2 J^3}$$

$$\boxed{m \cong a \cdot (T_c - T)^{1/2}} \qquad a = \sqrt{\frac{3T_c^2}{T_c^3}}$$

we obtain a behavior of m near T_c

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

Let us find susceptibility at $T<T_c$.

we have

$$\chi = \frac{\beta}{ch^2 \beta J m - \beta J}$$

we use an equality

$$\frac{1}{ch^2 \beta J m} = \frac{ch^2 - sh^2}{ch^2} = 1 - th^2(\beta J m) = 1 - m^2$$

Therefore,

$$\chi = \frac{\beta}{\frac{1}{1-m^2} - \beta J} = \frac{\beta(1-m^2)}{1-\beta J(1-m^2)}$$

$$= \frac{\beta(1-m^2)}{1-\beta J + \beta J m^2} =$$

$$= \frac{1-m^2}{\frac{1}{\beta J} - 1 + m^2} = \frac{1-m^2}{\frac{T}{T_c} - 1 + 3\left(1-\frac{T}{T_c}\right)} =$$

we find the susceptibility at $T<T_c$

$$\chi \approx \frac{1}{2\left(1-\frac{T}{T_c}\right)}$$

Landau theory

~~Let us show that~~ our exact solution

$$f(m) = \frac{1}{2} J m^2 - T \ln\left[2 ch(\beta J m + \beta H)\right]$$

corresponds to the Landau mean-field theory.
Let us consider $f(m)$ near critical point when $\beta J m, \beta H << 1$. We expand $f(m)$ over m.
Teylor expansion

$\varphi(x) = \ln[2\, ch\, x] =$

$$\varphi(x) = \varphi(x=0) + \varphi'(0) x + \frac{1}{2} \varphi''(0) x^2 + \frac{1}{3!} \varphi'''(0) x^3 + \frac{1}{4!} \varphi^{(IV)}(0) x^4 + \ldots$$

$$\varphi'(x) = \frac{sh x}{ch x} = th x$$

$$\varphi''(x) = \frac{ch x}{ch x} - \frac{sh^2 x}{ch^2 x} = \frac{ch^2 x - sh^2 x}{ch^2 x} = \frac{1}{ch^2 x}$$

$$\varphi'''(x) = -\frac{2\, sh x}{ch^3 x}$$

$$\varphi^{(IV)}(x) = -\frac{2\, ch x}{ch^3 x} + \frac{6\, sh^2 x}{ch^3 x}$$

$$\varphi(0) = \ln 1 = 0$$
$$\varphi'(0) = 0$$
$$\varphi''(0) = 1$$
$$\varphi'''(0) = 0$$
$$\varphi^{(IV)}(0) = -2$$

These are coefficient of the Teylor expansion of $\varphi(x)$

Teylor expansion of $\ln[\operatorname{ch} x]$:

$$\ln[\operatorname{ch} x] = \frac{1}{2}\varphi''(0)x^2 + \frac{1}{4!}\varphi^{(IV)}(0)x^4$$

$$= \frac{1}{2}x^2 + \frac{1}{\underset{4\cdot 3\cdot 2}{4!}}(-2)x^4$$

$$= \frac{1}{2}x^2 - \frac{1}{12}x^4$$

In our model

$$x = \beta J m + \beta H$$

Thus, the free energy is

$$f(m) \approx \frac{1}{2}Jm^2 - T\left[\frac{1}{2}(\beta J m + \beta H)^2 - \frac{1}{12}(\beta J m + \beta H)^4\right]$$

$$\approx \frac{1}{2}Jm^2 - \frac{T}{2}(\beta J m + \beta H)^2 + \frac{T}{12}\beta^4 J^4 m^4$$

$$= \frac{1}{2}Jm^2 - \frac{T}{2}\beta^2 J^2 m^2 - \frac{T}{2}\cdot 2\cdot \beta^2 J m H + \frac{1}{12}\frac{J^4}{T^3}m^4$$

$$\simeq \frac{1}{2} J\left(1-\frac{J}{T}\right) m^2 - \frac{J}{T} mH + \frac{1}{12}\frac{J^4}{T^3} m^4$$

$$T_c = J$$

Finally, at T near $T_c = J$, we obtain

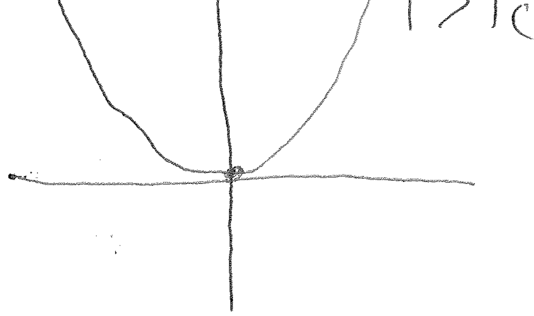
$$f(m) = \frac{1}{2} J\left(1-\frac{T_c}{T}\right) m^2 - mH + \frac{J}{12} m^4$$

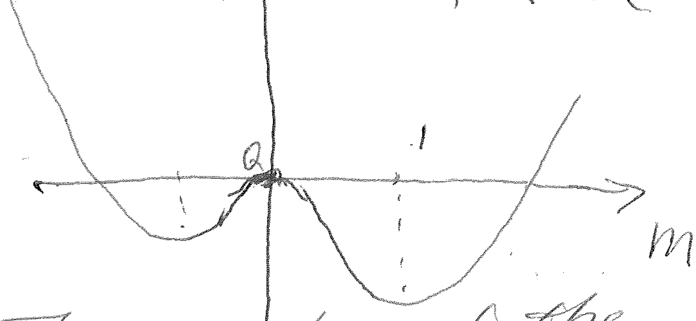
$$= \frac{1}{2}\frac{J}{T}(T-T_c)\, m^2 - mH + \frac{J}{12} m^4$$

Landau proposed (on the basis of analiticity of $f(m)$ near T_c)

$$f(m) = \frac{1}{2} a m^2 - mH + \frac{1}{4} A m^4$$

where $A>0$ and $\begin{cases} a>0 & \text{at } T>T_c \\ a<0 & \text{at } T<T_c \end{cases} \Rightarrow a = a_0\left(1-\frac{T_c}{T}\right)$





The asymmetry of the minima is due to magnetic field H.

Minimization $H=0$

$$\frac{d f(m)}{dm} = 0$$

$$\frac{d f(m)}{dm} = a_0 (T-T_c)\, m \cancel{- H} + A m^3 = 0$$

$M=0$ $$m\,(a_0 (T-T_c) + A m^2) = H \xrightarrow{\text{if } H=0} \boxed{m(a + A m^2) = 0}$$

a we have solutions

if $a_0 (T-T_c) > 0$ $\quad m = 0$

if $a_0 (T-T_c) < 0$ $\quad \begin{cases} m = 0 \\ m = \sqrt{\dfrac{a_0 (T_c - T)}{A}} = \sqrt{T_c - T}\,\sqrt{\dfrac{a_0}{A}} \end{cases}$ two solution

Order parameter is

$$\boxed{m \propto \sqrt{T_c - T}}$$

This is the mean-field result.

Magnetic susceptibility

$$\chi = \left.\frac{dm}{dH}\right|_{H=0}$$

We use the equation

$$a(T-T_c)\,m + A m^3 = H$$

Differention over H gives

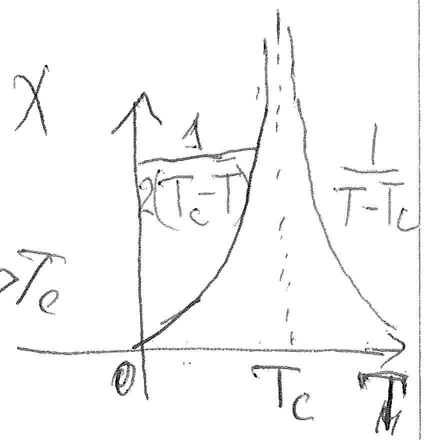
$$\frac{d}{dH}\left[a(T-T_c)\,m + Am^3\right] = 1$$

we get

$$a_0(T-T_c)\frac{dm}{dH} + 3Am^2\frac{dm}{dH} = 1$$

At $T>T_c$, $m^2=0$ and we get

$$a(T-T_c)\frac{dm}{dH} = 1$$



Therefore, the susceptibility at $T>T_c$

$$\chi = \frac{dm}{dH} = \frac{1}{a_0(T-T_c)} \xrightarrow[T\to T_c]{} \infty$$

At $T<T_c$, we get

$$\chi = \frac{dm}{dH} = \frac{1}{a_0(T-T_c)+3Am^2}$$

Using the solution $m=\sqrt{\frac{a_0}{A}(T_c-T)}$, we get

$$\chi = \frac{1}{2a_0(T_c-T)}$$

Thus the exact solution of the Ising model with all-to-all interaction confirms the phenomenological Landau theory.

Finite-size effects

All results presented above were obtained in the thermodynamic limit (infinite size limit)

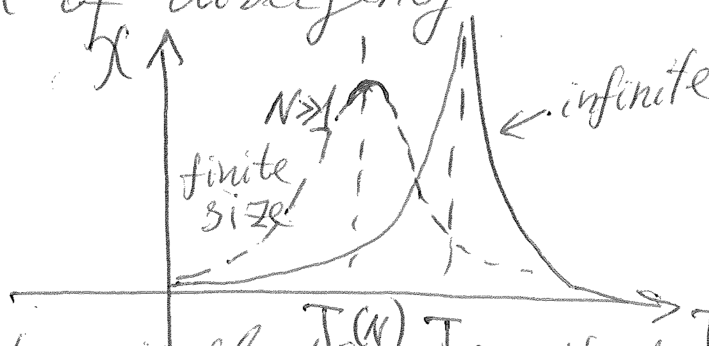
$$N \to \infty$$

In this limit, there is a critical temperature T_c below which the system is in the ordered state with non-zero magnetization. The divergence of susceptibility χ signals the phase transition of the second-order.

In order wards, the system stays an infinite time either in state $m_0 > 0$ (spins up) or $-m_0$ (spins down).

~~...~~ If size N is large but finite, then the life time in these states is large but finite. So, the system can spontaneously jump from one to the other state : $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \xrightarrow{\text{jump}} \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$

The susceptibility has a maximum at $T = T_c$ instead of divergency



$$T_c(N) < T_c$$

It is the spin fluctuations that ~~...~~ break down the phase transition.