

We said that to have a state of spontaneously broken symmetry at finite T ~~requires~~ one needs to be in thermodynamic limit $N \rightarrow \infty$.

Similarly, true singular phase transitions can only occur in this $N \rightarrow \infty$ limit. Proof as follows:
partition function sum:

$$Z(T, h) = \sum_{\{s_i\}} e^{-\beta H[s_i]}$$

For finite system (N finite) the number of configurations to sum over is 2^N is finite.

Z is therefore the sum of a finite number of analytic functions ("analytic" here in the sense of complex function theory - has no singularities as vary T, h). As such, Z must itself be an analytic function of T at h .

$\Rightarrow Z$ can have no singularities

\Rightarrow no singularities in any thermodynamic quantities

\Rightarrow no phase transitions.

Only in thermodynamic limit of $N \rightarrow \infty$ is Z now the sum of an infinite ~~and~~ number of analytic functions. Such an infinite sum need NOT be analytic, so phase transitions can exist.

Having outlined what we might expect from the Ising model, we would now like to compute properties and see what happens!

However, an exact solution is not in general possible. Exact solutions to Ising model exist in

$d=1$ dimension - we will do this later

$d=2$ dimension - famous solution by Onsager

in $d=3$ dimensions, the best one has is very accurate numerical simulations - no exact solution.

⇒ Approximate Solution

Mean Field or Curie-Weiss Molecular Field Approximation

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

Consider spin S_i . Approx the interaction of S_i with its neighbor S_j as an interaction with the thermal average value of $\langle S_j \rangle = m$.

Instead of S_i seeing the specific S_j that vary from config to config, we say S_i sees only the effective average value of S_j - which is the same value m for all sites j . $\langle S_j \rangle = m = \frac{1}{N} \sum_i \langle S_i \rangle$

$$\mathcal{H} \underset{\text{MF}}{\approx} -J \sum_{\langle i,j \rangle} S_i m - h \sum_i S_i$$

↑
sum over bonds

$$H_{MF} = -\frac{z}{2} J \sum_i s_i m - h \sum_i s_i$$

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

each bond is shared
by two sites - gives
the factor $\frac{1}{2}$

where z is the "coordination number" - the number of
nearest neighbors of site i . For a simple (3d)
cubic lattice, $z=6$. For a square lattice, $z=4$.

In this approx, the interaction of s_i with its
neighbors is just like the interaction of s_i with
an additional average magnetic field $\frac{z}{2} J m$
- hence the origin of the name "mean field" approx.

To complete the approx, we need to self-consistently
compute m using H_{MF} and self-consistently solve
for m from the resulting equation.

$$H_{MF} = \sum_i H_{MF}^{(i)} \quad \text{where } H_{MF}^{(i)} = -\left(\frac{z}{2} J m + h\right) s_i$$

we have non-interacting spins in MF approx

$$\Rightarrow \langle s \rangle = m = \frac{\sum_s e^{-\beta H_{MF}^{(i)}} s}{\sum_s e^{-\beta H_{MF}^{(i)}}}$$

s is a single spin
at any site

$$= \frac{e^{+\beta(\frac{z}{2} J m + h)} + e^{-\beta(\frac{z}{2} J m + h)}}{e^{+\beta(\frac{z}{2} J m + h)} + e^{-\beta(\frac{z}{2} J m + h)}}$$

$$m = \tanh \left[\beta \left(\frac{z}{2} J m + h \right) \right]$$

solve to get
 $m(T, h)$

Note $m(T, h) = -m(T, -h)$ as expected

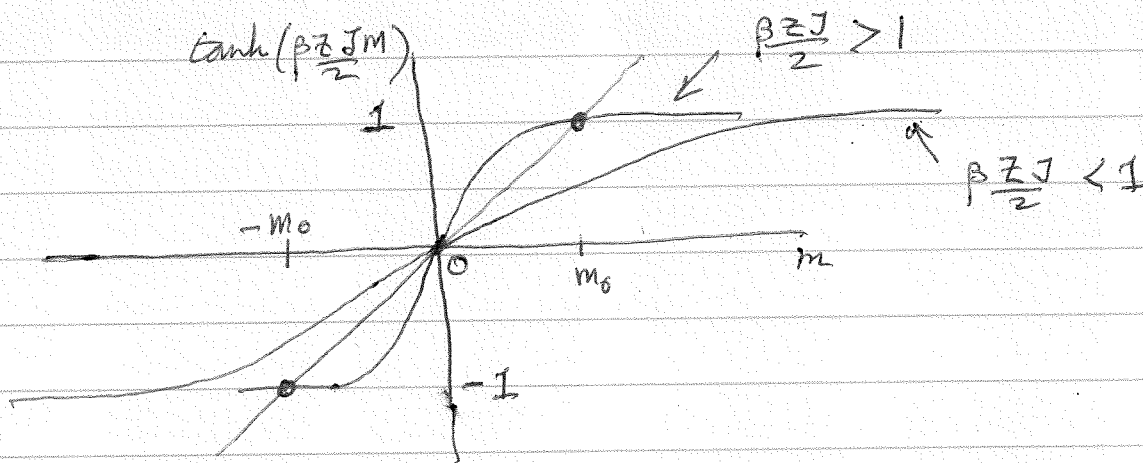
$$m = \tanh \left[\frac{\beta Z J m}{2} + \beta h \right]$$

consider first $h=0$

$$m = \tanh \left[\frac{\beta Z J m}{2} \right] \quad \text{could solve graphically}$$

since $\tanh x = x - \frac{1}{3}x^3 + O(x^5)$ we see that for $\frac{\beta Z J}{2} < 1$, the only solution will be $m=0$.

However for $\frac{\beta Z J}{2} > 1$ there are two additional solutions $m = \pm m_0$



$$\Rightarrow \text{critical temperature } \boxed{k_B T_c = \frac{ZJ}{2}}$$

$$T > T_c \Rightarrow m = 0$$

$$T < T_c \Rightarrow m = \pm m_0$$

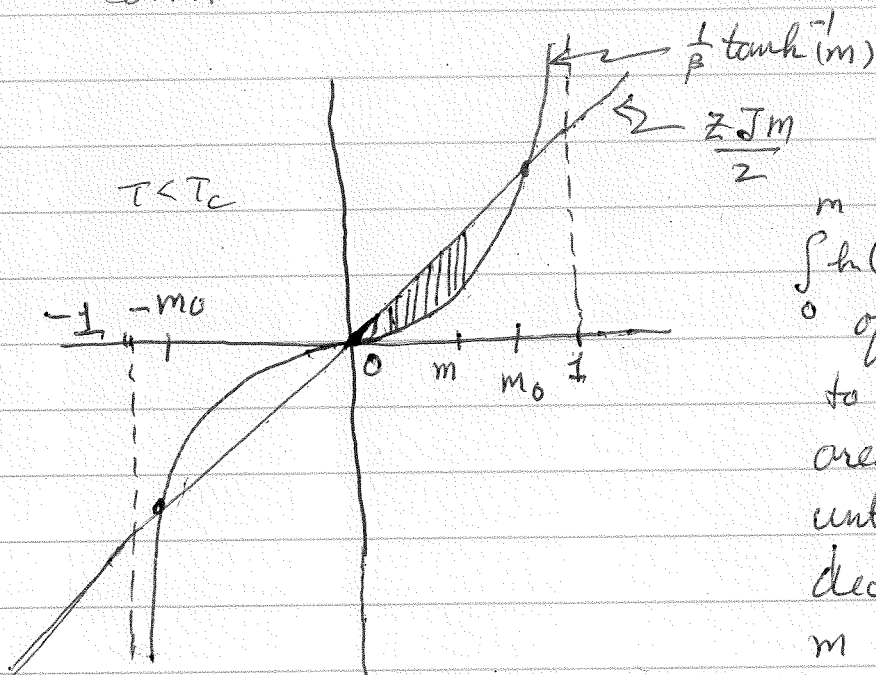
$m=0$ is unstable solution

For $T < T_c$, $m=0$ is unstable
 $m = \pm m_0$ are the equilib solutions. To see this

$$m = \tanh\left(\frac{\beta z J m}{2} + \beta h\right)$$

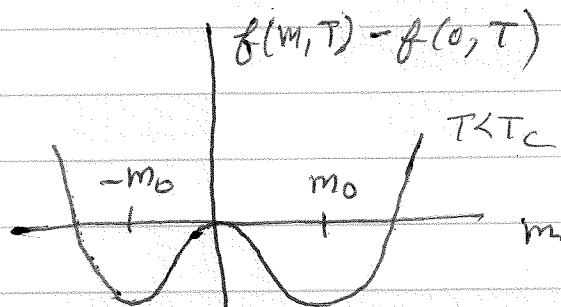
$$h = \frac{1}{\beta} \tanh^{-1} m - \frac{z J m}{2}$$

$$\left(\frac{\partial f}{\partial m}\right)_T = h \Rightarrow f(m, T) = \int_0^m h(m') dm' + f(0, T)$$



$\int_0^m h(m') dm'$ is the negative of the shaded area shown to the left. We see this area increases in magnitude until $m = m_0$, and then decreases in magnitude as m exceeds m_0 (since the curves cross at m_0)

Therefore we can plot the free energy, $f(m, T) - f(0, T)$



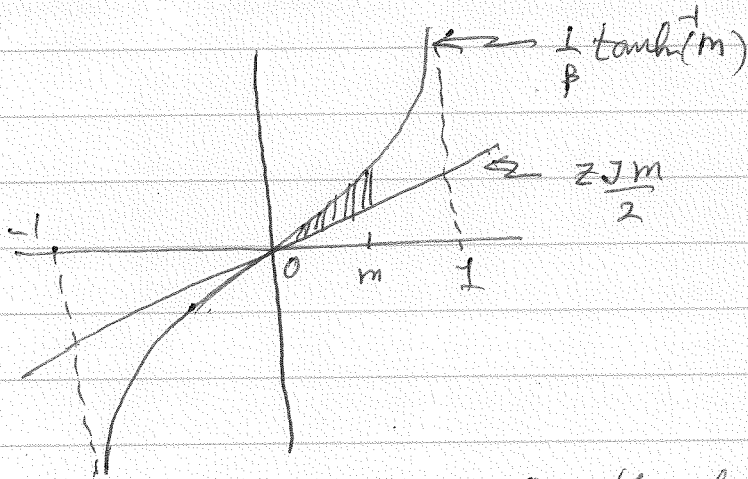
so $f(m_0, T) < f(0, T)$

m_0 gives the min of the free energy and so is the equilib solution

Gibbs free energy

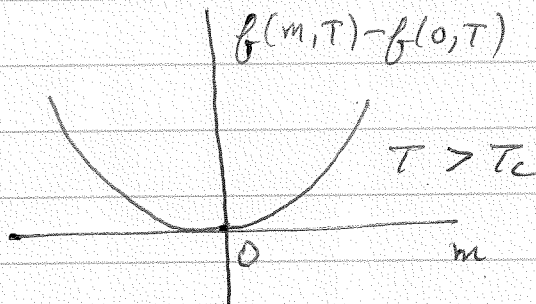
$$g(h=0, T) = \min_m f(m, T) \Rightarrow m = \pm m_0$$

For $T > T_c$ the situation looks like



now $\int_0^m h(m') dm'$ is the positive of the area shown to the left - it increases monotonically as m increases

so the free energy looks like



$\Rightarrow m=0$ is min of $f(m, T)$

$$g(h=0, T) = \min_m f(m, T)$$

$\Rightarrow m=0$ is equilib state

Recall - the plots of $f(m, T)$ shown above for $T > T_c$ and $T < T_c$ are exactly the same as we saw in discussing the van der Waals theory of the liquid-gas phase transition!

We can examine these points analytically if we consider behavior near T_c where m is small.

This analysis will introduce the critical exponents β, δ that characterize the critical point at $(T_c, h=0)$

$$m = \tanh\left(\beta \frac{zJ}{2} m + \beta h\right)$$

use $\frac{zJ}{2} = k_B T_c$, $\tanh x \approx x - \frac{1}{3}x^3$ for small x

for small h , near T_c where m small, expand the tanh

$$m = \left(\frac{T_c}{T} m + \frac{h}{k_B T}\right) - \frac{1}{3} \left(\frac{T_c}{T} m + \frac{h}{k_B T}\right)^3$$

for small $\frac{h}{k_B T} \ll m$,

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

$$(*) \quad m\left(1 - \frac{T_c}{T}\right) + \frac{1}{3} \left(\frac{T_c}{T}\right)^3 m^3 = \frac{h}{k_B T} \left(1 - \left(\frac{T_c}{T}\right)^2 m^2\right)$$

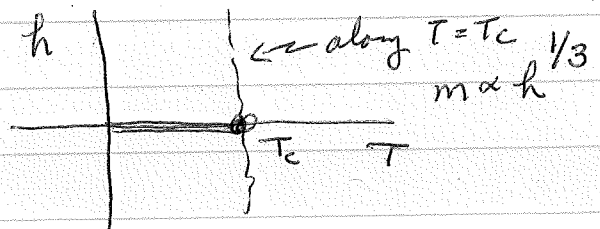
$$h = k_B T \left\{ \frac{m\left(1 - \frac{T_c}{T}\right) + \frac{1}{3} \left(\frac{T_c}{T}\right)^3 m^3}{1 - \left(\frac{T_c}{T}\right)^2 m^2} \right\}$$

$$(**) \quad \boxed{h \approx k_B T \left\{ m\left(1 - \frac{T_c}{T}\right) + \left[\left(1 - \frac{T_c}{T}\right)\left(\frac{T_c}{T}\right)^2 + \frac{1}{3} \left(\frac{T_c}{T}\right)^3\right] m^3 \right\}}$$

① At $T = T_c$ critical isotherm

$$h = \frac{k_B T_c}{3} m^3 \propto m^\delta \quad \delta = 3$$

or $m \propto h^{1/3}$



② At $h=0$ on coexistence line from (*) with $h=0$ we have

$$\left(1 - \frac{T_c}{T}\right)m + \left[\frac{1}{3}\left(\frac{T_c}{T}\right)^3 + \cancel{\left(\frac{T_c}{T}\right)^2} + \cancel{\left(\frac{T_c}{T}\right)}\right]m^3 = 0$$

as $T \rightarrow T_c^-$, $\left(1 - \frac{T_c}{T}\right) + \frac{1}{3}m^2 = 0$

$$m = \pm \sqrt{\frac{3(T_c - T)}{T}}$$

Define $t = \frac{T_c - T}{T_c}$ $m \propto \pm \sqrt{3t} \propto t^\beta$ $\beta = 1/2$

③ At $h=0$ on coexistence line as $T \rightarrow T_c$ from (**)

$$\frac{\partial h}{\partial m} = k_B T \left\{ \left(1 - \frac{T_c}{T}\right) + 3 \left[\left(1 - \frac{T_c}{T}\right) \frac{T_c}{T} + \frac{1}{3} \left(\frac{T_c}{T}\right)^3 \right] m^2 \right\}$$

$$\approx k_B T \left\{ \left(1 - \frac{T_c}{T}\right) + m^2 \right\} \quad \text{as } T \rightarrow T_c$$

As $T \rightarrow T_c^+$ from above, $m = 0$

$$\Rightarrow \frac{\partial h}{\partial m} = k_B T \left(1 - \frac{T_c}{T}\right) = k_B (T - T_c)$$

magnetic susceptibility $\Rightarrow \frac{\partial m}{\partial h} = \chi^+ = \frac{1}{k_B (T - T_c)} \propto \frac{1}{|t|^\gamma}$ $\gamma = 1$

Note: at high temp $T \gg T_c$, $\chi \sim \frac{1}{T}$ just like in Curie paramagnetism. Hence we say the $T > T_c$ phase is paramagnetic.

As $T \rightarrow T_c^-$ from below, $m^2 = 3 \left(\frac{T_c - T}{T} \right)$

$$\Rightarrow \frac{\partial h}{\partial m} = k_B T \left(\left(1 - \frac{T_c}{T}\right) + 3 \left(\frac{T_c - T}{T} \right) \right)$$

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

$$\frac{\partial m}{\partial h} = \chi^- = \frac{1}{2k_B (T_c - T)} \propto \frac{1}{|t|^\gamma} \quad \gamma = 1$$

Also $\lim_{T \rightarrow T_c} \left(\frac{\chi^+}{\chi^-} \right) = \frac{2k_B (T_c - T)}{k_B (T - T_c)} = 2$ ← amplitude ratio

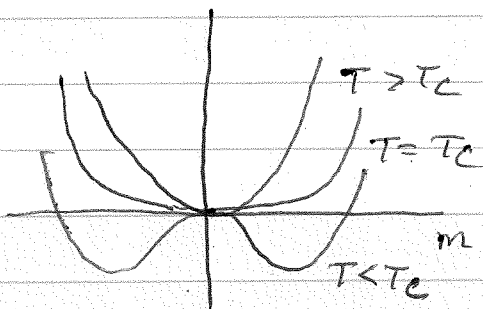
Our results here are identical to what we found for the van der Waal model of liquid-gas transition, if we make the identifications

$$h \leftrightarrow \delta p - \delta p^*(T) \quad \text{distance from coexistence curve}$$

$$m \leftrightarrow \delta v - \delta v_0$$

free energy $f(m, T) - f(0, T) = \int_0^m h(m') dm'$ case (**)
as $T \rightarrow T_c$

$$\Rightarrow f(m, T) - f(0, T) = k_B T \left\{ \frac{1}{2} \left(1 - \frac{T_c}{T}\right) m^2 + \frac{1}{12} m^4 \right\}$$



coefficient of m^2 term vanishes at T_c , goes negative below $T_c \Rightarrow$ minimum of $f(m, T)$ changes from $m=0$ to $m = \pm m_0(T)$

$$g(h=0, T) = \min_m f(m, T) \Rightarrow \text{min of } f \text{ gives equilibrium state}$$