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.

$\Rightarrow$ *Approximate Solution*

Mean Field or Curie-Weiss Molecular Field Approximation

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_i s_i$$

Consider spin s_i. Approx the interaction of s_i with its neighbor s_j as an interaction with the thermal average value of $\langle s_j\rangle \equiv m$.
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. $\langle s_j\rangle = m = \frac{1}{N}\sum_i \langle s_i\rangle$

$$\mathcal{H}_{MF} \simeq -J\sum_{\langle ij\rangle} s_i m - h\sum_i s_i$$

sum over bonds

$$\mathcal{H}_{MF} = -\frac{z}{2} J \sum_i s_i m - h \sum_i s_i$$

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

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) <u>cubic</u> lattice, $z=6$. For a (2d) <u>square</u> 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 $\mathcal{H}_{MF}$ and self-consistently solve for m from the resulting equation.

$$\mathcal{H}_{MF} = \sum_i \mathcal{H}_{MF}^{(1)} \quad \text{where } \mathcal{H}_{MF}^{(1)} = -\left(\frac{z}{2} J m + h\right) s$$

we have <u>non-interacting</u> spins in MF approx

$$\Rightarrow \langle s \rangle = m = \frac{\sum_s e^{-\beta \mathcal{H}_{MF}^{(1)}} s}{\sum_s e^{-\beta \mathcal{H}_{MF}^{(1)}}}$$

s is a single spin at any site

$$= \frac{e^{+\beta(\frac{z}{2} J m + h)}(+1) + e^{-\beta(\frac{z}{2} J m + h)}(-1)}{e^{+\beta(\frac{z}{2} J m + h)} + e^{-\beta(\frac{z}{2} J m + h)}}$$

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

solve to get $m(T, h)$

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

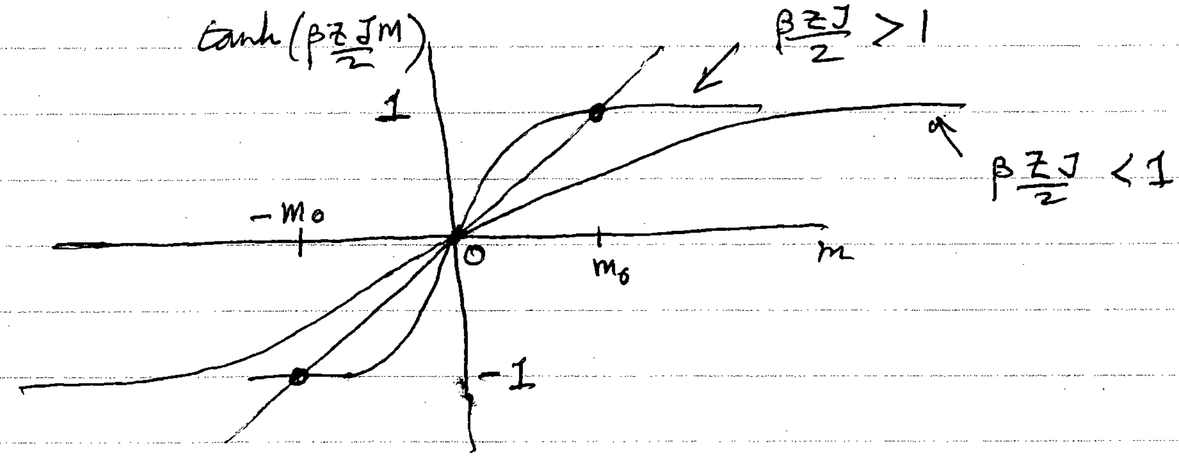
$$m = \tanh\left[\frac{\beta z J m}{2} + \beta h\right]$$

consider first $h=0$

$$m = \tanh\left[\frac{\beta z J m}{2}\right]$$ 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 $m = \pm m_0$



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

$T > T_c \Rightarrow m = 0$

$T < T_c \Rightarrow m = \pm m_0$ $\quad$ $m=0$ is unstable solution

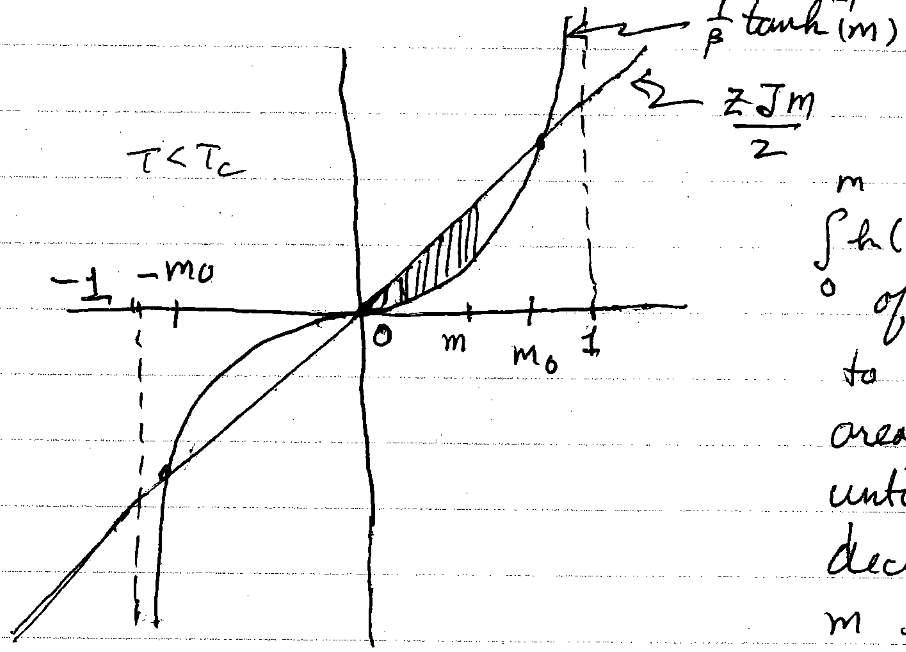
For $T < T_c$, $m = 0$ is unstable

$m = \pm m_0$ are the equilib solutions. To see this

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

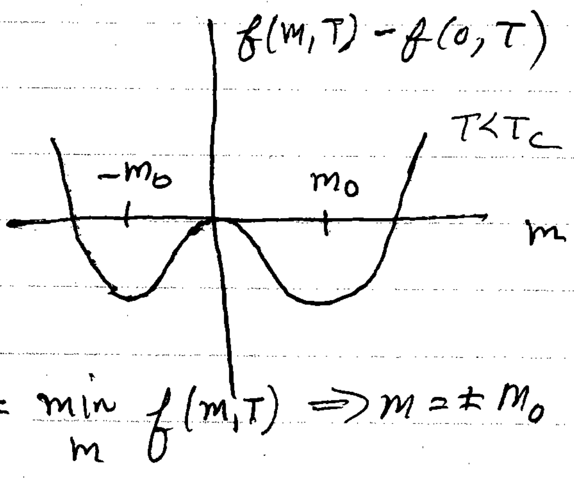
$$h = \frac{1}{\beta}\tanh^{-1} m - \frac{zJm}{2}$$

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



$\int_0^m h(m')\,dm'$ 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 $f(m,T) - f(0,T)$



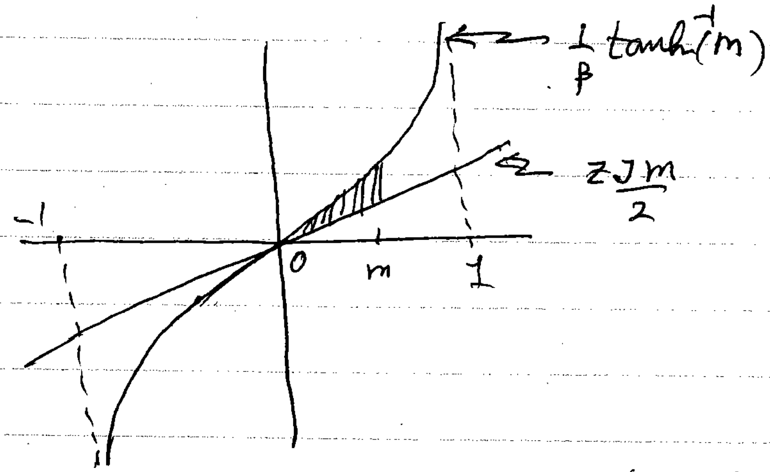
so $f(m_0,T) < f(0,T)$

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

Gibbs free energy

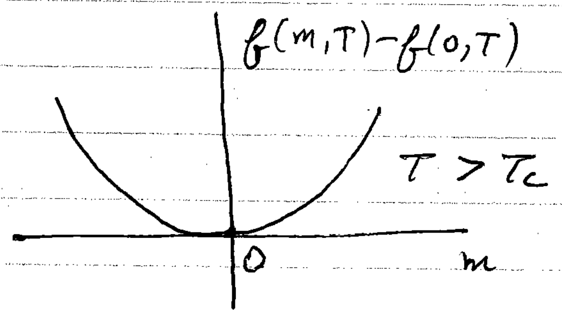
$$g(h=0,T) = \min_m f(m,T) \Rightarrow m = \pm m_0$$

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 minimum 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 δ, β, γ that characterize the critical point at $(T_c, h=0)$

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

use $\frac{zJ}{2} = k_B T_c$, $\tanh x \simeq x - \frac{1}{3}x^3$ 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 $\frac{h}{k_B T} \ll m$,

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

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

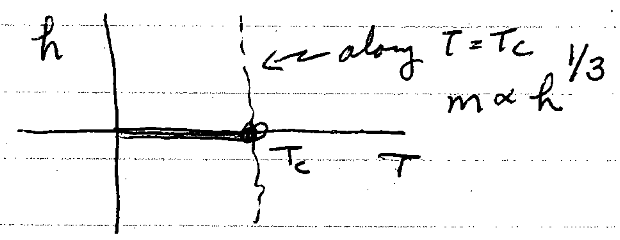
$$h = k_B T \left\{ \frac{m\left(1 - \frac{T_c}{T}\right) + \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3}{1 - \left(\frac{T_c}{T}\right)^2 m^2} \right\}$$

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

① At $T = T_c$ critical isotherm

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

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



(2) At $h=0$ on coexistence line

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

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

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

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

(3) At $h=0$ on coexistence line as $T \to T_c$

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

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

As $T \to T_c^+$ 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 $\Rightarrow \quad \frac{\partial m}{\partial h} = \chi^+ = \frac{1}{k_B(T-T_c)} \propto \frac{1}{|t|^{\gamma'}} \quad \gamma' = 1$

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

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

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

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

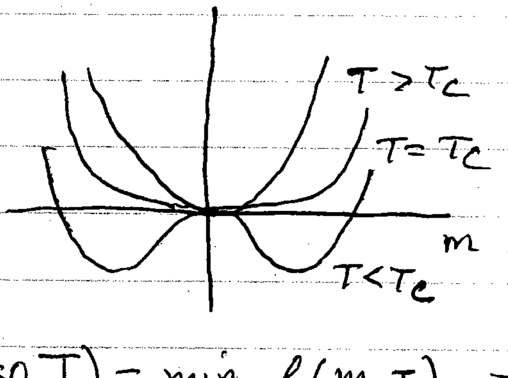
Also $\lim_{T \to T_c} \left(\frac{\chi^+}{\chi^-}\right) = \frac{2k_B (T_c - T)}{k_B (T - T_c)} = 2$ ← amplitude ratio

Our results here are <u>identical</u> to what we found for the v 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 $f(m,T) - f(0,T) = \int_0^m h(m')\,dm'$

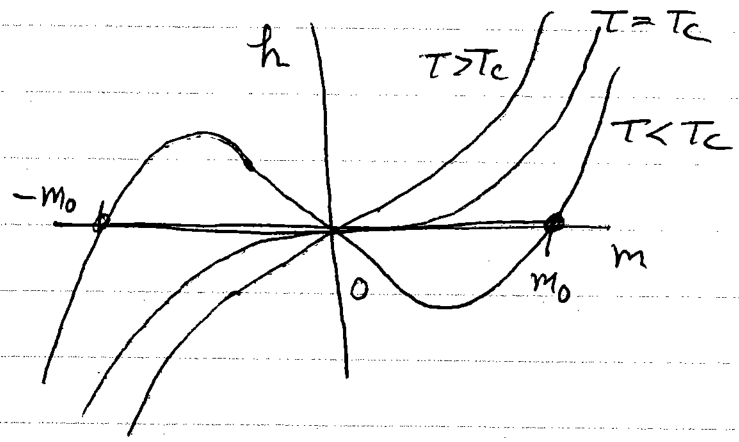
$$\Rightarrow f(m,T) - f(0,T) = k_B T \left\{ \frac{1}{2}\left(1 - \frac{T_c}{T}\right) m^2 + \frac{1}{12} m^4 \right\}$$



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

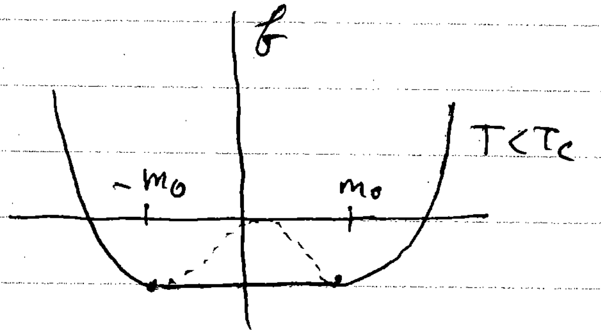
$g(h=0,T) = \min_m f(m,T)$ ⇒ min of f gives equilibrium state

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

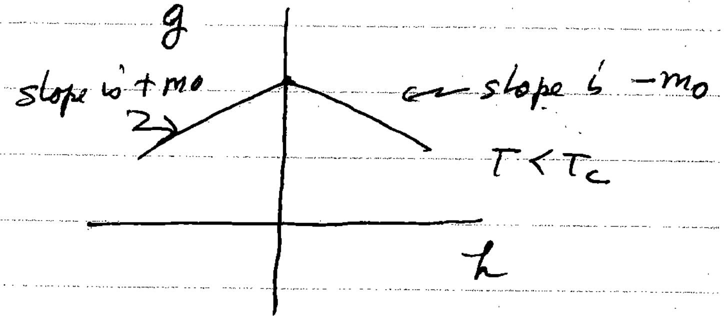


For $T < T_c$ we should "fix" the $h(m)$ curves with a Maxwell-like construction at $h=0$ from $m = -m_0(T)$ to $m = +m_0(T)$.

Similarly, $f(m,T)$ with Maxwell construction looks like



Helmholtz



Gibbs

$g(h)$ has discontinuous derivative at $h=0$ for $T < T_c$