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 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, \( \chi = \frac{d \theta \theta}{d \chi} \to \infty \) at \( T_c \)

Now \( \theta \theta = -\frac{\partial^2 \theta}{\partial \chi^2} \to \chi = -\frac{\partial^2 \theta}{\partial \chi^2} = \frac{1}{N} k_B T \frac{\partial^2 \ln Z}{\partial \chi^2} \)

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

\[
Z = \int e^{-\beta H + \beta \chi M}
\]

\[
\frac{\partial Z}{\partial \chi} = \int e^{-\beta H + \beta \chi M} (\beta M)
\]

\[
\frac{\partial^2 Z}{\partial \chi^2} = \int e^{-\beta H + \beta \chi M} (\beta M)^2
\]

\[
\chi = \frac{k_B T}{N} \frac{1}{\beta^2} \left\{ \langle M^2 \rangle - \langle M \rangle^2 \right\}
\]

\[
M = N \theta \theta
\]

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

fluctuation in total magnetization \( M \)
\[ m = \frac{M}{N} \quad \text{magnetization density} \]

\[ X = \frac{N}{k_B T} \sum \left( <m^2> - <m>^2 \right) \]

For \( T \neq T_c \), \( X \) is finite as \( N \to \infty \) in the thermodynamic limit.

\[ \Rightarrow <m^2> - <m>^2 \sim \frac{1}{N} \]

or fluctuations in magnetization density

\[ \sqrt{<m^2> - <m>^2} \sim \frac{1}{\sqrt{N}} \to 0 \quad \text{as} \quad N \to \infty \]

We can understand the \( \frac{1}{N^2} \) 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. \( \Rightarrow \)

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

the variance of \( m \) is the variance of \( m^{(i)} \) divided by \( N_0 \). So the standard deviation
of $m$, \[ \sqrt{\langle m^2 \rangle - \langle m \rangle^2} \propto \frac{1}{\sqrt{N}}. \]

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

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

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

$\Rightarrow$ 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 $T \to T_c$!

At $T = T_c$, the state of the system $\langle \vec{m}(\vec{r}) \rangle$ at position $\vec{r}$ has no effect on the state of the system at $\vec{r} + \vec{r}_i$ if $\vec{r}_i$ is sufficiently large, $|\vec{r}_i| \gg \xi$. At $T = T_c$, the state of the system at $\vec{r}$ influences the state of the system throughout its entire volume, $\xi \to \infty$.
Landau-Ginzburg approach

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

Free energy functional

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

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 $m(r)$.

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

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

$$F[m(r)] = \int d^d r \left\{ a m_0^2 + 2am_0 \delta m + a \delta m^2 + b m_0^4 + 4b m_0^2 \delta m + 6b m_0^3 \delta m^2 + c |\nabla \delta m|^2 \right\}$$

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

\[ SF = \int d^d r \left\{ [a' + \delta g \cdot \delta m_0^2] \delta m^2 + c \left| \delta \delta m \right|^2 \right\} \]

Integral is over vol \( L^d \)

Let \( a' = a + \delta g \cdot \delta m_0^2 \)

Fourier transforms

\[ \delta m(r) = \frac{1}{L^d} \sum_{g} e^{-i \vec{g} \cdot \vec{r}} \delta m_{\vec{g}} \]

\[ \delta m_{\vec{g}} = \frac{1}{L^d} \int d^d r e^{i \vec{g} \cdot \vec{r}} \delta m(r) \]

Then

\[ SF = \frac{1}{L^d} \frac{1}{L^d} \sum_{g} \sum_{g'} \left[ a' - c \vec{g} \cdot \vec{g}' \right] \delta m_{\vec{g}} \delta m_{\vec{g}'} \]

\[ \times \int d^d r e^{i \left( \vec{g} + \vec{g}' \right) \cdot \vec{r}} \]

\[ SF = \sum_{g} \left[ a' + c \delta^2 \right] \delta m_{g} \delta m_{g} \]

**Correlation function**

To average over fluctuations we should compute the partition function averaged over \( \delta m(r) \)
\[ Z = \prod_{r}^\infty \int d\delta m(r) e^{-\beta SF[\delta m(r)]} \]

Integrate over all values of \( \delta m(r) \) at all positions \( r \).

Now let's transform variables of integration from

\[ \{ \delta m(r) \} \rightarrow \{ \delta m_g \} \]

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

\[ Z = \prod_{g} \int d\delta m_g e^{-\beta SF[\delta m_g]} \]

Note however that \( \delta m_g \) is complex \( \Rightarrow \delta m_g = \delta m_g^r + i \delta m_g^i \)

real part complex part

Since \( \delta m(r) \) is real \( \Rightarrow \delta m_g^* = \delta m_g \), so \( \delta m_g^r \)

and \( \delta m_g^i \) are not independent. When we integrate over \( \delta m_g \) we should therefore integrate over real values \( \delta m_g^r \) and \( \delta m_g^i \), but restrict \( g \) to \( g > 0 \) so as not to double count \( \delta m_g^r \) and \( \delta m_g^i \).

\[ Z = \left( \prod_{g} \right) \int_{g > 0} d\delta m_g^r \int_{-\infty}^{\infty} d\delta m_g^i e^{-\beta SF[\delta m_g]} \]

Use \( SF = \sum_g \left( a' + g^2 \right) \delta m_g \delta m_g^* \)

\[ = \sum_g \left( a' + g^2 \right) \left( \delta m_g^2 + \delta m_g^2 \right) \]

\[ = 2 \sum_g \left( a' + g^2 \right) \left( \delta m_g^2 + \delta m_g^2 \right) \]

\[ s + g > 0 \quad \text{since we restricted \( g > 0 \) in SF terms.} \]
For an exponential of sum = product of exponentials,

\[ Z = \prod_{q} \left[ \int_{-\infty}^{\infty} d\delta m_q \int_{-\infty}^{\infty} d\delta m_{2q} \exp^{-2\beta(a' + c\delta^2)(\delta m_q^2 + \delta m_{2q}^2)} \right] \]

**Correlation function**

\[ \langle \delta m_q \delta m_{-q} \rangle = \langle \delta m_q^2 + \delta m_{2q}^2 \rangle \]

\[ = \int_{-\infty}^{\infty} d\delta m_q \int_{-\infty}^{\infty} d\delta m_{2q} \exp^{-2\beta(a' + c\delta^2)(\delta m_q^2 + \delta m_{2q}^2)} \]

\[ = \int_{-\infty}^{\infty} d\delta m_q \int_{-\infty}^{\infty} d\delta m_{2q} \exp^{-2\beta(a' + c\delta^2)(\delta m_q^2 + \delta m_{2q}^2)} \]

\[ = \frac{1}{4\beta(a' + c\delta^2)} + \frac{1}{4\beta(a' + c\delta^2)} = \frac{1}{2} \frac{k_B T}{(a' + c\delta^2)} \]

\[ \langle \delta m_q^2 \rangle \]

\[ \langle \delta m_{2q}^2 \rangle \]

**Real space correlation function** is then

\[ \langle \delta m(\mathbf{r}) \delta m(0) \rangle = \frac{1}{L^d} \sum \sum \exp^{i\mathbf{q} \cdot \mathbf{r}} \langle \delta m_q \delta m_{-q} \rangle \]

Because &F; involves only \( \delta m_q \delta m_{-q} = \delta m_q^2 + \delta m_{2q}^2 \)

\[ \langle \delta m_q \delta m_{-q} \rangle = 0 \text{ unless } q' = -q \]

\[ \langle \delta m(\mathbf{r}) \delta m(0) \rangle = \frac{1}{L^d} \sum \exp^{i\mathbf{q} \cdot \mathbf{r}} \langle \delta m_q \delta m_{-q} \rangle \]

\[ = \frac{1}{L^d} \sum \exp^{i\mathbf{q} \cdot \mathbf{r}} \frac{1}{2} \frac{k_B T}{a' + c\delta^2} \]

**contains limit**

\[ L \to \infty \]

\[ = \int \frac{d^d \mathbf{q}}{(2\pi)^d} \exp^{i\mathbf{q} \cdot \mathbf{r}} \frac{1}{2} \frac{k_B T}{a' + c\delta^2} \]
\[ e^{-r/l} \quad \text{Ornstein-Zernicke form} \]

where \( l = \sqrt{\frac{c}{a'}} \) is the "correlation length."

\( l \) gives the length scale over which fluctuations \( \Delta m(\vec{r}) \) decay.

The result for \( l \) comes from the integral having its poles at \( \vec{q} = \pm i (2a')/c \).

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

\[ l \sim \frac{1}{\sqrt{a'}} \sim \frac{1}{\sqrt{T - T_c}} \sim \frac{1}{|t|^n} \quad \text{with} \quad n = \frac{1}{2} \]

\( n \) is called the correlation length exponent.

For \( T < T_c \), \( a' = a + \alpha \Delta m^2 \)

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

\[ = 2a_0 (T_c - T) \]

\[ l \sim \frac{1}{\sqrt{a'}} \sim \frac{1}{\sqrt{T_c - T}} \sim \frac{1}{|t|^n} \quad \text{with} \quad n = \frac{1}{2} \]

As \( T \to T_c \) the correlation length diverges.

Since fluctuations propagate out a distance \( l \to \infty \) one can never divide the system up into independent boxes on any finite length scales.

This is why \( \sqrt{\langle m^2 \rangle - \langle m \rangle^2} \) do not vanish as \( 1/\sqrt{N} \) at \( T_c \). Fluctuations can be important at the critical point.
Contribution of fluctuations to the total free energy

\[ \delta F = \sum_{\Theta} (a_1 + cg^2) \delta m_\Theta \delta m_{-\Theta} \]
\[ = 2 \sum_{\Theta} (a_1 + cg^2) (\delta m_{2\Theta} \delta m_{2\Theta}) \]
\[ \delta F > 0 \]

\[ Z = \frac{T}{\mathcal{F}} \left[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-2 \beta (a_1 + cg^2) (\delta m_{2\Theta} \delta m_{2\Theta})} \right] \]

\[ = \frac{T}{\mathcal{F}} \left[ \frac{2\pi}{4 \beta (a_1 + cg^2)} \right]^{1/2} \left[ \frac{2\pi}{4 \beta (a_1 + cg^2)} \right]^{1/2} \]

\[ = \frac{T}{\mathcal{F}} \left[ \frac{\pi k_B T}{2 (a_1 + cg^2)} \right] \]

Cubic free energy due to fluctuations

\[ \delta G = -k_B T \ln Z = -k_B T \sum_{\Theta, \Phi} \ln \left( \frac{\pi}{2} \frac{k_B T}{a_1 + cg^2} \right) \]
\[ \delta G > 0 \]

\[ = -\frac{k_B T}{2} \sum_{\Theta} \ln \left( \frac{\pi}{2} \frac{k_B T}{a_1 + cg^2} \right) \]

\[ \text{new sum over all } \Theta, \text{ so multiply by } \frac{1}{2} \]

\[ = -\frac{k_B T}{2} \int d\rho \int \frac{d^3 T}{(2\pi)^3} \ln \left( \frac{\pi}{2} \frac{k_B T}{a_1 + cg^2} \right) \]
Contribution to specific heat per volume $8c$

$$8c = -\frac{T}{L^d} \frac{2^2 \pi b}{2 T^2}$$

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

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

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

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

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

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

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

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

$$8c = \frac{k_B}{2} \int \frac{d^d q}{(2\pi)^d} \left\{ 1 - \frac{2T a_0}{a' + cg^2} + \frac{T^2 a_0^2}{(a' + cg^2)^2} \right\}$$

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

classical and quantum corrections due to $T$-dependence
To see how the integrals behave as $T \to T_c$

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

Let $q^2 = t \xi^2$

\[ I_1 = t^{d/2} \int d^d q' \frac{a_0}{a_0 t + c + t \xi^2} = t^{d/2 - 1} \int d^d q' \frac{a_0}{a_0 + c \xi^2} \quad \text{(just some number)} \]

\[ I_1 \sim t^{d-1} = t^{d/2 - 1/2} \quad \xi^2 - d \quad \text{(since } \xi \sim t^{-1/2}) \]

Similarly

\[ I_2 = \int d^d q \frac{a_0^2}{(a_0 t + c q^2)^2} \propto t^{d-2} = t^{d/2 - 4} \propto \xi^{4-d} \]
The second integral is the more singular one.

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

In mean field theory, $G_{MF} \sim$ finite at $T_c$
$$\Sigma C \sim \pm \frac{d-4}{2}$$

$\Sigma C$ will diverge whenever $d < 4$

$\Rightarrow d > 4 \Rightarrow$ fluctuations negligible
mean field theory gives correct critical exponents

$\Rightarrow d < 4 \Rightarrow$ 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 $d <$ lower critical dimension, there is no phase transition at finite temperature.