

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

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

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  $j$ .  $\langle S_j \rangle = m = \frac{1}{N} \sum_i \langle S_i \rangle$

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

↑  
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 the 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.

$H_{MF} = \sum_i H_{MF}^{(i)}$  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

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

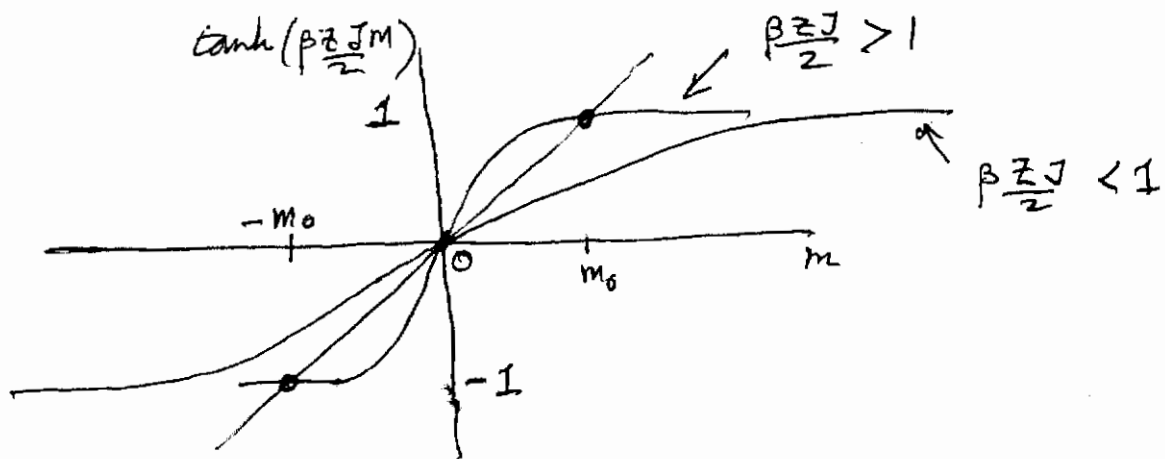
consider first  $h=0$

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

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  $m = \pm m_0$



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

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

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

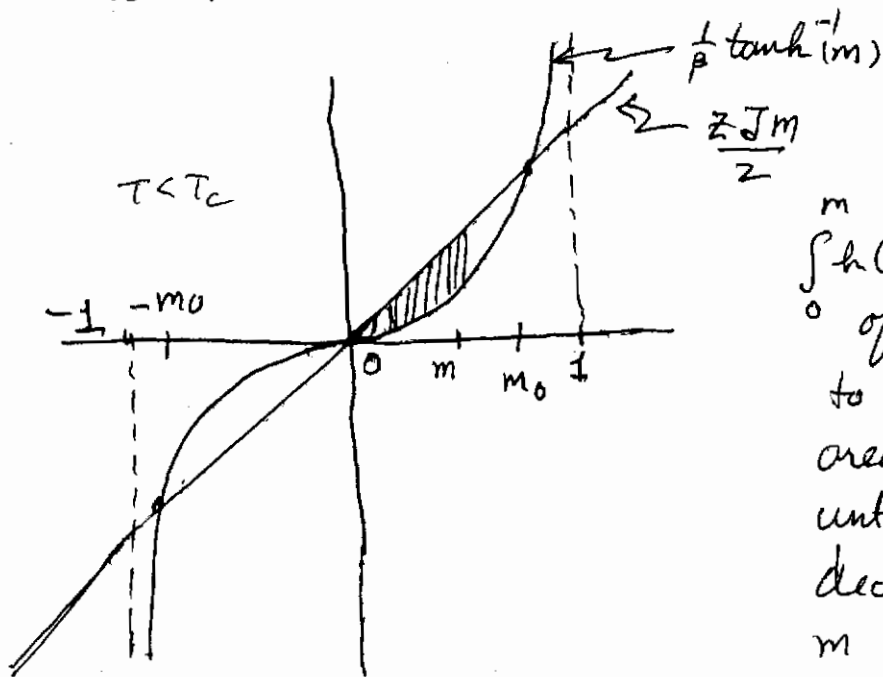
$m=0$  is unstable solution

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

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

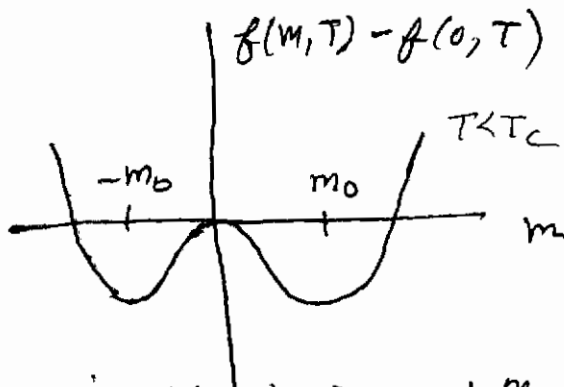
$$h = \frac{1}{\beta} \tanh^{-1} m - \frac{z J m}{2}$$

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



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



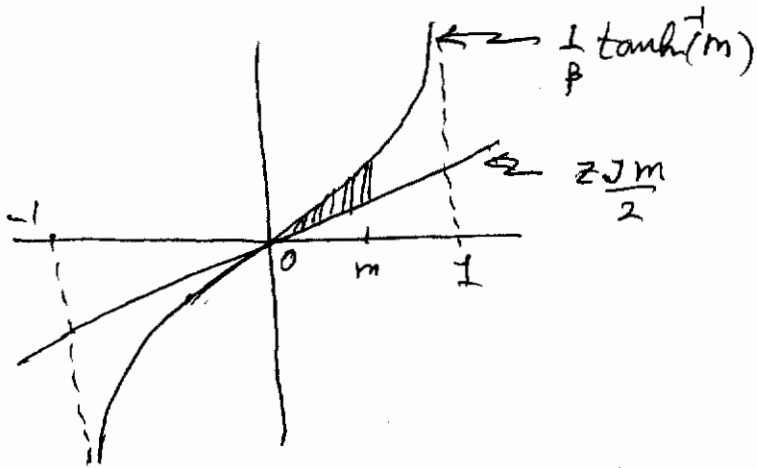
$$\text{so } f(m_0, T) < f(0, T)$$

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

Gibbs free energy

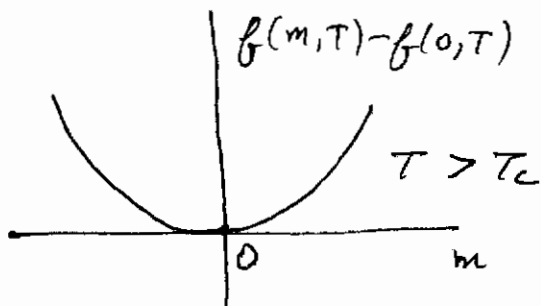
$$g(h=0, T) = \min_m f(m, T) \Rightarrow m = \pm m_0$$

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  $f(m, T)$

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

$\Rightarrow m=0$  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  $\beta, \delta$  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  $m \propto h^{1/3}$

