

What went wrong with mean field solution?

We said that need  $N \rightarrow \infty$  degrees of freedom to have a phase transition — but mean field theory is essentially a theory with only one 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 fluctuations around the average value of the order parameter.

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

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

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

$$Z = \int_{\{S_i\}} e^{-\beta H + \beta h M}$$

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

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

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

$$M = Nm$$

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

fluctuation in total magnetization  $M$ .

$m = M/N$  magnetization density

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

For  $T \neq T_c$ ,  $\chi$  is finite as  $N \rightarrow \infty$  in the thermodynamic limit

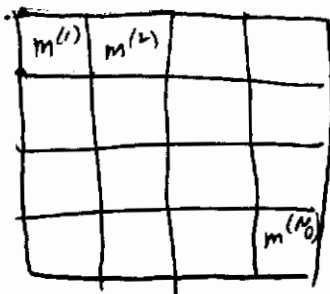
$$\Rightarrow \langle m^2 \rangle - \langle m \rangle^2 \sim \frac{1}{N}$$

or fluctuations in magnetization density

$$\sqrt{\langle m^2 \rangle - \langle m \rangle^2} \sim \frac{1}{\sqrt{N}} \rightarrow 0 \text{ as } N \rightarrow \infty$$

We can understand the  $1/\sqrt{N}$  dependence as follows.

Imagine we subdivide our total system into  $N_0$  subsystems. If each subsystem is sufficiently large we can expect the subsystems will be behaving independently of one another.  $\Rightarrow$  the



measured magnetization densities  $m^{(i)}$  in each subsystem ( $i$ ) would be a set of  $N_0$  independent and identically distributed random variables. ~~the~~ If

the total system average is the average of these  $m^{(i)}$ ,  $m = \frac{1}{N_0} \sum_i m^{(i)}$ , then

the variance of  $m$  is the variance of  $m^{(i)}$  divided by  $N_0$ . So the standard deviation

of  $m$ ,  $\sqrt{\langle m^2 \rangle - \langle m \rangle^2} \propto \frac{1}{\sqrt{N_0}}$ .

Now as long as the influence of the subsystem at position  $\vec{r}$  is no longer felt at a finite distance  $\xi$  away, one can choose the size of each subsystem to be  $\xi^d$  ( $d = \text{dimensionality}$ ) and  $N_0 = \frac{N}{\xi^d}$  so  $\sqrt{\langle m^2 \rangle - \langle m \rangle^2} \propto \sqrt{\frac{\xi^d}{N}} \propto \frac{1}{\sqrt{N}}$

For  $T = T_c$  however,  $\chi \rightarrow \infty$  as  $N \rightarrow \infty$

$\Rightarrow \sqrt{\langle m^2 \rangle - \langle m \rangle^2}$  does not vanish as quickly as  $1/\sqrt{N}$  as  $N \rightarrow \infty$ .

$\Rightarrow$  above argument about considering independent subsystems cannot apply.

$\Rightarrow$  The length scale  $\xi$  that describes how far the system is correlated in space must diverge as  $T \rightarrow T_c$ !

At  $T \neq T_c$ , the state of the system  $m(\vec{r})$  at position  $\vec{r}$  has no effect on the state of the system at  $\vec{r} + \vec{r}_0$  if  $\vec{r}_0$  is sufficiently large,  $|\vec{r}_0| \gg \xi$ . At  $T = T_c$ , the state of the system at  $\vec{r}$  influences the state of the system throughout its entire volume,  $\xi \rightarrow \infty$ !

## Landau-Ginzburg approach

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

free energy functional  $\swarrow$  general  $d$ -dimensional space

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

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

$b = \text{constant}$

$c = \text{constant}$  — 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  $T < T_c$

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

$$F[m(\vec{r})] = \int d^d r \left\{ a m_0^2 + 2a m_0 \delta m + a \delta m^2 + b m_0^4 + 4b m_0^3 \delta m + 6b m_0^2 \delta m^2 + c |\nabla \delta m|^2 \right\}$$

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

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

The remaining quadratic terms are

$$\delta F = \int d^d r \left\{ [a + \frac{6}{2} b m_0^2] s m^2 + c |\nabla s m|^2 \right\}$$

↑ integral is over vol  $L^d$

$$\text{let } a' = a + \frac{6}{2} b m_0^2$$

Fourier transform

$$s m(\vec{r}) = \frac{1}{L^{d/2}} \sum_{\vec{g}} e^{i \vec{g} \cdot \vec{r}} s m_{\vec{g}}$$

sum over all  $\vec{g}$  s.t.  
 $g_{\mu} = \frac{2\pi n_{\mu}}{L}$ ,  $n_{\mu}$  integer

$$s m_{\vec{g}} = \frac{1}{L^{d/2}} \int d^d r e^{-i \vec{g} \cdot \vec{r}} s m(\vec{r})$$

Then

$$\delta F = \frac{1}{L^{d/2}} \frac{1}{L^{d/2}} \sum_{\vec{g}} \sum_{\vec{g}'} [a' - c \vec{g} \cdot \vec{g}'] s m_{\vec{g}} s m_{\vec{g}'} \\ \times \underbrace{\int d^d r e^{i(\vec{g} + \vec{g}') \cdot \vec{r}}}_{L^d \delta(\vec{g} + \vec{g}')}$$

$$\delta F = \sum_{\vec{g}} [a' + c g^2] s m_{\vec{g}} s m_{-\vec{g}}$$

Correlation function

To average over fluctuations we should compute the partition function averaged over  $s m(\vec{r})$

$$Z = \prod_{\vec{r}} \int_{-\infty}^{\infty} d\delta m(\vec{r}) e^{-\beta \delta F[\delta m(\vec{r})]}$$

↑ integrate over all values of  $\delta m(\vec{r})$   
at all positions  $\vec{r}$

Now lets transform variables of integration from  $\{\delta m(\vec{r})\} \rightarrow \{\delta m_{\vec{q}}\}$

Our Fourier transforms were defined so that the Jacobian of this transformation is unity.

$$Z = \prod_{\vec{q}} \int d\delta m_{\vec{q}} e^{-\beta \delta F[\delta m_{\vec{q}}]}$$

Note however that  $\delta m_{\vec{q}}$  is complex  $\Rightarrow \delta m_{\vec{q}} = \delta m_{1\vec{q}} + i \delta m_{2\vec{q}}$   
real part      complex part

Since  $\delta m(\vec{r})$  is real  $\Rightarrow \delta m_{\vec{q}}^* = \delta m_{-\vec{q}}$ , so  $\delta m_{\vec{q}}$  and  $\delta m_{-\vec{q}}$  are not independent. When we integrate over  $\delta m_{\vec{q}}$  we should therefore integrate over real values  $\delta m_{1\vec{q}}$  and  $\delta m_{2\vec{q}}$  but restrict  $\vec{q}$  to  $q_3 > 0$  so as not to double count  $\delta m_{\vec{q}}$  and  $\delta m_{-\vec{q}}$ .

$$Z = \left( \prod_{\substack{\vec{q} \\ s.t. q_3 > 0}} \int_{-\infty}^{\infty} d\delta m_{1\vec{q}} \int_{-\infty}^{\infty} d\delta m_{2\vec{q}} \right) e^{-\beta \delta F[\delta m_{1\vec{q}} + i \delta m_{2\vec{q}}]}$$

$$\text{Use } \delta F = \sum_{\vec{q}} (a' + c q^2) \delta m_{\vec{q}} \delta m_{-\vec{q}}$$

$$= \sum_{\vec{q}} (a' + c q^2) (\delta m_{1\vec{q}}^2 + \delta m_{2\vec{q}}^2)$$

$$= 2 \sum_{\substack{\vec{q} \\ s.t. q_3 > 0}} (a' + c q^2) (\delta m_{1\vec{q}}^2 + \delta m_{2\vec{q}}^2)$$

since we restricted sum to  $q_3 > 0$   
we multiply by 2 to include  $q_3 < 0$  terms

now use exponential of sum = product of exponentials

$$\Rightarrow Z = \prod_{\mathbf{g}} \left[ \int_{-\infty}^{\infty} d\delta m_{1\mathbf{g}} \int_{-\infty}^{\infty} d\delta m_{2\mathbf{g}} e^{-2\beta(a' + c\mathbf{g}^2)(\delta m_{1\mathbf{g}}^2 + \delta m_{2\mathbf{g}}^2)} \right]$$

$st \delta_{\mathbf{g}} > 0$

$\Rightarrow$  Correlation function

$$\begin{aligned} \langle \delta m_{\mathbf{g}} \delta m_{-\mathbf{g}} \rangle &= \langle \delta m_{1\mathbf{g}}^2 + \delta m_{2\mathbf{g}}^2 \rangle \\ &= \frac{\int_{-\infty}^{\infty} d\delta m_{1\mathbf{g}} \int_{-\infty}^{\infty} d\delta m_{2\mathbf{g}} e^{-2\beta(a' + c\mathbf{g}^2)(\delta m_{1\mathbf{g}}^2 + \delta m_{2\mathbf{g}}^2)} (\delta m_{1\mathbf{g}}^2 + \delta m_{2\mathbf{g}}^2)}{\int_{-\infty}^{\infty} d\delta m_{1\mathbf{g}} \int_{-\infty}^{\infty} d\delta m_{2\mathbf{g}} e^{-2\beta(a' + c\mathbf{g}^2)(\delta m_{1\mathbf{g}}^2 + \delta m_{2\mathbf{g}}^2)}} \end{aligned}$$

$$= \frac{1}{4\beta(a' + c\mathbf{g}^2)} + \frac{1}{4\beta(a' + c\mathbf{g}^2)} = \frac{1}{2} \frac{k_B T}{(a' + c\mathbf{g}^2)}$$

$\uparrow$   $\langle \delta m_{1\mathbf{g}}^2 \rangle$                        $\uparrow$   $\langle \delta m_{2\mathbf{g}}^2 \rangle$

Real space correlation function is then

$$\langle \delta m(\vec{r}) \delta m(0) \rangle = \frac{1}{L^{d/2}} \frac{1}{L^{d/2}} \sum_{\mathbf{g}} \sum_{\mathbf{g}'} e^{i\vec{g} \cdot \vec{r}} \langle \delta m_{\mathbf{g}} \delta m_{\mathbf{g}'} \rangle$$

Because SF involves only  $\delta m_{\mathbf{g}} \delta m_{-\mathbf{g}} = \delta m_{1\mathbf{g}}^2 + \delta m_{2\mathbf{g}}^2$ ,  
 $\langle \delta m_{\mathbf{g}} \delta m_{\mathbf{g}'} \rangle = 0$  unless  $\mathbf{g}' = -\mathbf{g}$

$$\langle \delta m(\vec{r}) \delta m(0) \rangle = \frac{1}{L^d} \sum_{\mathbf{g}} e^{i\vec{g} \cdot \vec{r}} \langle \delta m_{\mathbf{g}} \delta m_{-\mathbf{g}} \rangle$$

$$= \frac{1}{L^d} \sum_{\mathbf{g}} e^{i\vec{g} \cdot \vec{r}} \frac{1}{2} \frac{k_B T}{a' + c\mathbf{g}^2}$$

continuum limit  $L \rightarrow \infty$

$$= \int \frac{d^d \mathbf{g}}{(2\pi)^d} e^{i\vec{g} \cdot \vec{r}} \frac{1}{2} \frac{k_B T}{a' + c\mathbf{g}^2}$$

$$\sim \frac{e^{-r/\xi}}{r^{d-2}} \quad \text{Ornstein-Zernicke form}$$

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

$\xi$  gives the length scale over which fluctuations  $S_m(\vec{r})$  decay

This result for  $\xi$  comes from the integral having its poles at  $|\vec{q}| = \pm i \sqrt{a'/c}$

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

$$\xi \sim \frac{1}{\sqrt{a'}} \sim \frac{1}{\sqrt{T - T_c}} \sim \frac{1}{|t|^\nu} \quad \text{with } \nu = 1/2$$

$\nu$  is called the correlation length exponent

For  $T < T_c$ ,  $a' = a + 6b m_0^2$

$$= a - 6b \left( \frac{a}{2b} \right) = -2a$$

$$= 2a_0(T_c - T)$$

$$\xi \sim \frac{1}{\sqrt{a'}} \sim \frac{1}{\sqrt{T_c - T}} \sim \frac{1}{|t|^\nu} \quad \text{with } \nu = 1/2$$

As  $T \rightarrow T_c$  the correlation length diverges.

Since fluctuations propagate out a distance  $\xi \rightarrow \infty$  one can never divide the system up into independent boxes on any finite length scales.

This is why  $\sqrt{\langle m^2 \rangle - \langle m \rangle^2}$  does not vanish as  $\frac{1}{\sqrt{N}}$  at  $T_c$ .  $\rightarrow$  fluctuations can be important at the critical point



## Contribution of fluctuations to the total free energy

$$\begin{aligned}\delta F &= \sum_{\vec{q}} (a' + c q^2) \delta m_{\vec{q}} \delta m_{-\vec{q}} \\ &= 2 \sum_{\substack{\vec{q} \\ \text{st } q_z > 0}} (a' + c q^2) (\delta m_{1\vec{q}}^2 + \delta m_{2\vec{q}}^2)\end{aligned}$$

$$Z = \prod_{\substack{\vec{q} \\ \text{st } q_z > 0}} \left[ \int_{-\infty}^{\infty} d\delta m_{1\vec{q}} \int_{-\infty}^{\infty} d\delta m_{2\vec{q}} e^{-2\beta (a' + c q^2) (\delta m_{1\vec{q}}^2 + \delta m_{2\vec{q}}^2)} \right]$$

$$= \prod_{\substack{\vec{q} \\ \text{st } q_z > 0}} \left[ \frac{2\pi}{4\beta (a' + c q^2)} \right]^{1/2} \left[ \frac{2\pi}{4\beta (a' + c q^2)} \right]^{1/2}$$

$\uparrow$  from  $\delta m_{1\vec{q}}$                        $\uparrow$  from  $\delta m_{2\vec{q}}$

$$= \prod_{\substack{\vec{q} \\ \text{st } q_z > 0}} \left[ \frac{\pi}{2} \frac{k_B T}{a' + c q^2} \right]$$

Gibbs free energy due to fluctuations

$$\delta G = -k_B T \ln Z = -k_B T \sum_{\substack{\vec{q} \\ \text{st } q_z > 0}} \ln \left( \frac{\pi}{2} \frac{k_B T}{a' + c q^2} \right)$$

$$= -\frac{k_B T}{2} \sum_{\vec{q}} \ln \left( \frac{\pi}{2} \frac{k_B T}{a' + c q^2} \right)$$

$\uparrow$  now sum over all  $\vec{q}$ , so multiply by  $\frac{1}{2}$

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

Contribution to specific heat per volume  $sc$

$$sc = -\frac{T}{L^d} \frac{\partial^2 \delta G}{\partial T^2}$$

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

(result will be similar for  $T < T_c$  where  $a' = 2a_0(T_c - T)$ )

$$\frac{1}{L^d} \frac{\partial \delta G}{\partial T} = -\frac{k_B}{2} \int \frac{d^d q}{(2\pi)^d} \ln\left(\frac{\pi}{2} \frac{k_B T}{a' + cg^2}\right)$$

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

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

$$\frac{1}{L^d} \frac{\partial^2 \delta G}{\partial T^2} = -\frac{k_B}{2} \int \frac{d^d q}{(2\pi)^d} \left\{ \frac{1}{T} - \frac{a_0}{a' + cg^2} \right\}$$

$$+ \frac{k_B}{2} \int \frac{d^d q}{(2\pi)^d} \frac{a_0}{a' + cg^2}$$

$$- \frac{k_B T}{2} \int \frac{d^d q}{(2\pi)^d} \frac{a_0^2}{(a' + cg^2)^2}$$

$$sc = \frac{k_B}{2} \int \frac{d^d q}{(2\pi)^d} \left\{ 1 - \frac{2T a_0}{a' + cg^2} + \frac{T^2 a_0^2}{(a' + cg^2)^2} \right\}$$

↑  
this gives classical  
 $\frac{1}{2} k_B$  per degree  
of freedom

↑  
corrections due  
to  $T$ -dependence  
of  $a(T)$  in  $\delta F$

To see how the integrals behave as  $T \rightarrow T_c$

$$I_1 = \int d^d g \frac{a_0}{a_0 t + c g^2} \quad \text{where } t = T - T_c$$

$$\text{let } g^2 = t g'^2$$

$$I_1 = t^{d/2} \int d^d g' \frac{a_0}{a_0 t + c t g'^2} = t^{d/2 - 1} \int d^d g' \frac{a_0}{a_0 + c g'^2}$$

$$I_1 \sim t^{d/2 - 1} = t^{d/2 - 2} \propto \xi^{2-d} \quad \text{just some number}$$

(since  $\xi \sim t^{-1/2}$ )

Similarly

$$I_2 = \int d^d g \frac{a_0^2}{(a_0 t + c g^2)^2} \propto t^{d/2 - 2} = t^{d/2 - 4} \propto \xi^{4-d}$$

The second integral is the more singular one

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

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

$\delta C$  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 upper critical dimension  
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 lower critical dimension - depends on  $n$

For  $d < \text{lower critical dimension}$ , there is no phase transition at finite temperature