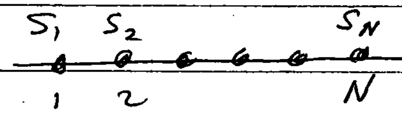
Ising model in 1-dimension

$h=0$ for simplicity



$$\mathcal{H} = -J\sum_{i=1}^{N} s_i s_{i+1}$$

Define $\sigma_i = s_i s_{i+1}$, $i = 1, \cdots, N-1$

$$\sigma_i = \pm 1$$

$$\mathcal{H} = -J\sum_{i=1}^{N-1}\sigma_i \qquad s_1 s_j = \prod_{i=1}^{j-1}\sigma_i = (s_1 s_2)(s_2 s_3)\cdots(s_{j-1}s_j)$$

$$= s_1 s_2^2 s_3^2 \cdots s_{j-1}^2 s_j$$

$$= s_1 s_j$$

For every set of $\{\sigma_i\}_{i=1}^{N-1}$ there are 2 possible spin configurations depending on whether $s_1 = +1$ or -1

For a given value of s_1, then

$$s_j = \frac{1}{s_1}\prod_{i=1}^{j-1}\sigma_i$$

So

$$Z = \sum_{\{s_i\}} e^{\beta J\sum_{i=1}^{N} s_i s_{i+1}} = 2\sum_{\{\sigma_i\}} e^{\beta J\sum_{j=1}^{N-1}\sigma_j} = 2\prod_{i=1}^{N-1}\sum_{\sigma_i=\pm1} e^{\beta J\sigma_i}$$

two values for s_1

$$Z = 2\left[\sum_{\sigma=\pm1} e^{\beta J\sigma}\right]^{N-1} = 2\left[2\cosh\beta J\right]^{N-1}$$

Gibbs free energy

$$G(h=0,T) = -k_B T \ln Z = -k_B T \ln 2 - k_B T (N-1) \ln (2\cosh \beta J)$$

$$g = \lim_{N\to\infty} \frac{G}{N} = -k_B T \ln(2\cosh\beta J)$$

entropy $s = -\left(\frac{\partial g}{\partial T}\right)_{h=0}$ specific heat at const $h=0$ $C = T\left(\frac{\partial s}{\partial T}\right)_{h=0}$

$$= -T\left(\frac{\partial^2 g}{\partial T^2}\right)$$

$$s = k_B \ln(2\cosh\beta J) + \frac{k_B T \; 2}{2\cosh(\beta J)} \frac{\partial}{\partial T}[\cosh(\beta J)]$$

$$= k_B \ln(2\cosh\beta J) + \frac{k_B T}{\cosh(\beta J)} \sinh(\beta J) J \frac{d\beta}{dT}$$

$$= k_B \ln(2\cosh\beta J) - \frac{J}{T}\tanh\beta J$$

$$s = k_B [\ln(2\cosh\beta J) - \beta J \tanh\beta J]$$

At $T\to\infty$, $\beta\to 0$,

$$\cosh\beta J \simeq 1+\frac{1}{2}(\beta J)^2$$

$$\tanh(\beta J) \simeq \beta J$$

$$s \simeq k_B [\ln[2+(\beta J)^2] - (\beta J)^2]$$

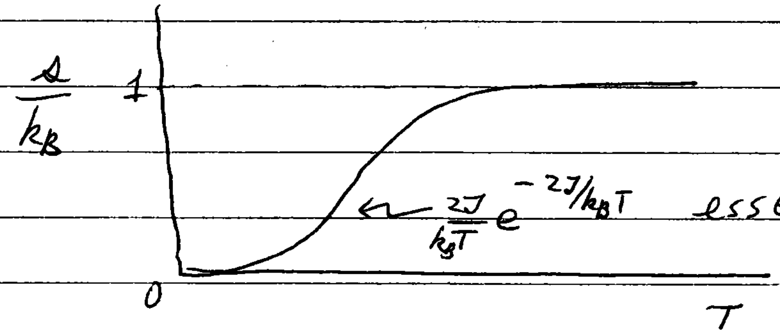
$$\simeq k_B \ln 2 = k_B$$

At $T\to 0$, $\beta\to\infty$

$$\cosh\beta J \simeq e^{\beta J}$$

$$\tanh \simeq \frac{1-e^{-2\beta J}}{1+e^{-2\beta J}} \simeq 1-2e^{-2\beta J}$$

$$s \simeq k_B\left[\ln e^{\beta J} - \beta J(1-2e^{-2\beta J})\right] \simeq \frac{2J}{T} e^{-2J/k_B T}$$



essential singularity at $T=0$

$$C = T\left(\frac{\partial s}{\partial T}\right) = k_B T \left\{ \cancel{\frac{-2J\sinh\beta J}{2\cosh\beta J}\frac{1}{k_B T^2}} + \cancel{\frac{J}{k_B T^2}\tanh\beta J} \right.$$

$$\left. + \frac{\beta J^2}{k_B T^2}\frac{\partial}{\partial(\beta J)}\tanh\beta J \right\}$$

$$= \frac{J^2}{k_B T^2}\frac{\partial}{\partial(\beta J)}\left(\tanh\beta J\right) = \frac{J^2}{k_B T^2}\frac{1}{(\cosh\beta J)^2}$$

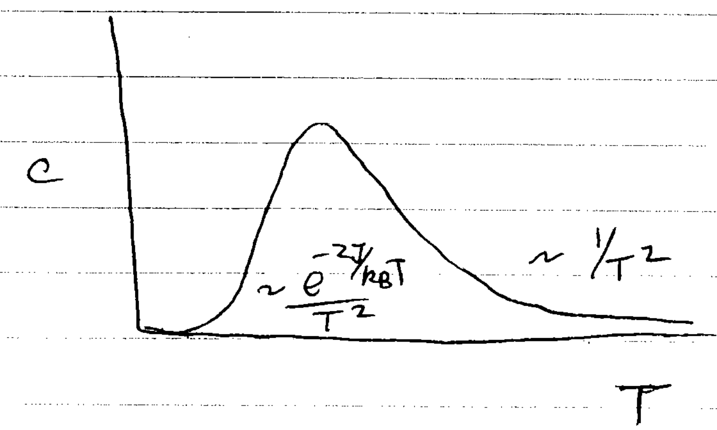
$$\boxed{C = k_B\left(\frac{\beta J}{\cosh\beta J}\right)^2}$$

as $T\to\infty$, $\beta\to 0$

$$C \simeq k_B\left(\frac{J}{k_B T}\right)^2$$

as $T\to 0$, $\beta\to\infty$

$$C \simeq k_B\left(\frac{J}{k_B T}\right)^2 e^{-2J/k_BT}$$



essential singularity at $T=0$

$\Rightarrow$ No singularity at any finite T.

$\Rightarrow$ No phase transition at any finite T

What went wrong with mean field solution?

We said that need $N \to \infty$ degrees of freedom to have a phase transition — but mean field theory is essentially a theory with only <u>one</u> degree of freedom – the order parameter. The singular behavior in the mean field theory comes when we "fix" the mean field solution using the Maxwell construction. But there is no true consideration of the many degrees of freedom which give <u>fluctuations</u> around the average value of the order parameter.

For Ising model, $\chi = \frac{dm}{dh} \to \infty$ at T_c

Now $\quad m = -\frac{\partial g}{\partial h} \quad \Rightarrow \quad \chi = -\frac{\partial^2 g}{\partial h^2} = \frac{1}{N} k_B T \frac{\partial^2 \ln Z}{\partial h^2}$

$$\chi = \frac{k_B T}{N} \left\{ \frac{1}{Z} \frac{\partial^2 Z}{\partial h^2} - \left(\frac{1}{Z} \frac{\partial Z}{\partial h} \right)^2 \right\}$$

$$Z = \int_{\{s_i\}} e^{-\beta H + \beta h M} \qquad \frac{\partial Z}{\partial h} = \int e^{-\beta H + \beta h M} (\beta M)$$

$$\frac{\partial^2 Z}{\partial h^2} = \int e^{-\beta H + \beta h M} (\beta M)^2$$

$$\chi = \frac{k_B T}{N} \beta^2 \left\{ \langle M^2 \rangle - \langle M \rangle^2 \right\} \qquad M = Nm$$

$$\chi = \frac{1}{k_B T} \frac{\langle M^2 \rangle - \langle M \rangle^2}{N}$$

fluctuation in total magnetization M

$$\chi = \frac{N}{k_B T} \left\{ \langle m^2 \rangle - \langle m \rangle^2 \right\}$$

away from T_c, χ is finite

$$\Rightarrow \quad \langle m^2 \rangle - \langle m \rangle^2 = \sigma_M^2 \propto \frac{1}{N}$$

$\sigma_M \propto \frac{1}{\sqrt{N}}$ fluctuation in average magnetization density $\to 0$ as $N \to \infty$

But at T_c, $\chi \to \infty$

$\Rightarrow \sigma_M \to \infty$ fluctuations in average magnetization diverge $\Rightarrow$ must include the effect of fluctuations to correctly describe the critical behavior

~~How to fix Landau Theory - take m(r) spatially varying~~

~~$f(m,T) = a m^2 + b m^4 + (\vec{\nabla} m)^2$~~

~~↑ spatial derivatives cost in energy~~

Landau-Ginzburg approach

Order parameter may vary slowly in space to represent a fluctuation from a perfectly ordered system.

free energy functional

general d-dimensional space

$$F[m(\vec{r})] = \int d^d r \left\{ a m^2 + b m^4 + c |\vec{\nabla} m|^2 \right\}$$

where $a = a_0 (T - T_c)$ vanishes at T_c as before

b = constant

c = constant — measures stiffness to spatial variations in $m(\vec{r})$.

Consider small fluctuations away from the mean field solution m_0. $m_0 = 0$ for $T > T_c$, $m_0 = \sqrt{\frac{a_0 (T_c - T)}{2b}}$ for $T < T_c$

$m(\vec{r}) = m_0 + \delta m(\vec{r})$ expand F to $O(\delta m^2)$

$$F[m(\vec{r})] = \int d^d r \left\{ a m_0^2 + 2 a m_0 \delta m + a \delta m^2 + b m_0^4 + 4 b m_0^3 \delta m + 12 b m_0^2 \delta m^2 + c |\vec{\nabla} \delta m|^2 \right\}$$

the constant terms $a m_0^2 + b m_0^4$ give the mean field free energy.

the linear terms $(2 a m_0 + 4 b m_0^3) \delta m$ vanish because m_0 minimizes F.

The remaining quadratic terms are

$$\delta F = \int d^d r \left\{ \left[a + 12 b m_0^2\right] \delta m^2 + c \, |\vec{\nabla} \delta m|^2 \right\}$$

$$= \int d^d q \left[a + 12 b m_0^2 + c q^2 \right] \delta m_q \delta m_{-q}$$

where δm_q is the Fourier transf of $\delta m(\vec{r})$

Correlation function

To average over fluctuations, we should compute the partition function

$$Z = \prod_q \int d\delta m_q \, e^{-\beta \delta F[\delta m]}$$

$$\Rightarrow \quad \langle \delta m_q \delta m_{-q} \rangle = \frac{\int d\delta m_q \, e^{-\beta[a + 12 b m_0^2 + c q^2] \delta m_q \delta m_{-q}} \, \delta m_q \delta m_{-q}}{\int d\delta m_q \, e^{-\beta[a + 12 b m_0^2 + c q^2] \delta m_q \delta m_{-q}}}$$

$$\langle \delta m_q \delta m_{-q} \rangle = \frac{k_B T}{2(a + 12 b m_0^2 + c q^2)}$$ doing the Gaussian integrations

take Fourier transf

$$\int d^d q \, e^{i \vec{q} \cdot \vec{r}} \langle \delta m_q \delta m_{-q} \rangle = \langle \delta m(\vec{r}) \delta m(0) \rangle = \int d^d q \, e^{i q \cdot r} \frac{k_B T}{a' + c' q^2}$$

$$a' = 2a + 24 b m_0^2$$

$$c' = 2c$$

$$\langle \delta m(r)\,\delta m(0)\rangle = \int d^d q \, \frac{e^{i q \cdot r}\, k_B T}{a' + c' q^2} \sim \frac{e^{-r/\xi}}{r^{d-2}}$$ ← Ornstein Zernike form

where $\xi = \sqrt{\frac{c'}{a'}}$ is decay length, or "correlation" length

comes because pole of integrand is at $q = \pm i \sqrt{\frac{a'}{c'}}$

For $T > T_c$, $a' = 2a = 2a_0(T - T_c)$ (since $m_0 = 0$)

$$\xi \propto \frac{1}{|T - T_c|^{\nu}} \qquad \nu = 1/2 \quad \text{correlation length exponent}$$

For $T < T_c$, $a' = 2a + 24 b m_0^2$

$$= 2a_0(T - T_c) + 24b\left(\frac{a_0(T_c - T)}{2b}\right)$$

$$= 10 a_0 (T_c - T)$$

$$\Rightarrow \xi \propto \frac{1}{|T_c - T|^{\nu}} \qquad \nu = 1/2$$

As $T \to T_c$ the correlation length diverges
fluctuations at $\vec{r}$ propagate out a distance ξ
so as $T \to T_c$ length scale of fluctuations diverges
$\Rightarrow$ fluctuations important at critical point!

Contribution to total free energy from fluctuations δm

$$\delta F = \int d^d q \, [a + 12 b m_0^2 + c q^2] \delta m_q \delta m_{-q}$$

let $a + 12 b m_0^2 = a' = a_0' |T - T_c|$

where $a_0' = a_0$ for $T > T_c$

$= a_0$ for $T < T_c$

$$Z = \prod_q \left[\int d\delta m_q \, e^{-\beta [a' + c q^2] \delta m_q \delta m_{-q}} \right.$$

$$= \prod_q \left(\frac{2\pi k_B T}{2(a' + c q^2)} \right)^{1/2}$$

$$\delta G = -k_B T \ln Z = -\frac{k_B T}{2} \int d^d q \, \ln \left(\frac{\pi k_B T}{a' + c q^2} \right)$$

contribution to specific heat

$$\delta C = -T \frac{\partial^2 \delta G}{\partial T^2}$$

Consider $T > T_c$ so $a' = a_0 (T - T_c)$

$$\frac{\partial \delta G}{\partial T} = -\frac{k_B}{2} \int d^d q \, \ln \left(\frac{\pi k_B T}{a' + c q^2} \right)$$

$$- \frac{k_B T}{2} \int d^d q \left\{ \frac{1}{T} - \frac{a_0}{a' + c q^2} \right\}$$

comes from T dependence of $a' = a_0 (T - T_c)$

$$\frac{\partial^2 \delta G}{\partial T^2} = -\frac{k_B}{2}\int d^dq \left\{ \frac{1}{T} - \frac{a_0}{a' + cq^2} \right\}$$

$$+ \frac{k_B}{2}\int d^dq \left\{ \frac{a_0}{a'+cq^2} \right\}$$

$$- \frac{k_B T}{2}\int d^dq \left\{ \frac{a_0^2}{(a'+cq^2)^2} \right\}$$

$$= -\frac{k_B}{2}\int d^dq \frac{1}{T} + k_B \int d^dq \frac{a_0}{a'+cq^2} - \frac{k_B T}{2}\int d^dq \frac{a_0^2}{(a'+cq^2)^2}$$

$$\delta C = -T\frac{\partial^2 \delta G}{\partial T^2} = \frac{k_B}{2}\int d^dq - k_B T\int d^dq \frac{a_0}{a'+cq^2} + \frac{k_B T^2}{2}\int d^dq \frac{a_0^2}{(a'+cq^2)^2}$$

Classical $\frac{1}{2}k_B$ per degree of freedom

corrections due to T-dependence of coefficient $a(T)$ in δF

To see how the integrals behave as $T \to T_c$,

$$\int d^dq \frac{a_0}{a_0 t + cq^2} \qquad \text{where } t = T - T_c \qquad \text{let } q^2 = t q'^2$$

$$= t^{d/2}\int d^dq' \frac{a_0}{a_0 t + c t q'^2} = t^{\frac{d}{2}-1} \underbrace{\int d^dq' \frac{a_0}{a_0 + cq'^2}}_{\text{some number}}$$

$$\propto t^{\frac{d}{2}-1} = t^{\frac{d-2}{2}} \propto \xi^{2-d}$$

Similarly

$$\int d^dq \frac{a_0}{(a_0 t + cq^2)^2} \propto t^{\frac{d}{2}-2} = t^{\frac{d-4}{2}} \propto \xi^{4-d}$$

The second integral is the more singular one

For mean field theory to be valid as $T \to T_c$,
we want the correction δC to be small compared
to C_{MF} the mean field value.

In mean field theory, $C_{MF} \sim$ finite at T_c
$\delta C \sim t^{\frac{d-4}{2}}$

δC will diverge whenever $d < 4$

$\rightarrow$ $d > 4 \Rightarrow$ fluctuations negligible
mean field theory gives correct critical exponents
$d < 4 \rightarrow$ fluctuations give singular corrections
mean field theory breaks down
$\Rightarrow$ Renormalization Group approach.

$d_c = 4$ is called the <u>upper critical dimension</u>
the value of d_c can vary with the
symmetry of $F[m(r)]$.
$d_c = 4$ for spherically symmetric
n component spin models
mean field theory is OK only when $d > d_c$

Also a <u>lower critical dimension</u> - depends on n
For $d <$ lower critical dimension, there is no phase
transition at finite temperature

Note: The mean field approx is exact in the limit that every spin interacts with every other spin (not just nearest neighbors). Then

$$\mathcal{H} = -\tilde{J} \sum_{i,j} s_i s_j - h \sum_i s_i$$

$$= -\tilde{J} \sum_i s_i \left(\sum_j s_j \right) - h \sum_i s_i$$

$$= -\tilde{J} \sum_i s_i \, Nm - h \sum_i s_i$$

$$\mathcal{H} = -\left(\frac{z J}{2} m + h \right) \sum_i s_i$$

where we took $J \equiv \frac{2}{z} \frac{\tilde{J}}{N}$. For infinite range coupling model, need to take coupling $J \propto \frac{1}{N}$ so that total energy scales with $E \propto N$ as desired.

In the above, $m[s_i] = \frac{1}{N} \sum_j s_j$ depends on the config $\{s_i\}$, however it is the same for every spin s_i