"Mean field" description of the ordering transition

Consider Ising ferromagnet as an example

\[ H = -J \sum_{i,j} S_i S_j - h \sum_i S_i \]

(qualitatively similar approach works for \( n \)-vector models as well)

Single spin in a field:

\[ H_{\text{spin}} = -hS \]

\[ Z_{\text{spin}} = e^{\beta h} + e^{-\beta h} = 2 \cosh(\beta h) \]

\[ F_{\text{spin}} = -k_B T \ln (2 \cosh(\beta h)) \]

\[ m = \langle S \rangle = \frac{e^{\beta h} - e^{-\beta h}}{e^{\beta h} + e^{-\beta h}} = \tanh(\beta h) = \frac{1}{e^{\beta h} + 1} \]

\[ = \frac{\partial F}{\partial h} \]

Collection of \( N \) noninteracting spins - multiply by \( N \) to obtain total free energy and magnetization; (properties per spin remain unchanged)

Interacting spins - try "effective medium" approximation or "mean field"

Consider a spin \( i \)

Piece in \( H \):

\[ - \left( J \sum_{j \text{-neighbours of } i} S_j + h \right) S_i \]

\[ \text{hess} = \text{effective field acting on } S_i \]

\[ \text{hess depends on the configuration of spins nearby} \]
Mean field approximation: consider "average" hess obtained by $S_j \rightarrow \langle S_j \rangle$

$$\text{hess} = h + J \sum_{j=\text{neighbours of } i} \langle S_j \rangle = h + J z \cdot m$$

(remark: this is equivalent to the uniform density approximation in our treatment of interacting particles; here $J \cdot z \sim$ integral of the attractive part of the interaction assuming uniform dens.,)

only here interaction extends only to nearest neighbors)

But $m = \langle S_i \rangle$ is itself determined by hess

$\Rightarrow$ self-consistent field condition

$$m = \tanh (\beta \text{hess}) = \tanh (\beta (h + J z m))$$

want to solve for $m$ as a function of $h$.

Example: at high temperatures and in small field

$\frac{K_B T}{J} \gg 1$, $h \ll \frac{K_B T}{J}$

(e.g. susceptibility is measured with $h \rightarrow 0$)

expect also $m$ to be small:

$$m = \tanh \left( \frac{\beta (h + J z m)}{K_B T} \right) \propto \frac{h + J z m}{K_B T}$$

Curie-Weiss

$$m = \frac{h}{K_B T - J z} ; \chi = \left( \frac{m}{h} \right) = \frac{1}{K_B T - J z}$$

if $J$ ferromagnetic $\rightarrow$ susceptibility is larger than for free spins - "spins are happy to cooperate"
(If \( J \) is antiferromagnetic, the susceptibility is smaller than free spins: spins like to be antiparallel, so aligning neighbours with the field effectively decreases the field on a given spin).

Remark: all discussions of dielectric constant or magnetic permeability constant are essentially effective "medium descriptions" in the above sense. If the "medium corrections" are small, we would stop here. Important aspect in electrostatics and magnetostatics is the long-range nature of the interactions, so one needs to work harder to calculate the average field due to the rest of the system — usually done by using e.g., Gauss' law.
Note: \[ \chi = \frac{1}{k_B T - J_z} \to \infty \text{ for } T \to T_c = \frac{J_z}{k_B} \]

\[ m = \tanh \left( \frac{h + J_z m}{k_B T} \right) \Rightarrow m(h) \]

Can argue that for \( T > T_c \) this has unique solution.

While for \( T < T_c \) the solution is not unique and the stable branch starts with nonzero magnetization @ \( h=0 \)

Indeed, consider \( h=0 \) first:

Graphical Solution:

\[ m = \tanh \left( \frac{J_z m}{k_B T} \right) \]

For small \( m \), behaves as \( \sim \frac{J_z m}{k_B T} \) \( \Rightarrow \) slope \( \frac{J_z}{k_B T} \)

- For \( k_B T > J_z \), the initial slope is \( <1 \), and there is unique solution \( m=0 \)

- For \( k_B T < J_z \), the initial slope is \( >1 \), and there are three solutions: \( m=0 \), \( m_+ \), \( m_- = -|m+| \)

\( k_B T_c = J_z \) - critical point
For $R \neq 0$, \( \tanh \left( \frac{J^2 m + h}{k_B T} \right) = \tanh \left( \frac{J^2 (m + \frac{h}{J^2})}{k_B T} \right) \)

gives the same "tanh" curve shifted to the left by \( \frac{h}{J^2} \).

- Globally stable solution
- Unique solution
- Unstable solution
- Locally stable solution (meta-stable)

"Variational" perspective on this mean-field (so-called Bragg-Williams theory)
Consider trial density matrix where spins are independent — for example, can define the trial density matrix by \( hess \)

\[ H_0 = -hess \sum_i S_i \]

or equivalently
\[
\begin{align*}
p_+ &= \frac{e^\beta hess}{Z_{1spin}} \\
p_- &= \frac{e^{-\beta hess}}{Z_{1spin}} \quad p_+ - p_- = m = \tanh(\beta hess)
\end{align*}
\]

(can parametrize the trial state by either \( hess \) or \( m \))

\[ F_{\text{trial}} = \langle H \rangle_{\text{trial}} + k_B T \cdot \text{Tr}(\text{log } S_{\text{trial}}) \]
\[
\langle H \rangle_{\text{trial}} = -J \sum_{m} \langle s_i \rangle \langle s_j \rangle - h \sum_{m} \langle s_i \rangle = \\
= N \left( -J m^2 \frac{Z}{2} - h m \right) \\
\text{Each bond is shared between 2}
\]

\[
\text{Tr}_{\text{trial}} \ln_{\text{trial}} = N \left( p_+ \ln p_+ + p_- \ln p_- \right) = \\
= N \left( \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right)
\]

\[
\Rightarrow F_{\text{trial}} = -J m^2 \frac{Z}{2} - h m + k_B T \left\{ \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right\}
\]

Minimize w.r.t. \( m \):

\[
0 = \frac{\partial F}{\partial m} : 0 = -J m Z - h + k_B T \left\{ \frac{1}{2} \ln \frac{1+m}{2} + \frac{1+m}{2} \cdot \frac{2}{1+m} \cdot \frac{1}{2} + \right. \\
+ \frac{1}{2} \ln \frac{1-m}{2} + \frac{1-m}{2} \cdot \frac{2}{1-m} \cdot \frac{1}{2} \left\} = -J m Z - h + k_B T \ln \frac{1+m}{1-m}
\]

\[
\frac{1}{2} \ln \frac{1+m}{1-m} = \frac{h + J m^2}{k_B T}
\]

\[
\text{atanh}(m)
\]

\[
\updownarrow \text{tanh}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^{2x} - 1}{e^{2x} + 1} = \frac{\frac{1+m}{1-m} - 1}{\frac{1+m}{1-m} + 1} = m \checkmark
\]

\[
\Rightarrow m = \tanh \frac{h + J m^2}{k_B T} \quad \text{precisely the self-consistency condition!}
\]
This is not magic but dictated by the structure of the variational meanfield:

$$F_{\text{trial}} = -\sum_{\langle ij \rangle} J_{ij} m(h_i) m(h_j) + \sum_i \left( F_{\text{spin}}(h_i) + h_i m(h_i) \right)$$

$$F_0 - \langle H_0 \rangle_0$$

Minimize wrt $h_i$:

$$\frac{\delta F_{\text{trial}}}{\delta h_i} = -\sum_{j: \text{neighbours of } i} J_{ij} m(h_j) \frac{8m(h_i)}{8h_i}$$

$$+ \left( \frac{\partial F_{\text{spin}}}{\partial h_i} + m(h_i) + h_i \frac{8m(h_i)}{8h_i} \right)$$

$$= (h_i - \sum_{j \neq i} J_{ij} m(h_j)) \frac{8m}{8h_i} = \text{require equal to 0.}$$

$$\Rightarrow h_i = \sum_{j \neq i} J_{ij} m(h_j)$$

- self-consistent field equation
Analysis of the solutions of the self-consistency conditions is the same as before, but now for each solution we can calculate $F_{\text{trial}}(m)$, and check which one is global minimum (if there are several).

Analysis of $F_{\text{trial}}$ for small $m$:

\[
F_{\text{trial}} \propto -Jm^2 \cdot \frac{Z}{2} - hm + k_B T \left\{ \frac{1+m}{2} (-\ln 2 + \right.
\left. + m - m^2 + m^3 - m^4 \right) + \frac{1-m}{2} (-\ln 2 - m - m^2 - m^3 - m^4 ) \right\}^2
\]

\[
= -Jm^2 \cdot \frac{Z}{2} - hm + k_B T \left\{ \frac{1}{2} (-\ln 2 - \frac{m^2}{2} - \frac{m^4}{4} ) + m \cdot \left( m + \frac{m^3}{3} \right) \right\}^2
\]

\[
= -T \cdot k_B \ln 2 + \frac{(k_B T - J^2) m^2}{2} + \frac{k_B T}{12} m^4 - hm
\]

$h=0$

\[
\frac{k_B T - J^2}{2} m^2 + \frac{k_B T}{2} m^4
\]

$T > T_c = \frac{J^2}{k_B}$

unique minimum at $m=0$

$T < T_c$

local maximum

equivalent minima
\[ T = T_c \]

\[ F \quad m \]

very "flat" \( \sim m^4 \)

add \(-hm\) to

\[ h \neq 0 \] the above curves

\[ T > T_c \]

\[ T < T_c \]

local minimum

Analysis near the critical point

* Self-consistency condition to \( O(m^3) \):

\[ (k_B T - Jz) m + \frac{k_B T}{3} m^3 - h = 0 \]

\( \iff \frac{h + Jz m}{k_B T} = \frac{1}{3} (m + \frac{m^3}{3}) \)

For \( h = 0 \) and \( T < T_c \)

order param: Magnetization

\[ m \approx \sqrt{\frac{3(Jz - k_B T)}{k_B T}} \]

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

order parameter exponent:

\[ \beta = \frac{1}{2} \] in mean field
Singularity in the susceptibility

\[ T > T_c : \quad m(h) \propto \frac{h}{k_B T - J_z} \]

\[ \chi(T > T_c) \approx \frac{1}{k_B T - J_z} = \frac{1}{k_B(T - T_c)} = \frac{A_+}{(T - T_c)^{\delta_+}} \]

\( \delta_+ = 1 \) in mean field

\[ T < T_c : \quad \bar{m} = \sqrt[3]{\frac{3(J_z - k_B T)}{k_B T}} \]

Write \( m = \bar{m} + \delta m \)

\[ (k_B T - J_z)(\bar{m} + \delta m) + \frac{k_B T}{3} (\bar{m}^3 + 3 \bar{m} \delta m \bar{m} + O(\delta m^2)) - h = 0 \]

\[ \Rightarrow \delta m \left( k_B T \bar{m}^2 + k_B T - J_z \right) = h \]

\[ \delta m = \frac{h}{3(J_z - k_B T)} \]

\[ \Rightarrow \chi(T < T_c) = \frac{1}{2k_B(T_c - T)} = \frac{A_-}{(T_c - T)^{\delta_-}} \]

\( \delta_+ = 1 \)

\( \frac{A_+}{A_-} = 2 \)

in mean field

\( \delta_- = \) ("critical isotherm")

Behaviour at the critical temperature:

\[ T = T_c \]

\[ m(h) = \left( \frac{2}{k_B T} \right)^{1/3} h^{1/3} \sim h^{1/8} \]

\( S = 3 \)

in mean field
Singularity in the specific heat

- $F_{\text{trial}} (T > T_c) = -k_B T \ln 2$

\[ C = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} (F + TS) = \frac{\partial}{\partial T} (F - T \frac{\partial F}{\partial T}) = -T \frac{\partial^2 F}{\partial T^2} = 0 \]

- $F_{\text{trial}} (T < T_c) = -k_B T \ln 2 + \frac{k_B (T - T_c)}{2} m(r)^2 + \frac{k_B T}{12} m(r)^4$

\[ C = \frac{3}{2} \frac{k_B}{T} \left[ -k_B T \ln 2 + k_B (T - T_c) \frac{3(T_c - T)}{2} + \frac{k_B T}{12} \frac{3(T_c - T)^2}{k_B T} \right] \]

\[ C \sim \frac{3}{2} \frac{k_B}{T} \quad \text{near } T_c \]

In the mean field, $C$ is discontinuous across the transition $

C \sim |t|^{-\alpha}$ with formal $\alpha = 0$

- One more exponent - so-called "correlation length exponent" $\xi \sim |t|^{-\gamma}$ will be discussed when we consider Landau - Ginzburg theory with inhomogeneous order parameter (spatially varying)
Remarks

* Ordering transition in the Ising ferromagnet is an example of continuous phase transition: the ordered phase grows continuously below $T_c$. (Order parameter)

Thermodynamic potentials ($U, S, F, ...$) are continuous at $T_c$, but their derivatives ("susceptibilities") are not in general.

<table>
<thead>
<tr>
<th>$h=0$</th>
<th>$m(T&lt;T_c) \sim (T_c-T)^\beta$</th>
<th>$m(h,T=T_c) \sim h^{1/8}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x(T&gt;T_c) \sim \frac{A_x}{</td>
<td>T-T_c</td>
<td>^\delta_x}$</td>
</tr>
<tr>
<td>$C(T&gt;T_c) \sim \frac{A_c}{</td>
<td>T-T_c</td>
<td>^\alpha}$</td>
</tr>
</tbody>
</table>

$\alpha, \beta, \delta, \gamma, \delta$ - critical exponents

Mean field exponents: $\left[ \beta = \frac{1}{m+2}, \gamma = 1, \delta = 0, \delta = 3 \right]$ - "universal" in mft.

In general, $\alpha, \beta, \delta, \gamma, \delta$ are universal (system-indep) for problems within the same symmetry class (Ising, XY, Heisenberg).

For $n$-vector models, mean field exponents are the same, but this is not true for $d \leq 3$: different $O(n)$ models each has its own exponents.

* Mean field exponents are accurate when $d \geq 4$, but fail for $d \leq 3$. The reason is that mft ignores fluctuations, which are important at the second-order transition since the two phases are quantitatively the same and the system easily "fluctuates"
Analogy between Ising transition and critical point in the liquid-gas transition

\[ h \]

mostly \uparrow \text{ phase}
mostly \downarrow \text{ phase}

\[ T_c \]

\[ \text{liquid} \]
\[ \text{gas} \]

\[ M \]

\[ M(h \to 0+) \]

\[ \phi \]

\[ \frac{1}{T} \]

Cannot exist as a uniform phase \rightarrow phase-separated into "mostly-\uparrow" and "mostly-\downarrow"

different \( h \) values correspond to different points in the \( M-T \) phase diagram

Critical properties of the Ising model near \( T_c \) \iff critical properties of the liquid-gas transition near the crit. point.