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

However, an <u>exact solution</u> 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.

⇒ <u>Approximate Solution</u>

<u>Mean Field</u> or Curie-Weiss Molecular Field Approximati

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

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. $\langle s_j\rangle = m = \frac{1}{N}\sum_i \langle s_i\rangle$

$$\mathcal{H}_{MF} \simeq -J\underbrace{\sum_{\langle ij\rangle}}_{\text{sum over bonds}} s_i m - h\sum_i s_i$$

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

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

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

where z is the "coordination number" - the number of nearest neighbors of site i. For a simple (3d) cubic lattice, $z=6$. For a (2d) 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 $\mathcal{H}_{MF}$ and self-consistently solve for m from the resulting equation.

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

we have non-interacting spins in MF approx

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

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 $m(T, h)$

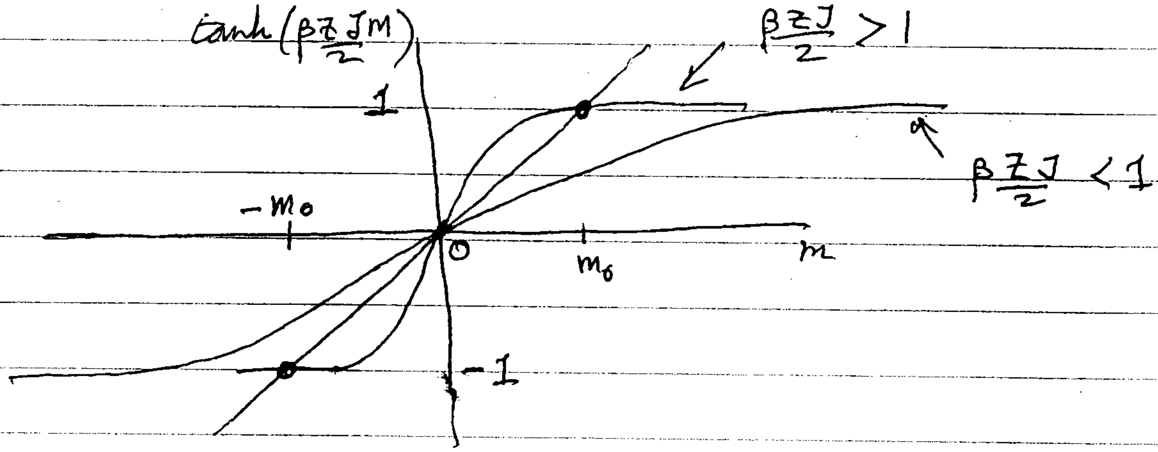
Note $m(T, h) = -m(T, -h)$ as expected

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

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 $\boxed{k_B T_c = \frac{Z J}{2}}$

$T > T_c \Rightarrow m = 0$

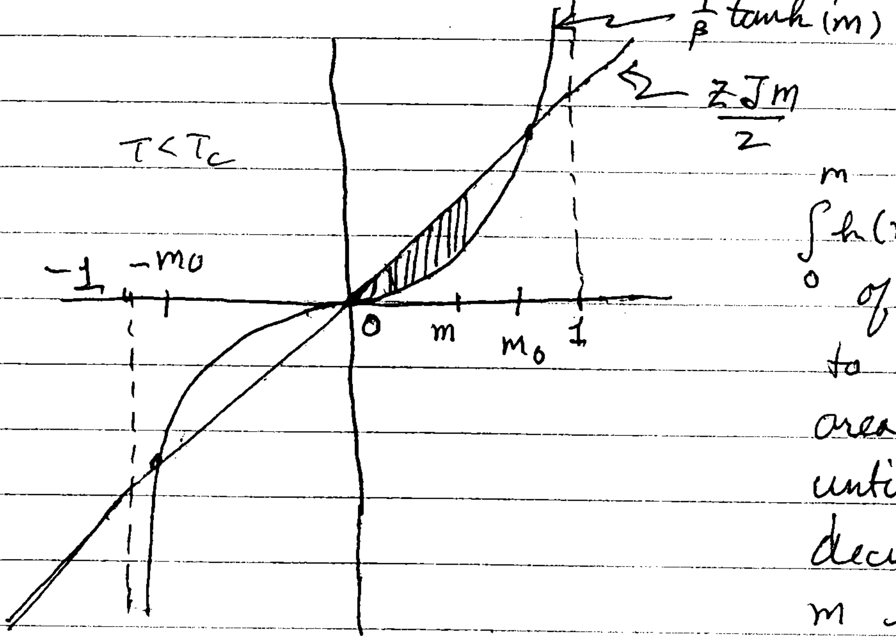
$T < T_c \Rightarrow m = \pm m_0$ $\qquad$ $m = 0$ is unstable solution

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

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

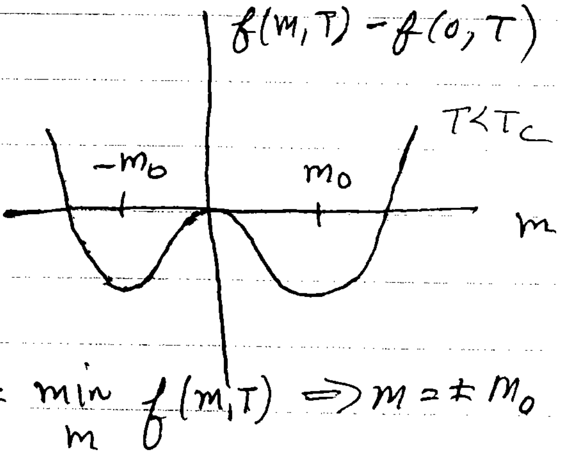
$$h = \frac{1}{\beta}\tanh^{-1} m - \frac{zJm}{2}$$

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



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

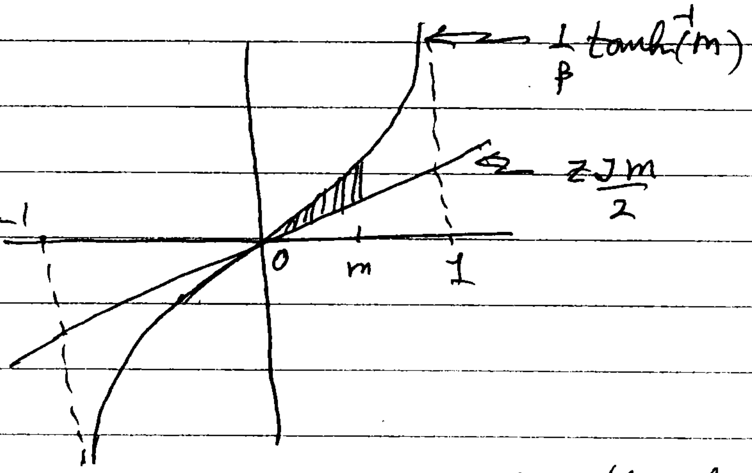


so $f(m_0,T) < f(0,T)$

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

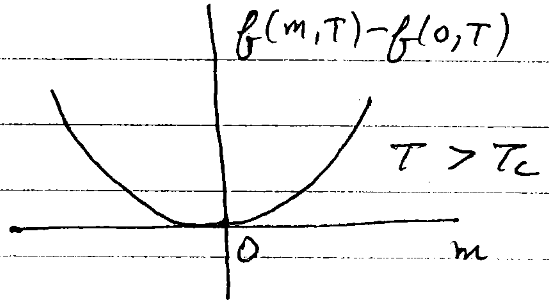
Gibbs free energy
$g(h=0,T) = \min_m f(m,T) \Rightarrow m = \pm m_0$

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 minim 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

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

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

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

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

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

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

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

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

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

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

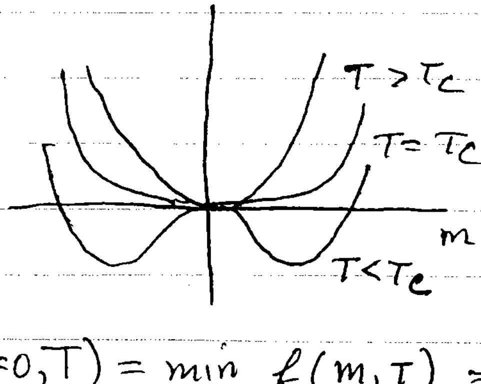
Our results here are identical to what we found for the v der Waal model of liquid-gas transition, if we make the identifications

$h \leftrightarrow \delta p - \delta p^*(T)$ distance from coexistence cu

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

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

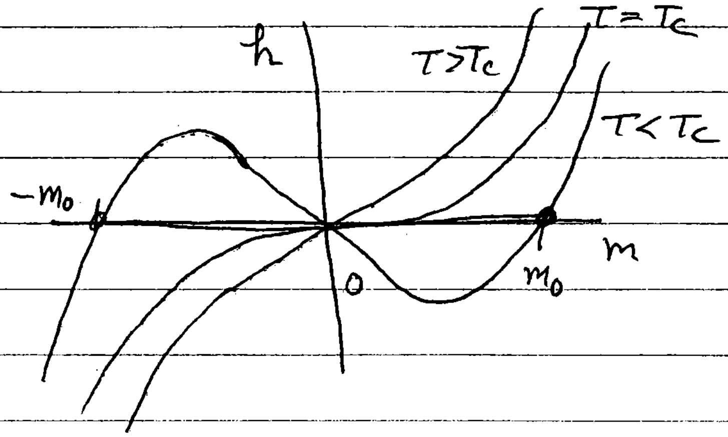
$$\Rightarrow f(m,T) - f(0,T) = k_B T\left\{\frac{1}{2}\left(1 - \frac{T_c}{T}\right)m^2 + \frac{1}{12}m^4\right\}$$



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

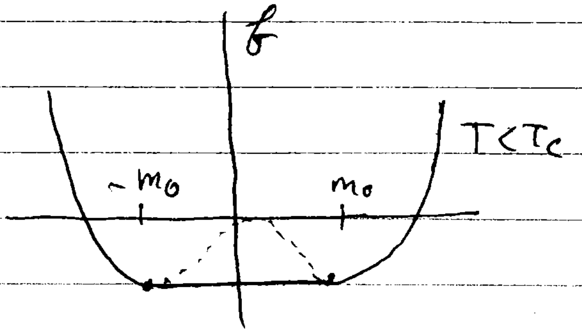
$g(h=0,T) = \min_m f(m,T) \Rightarrow$ min of f gives equilibrium state

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

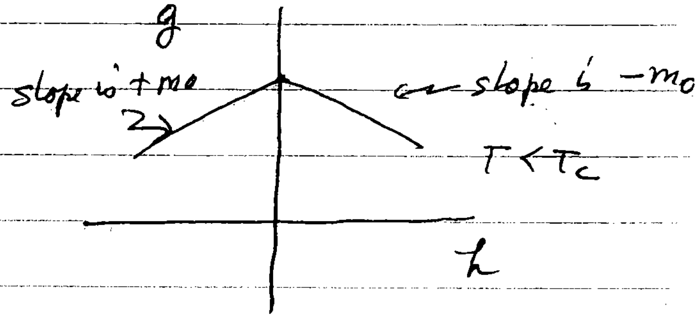


For $T<T_c$ we should "fix" the $h(m)$ curves with a Maxwell-like construction at $h=0$ from $m=-m_0(T)$ to $m=+m_0(T)$.

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



Helmholtz

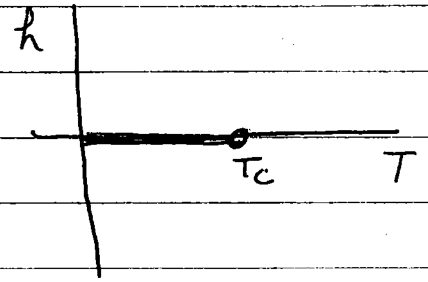


Gibbs

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

Landau's Theory of phase transitions

Ising model



order parameter m - $\begin{cases} \text{zero} & T > T_c \\ \text{non-zero} & T < T_c \end{cases}$

ordering field h

applying $h \neq 0$ reduces symmetry of Hamiltonian, induces $m \neq 0$.

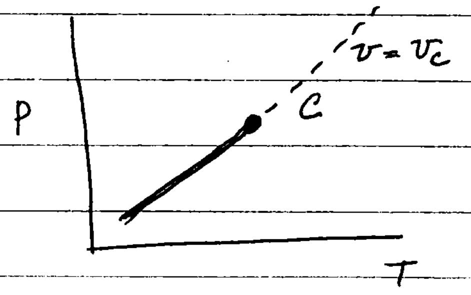
For ordering field $h=0$, Hamiltonian has higher symmetry. A finite order parameter $m \neq 0$ breaks this symmetry.

For $h=0$, 2nd order phase transition at T_c such that $m=0$ for $T > T_c$ $\Rightarrow$ thermodynamic state has full symmetry of $\mathcal{H}$. When $T < T_c$ the order parameter becomes finite $m \neq 0$ $\rightarrow$ thermodynamic state breaks symmetry of $\mathcal{H}$. Spontaneous symmetry breake

For $T < T_c$ varying the ordering field h through zero results in a discontinuous jump in the order parameter – 1st order transition line

~~At~~ the 2nd order transition at T_c, that ends the 1st order transition line, m goes to zero continuously as $T \to T_c^-$.

For liquid-gas transition



1st order line does not have any particular symmetry with respect to the natural thermodynamic variables

dashed line is critical isochore – line of constant $v = v_c$ smoothly extends from 1st order transition line.

Define ordering field δp as distance from critical isochore. Define order parameter $\delta v = v - v_c$ as difference in specific volume (or density) from critical value.

Landau methodolgy

① Given a physical system with a phase transition, first identify the order parameter m – a quantity that vanishes in the high T disordered phase, and is non zero in the low T ordered phase. Often this can be the hard part! cf. spin glass problem

② Near the 2nd order critical pt, the order parameter is small. ⇒ expand the Helmholtz free energy $f(m,T)$ in a Taylor series in m, keeping all terms which have the appropriate symmetry of the problem.

For Ising model

$$f(m,T) \simeq f_0 + am^2 + bm^4 + \cdots$$

only even powers of m appear since $\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j$ is symmetric under $\{s_i\} \to \{-s_i\}$.

For liquid - gas transition

$$f(\delta v,T) \simeq f_0 + a\,\delta v^2 + b\,\delta v^3 + c\,\delta v^4 + \cdots$$

no symmetry of $\mathcal{H}$ to rule out odd powers of order parameter δv. - but still no linear δv term since $f(\delta v=0,T)$ must be a minimum when $T>T_c$. - or equivalently, if there was a δv linear term in $f(\delta v,T)$, it would mean we were not properly expanding about critical isochore.

But we saw that by the trick of transformation of variables, $\delta v = \delta v_0 + u$, we can effectively eliminate the δv^3 term and make the problem look just like the Ising model.

$$f(m,T) = f_0(T) + a(T)m^2 + b(T)m^4 + \cdots$$

↑ ignore higher order terms

Stability ⇒ $b(T) > 0$, $f(m,T)$ must have global minimum

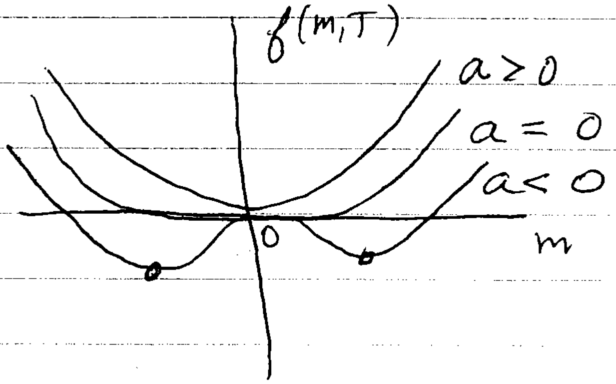
State of system is obtained by minimizing $f(m,T)$ with respect to m. Or equivalently; Gibbs free energy is

$$g(h,T) = \min_m \left[f(m,T) - hm \right]$$

On the 1st order line the ordering field $h=0$

$$\Rightarrow \quad g(0,T) = \min_m \left[f(m,T) \right]$$

⇒ 2nd order critical point occurs when $a(T) = 0$



When $a \geq 0$ then $m=0$ minimizes $f(m,T)$ ⇒ thermodynamic state has symmetry of H

When $a<0$, then $m = \pm m_0$ minimizes $f(m,T)$ ⇒ thermodynamic state breaks symmetry

minimum of $f(m,T)$ increases continuously from $m=0$ as a decreases below zero

Expading near T_c to lowest orders,

$$b(T) \approx b(T_c) \equiv b_0 \quad \text{a constant}$$

$$a(T) \approx a_0[T-T_c] \quad a_0 \text{ a constant}$$

① Behavior of order parameter near T_c

$T < T_c$ minimize $f(m,T)$

$$\Rightarrow \quad 2am + 4bm^3 = 0$$

$$2a + 4bm^2 = 0 \quad \text{for } m \neq 0$$

$$m^2 = -\frac{a}{2b}$$

$$\boxed{m_0 = \pm\sqrt{\frac{a_0(T_c-T)}{2b_0}}} \propto |t|^\beta \quad \boxed{\beta = 1/2}$$

$$t = \left(\frac{T_c - T}{T_c}\right)$$

same β as found earlier

② $h(m)$ curve at critical isotherm $T = T_c$

$$g(h,T_c) = \min_m \left[f(m,T) - hm \right]$$

$$= \min_m \left[f_0 + b_0 m^4 - hm \right] \quad a = 0 \text{ at } T_c$$

$$\Rightarrow \quad 4b_0 m^3 - h = 0 \quad \Rightarrow \quad \boxed{h = 4b_0 m^3}$$

$$h \propto m^\delta \quad \boxed{\delta = 3}$$ same as before

③ susceptibility $\chi = \frac{\partial m}{\partial h}$ at $h = 0$

$$g(h,T) = \min_m \left[f(m,T) - h m \right]$$

$$\Rightarrow \quad 2am + 4bm^3 = h$$ "equation of state"

$$\chi^{-1} = \frac{\partial h}{\partial m} = 2a + 12bm^2$$

$$\chi = \frac{1}{2a + 12bm^2}$$

For $T > T_c$, $h = 0 \Rightarrow m^2 = 0$

$$\boxed{\chi^+ = \frac{1}{2a}} = \frac{1}{2a_0(T - T_c)} \propto \frac{1}{|t|^{\gamma'}}, \quad \boxed{\gamma' = 1}$$

For $T < T_c$, $h = 0 \Rightarrow m^2 = m_0^2 = \frac{-a}{2b} = \frac{a_0(T_c - T)}{2b_0}$

$$\chi^- = \frac{1}{2a_0(T - T_c) + \frac{12 b_0 a_0}{2b_0}(T_c - T)}$$

$$\boxed{\chi^- = \frac{1}{4a_0(T_c - T)}} \propto \frac{1}{|t|^{\gamma}} \quad \boxed{\gamma = 1}$$

$$\boxed{\lim_{T \to T_c} \frac{\chi^+}{\chi^-} = 2}$$ amplitude ratio

all same as before

④ specific heat at $h=0$ along 1st order transition line

from ① we have $m_0^2 = \frac{-a}{2b}$ $\quad T<T_c$, $\quad m_0^2 = 0 \quad T>T_c$

$$\Rightarrow g(h=0,T) = f(m_0,T) = f_0(T), \quad T>T_c$$

$$= f_0(T) + a\left(\frac{-a}{2b}\right) + b\left(\frac{-a}{2b}\right)^2, \quad T<T$$

$T<T_c$: $$f(m_0,T) = f_0(T) - \frac{a^2}{2b} + \frac{a^2}{4b} = f_0(T) - \frac{a^2}{4b}$$

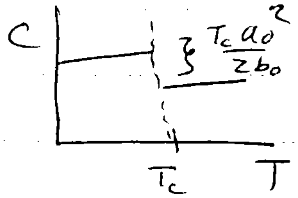
$$= f_0(T) - \frac{a_0^2}{4b_0}(T-T_c)^2$$

specific heat

$$s = -\frac{\partial g}{\partial T} \Rightarrow C = T\left(\frac{\partial s}{\partial T}\right)_{h=0} = -T\frac{\partial^2 g}{\partial T^2}$$

$$C = -T\frac{d^2}{dT^2} f(m_0(T),T)$$

$$= \begin{cases} -T\dfrac{d^2 f_0}{dT^2} & T>T_c \\ -T\dfrac{d^2 f_0}{dT^2} + \dfrac{T a_0^2}{2b_0} & T<T_c \end{cases}$$



$$\Rightarrow C(T\to T_c^-) - C(T\to T_c^+) = \frac{T_c a_0^2}{2b_0}$$

jump in specific heat at T_c

The piece $\frac{\partial^2 f_0}{\partial T^2}$ is the non singular piece of the specific heat. f_0 is the same as the "reference" free energy we used earlier when integrating the equation of state in the mean field or the van der Waals approx.

We can define a critical exponent α for the specific heat by $C \propto |t|^\alpha$, or

$$\alpha = \lim_{t \to 0} \left[\frac{\ln C}{\ln |t|} \right]$$

For Landau theory this gives $\boxed{\alpha = 0}$

Summary: Landau theory = mean field theory

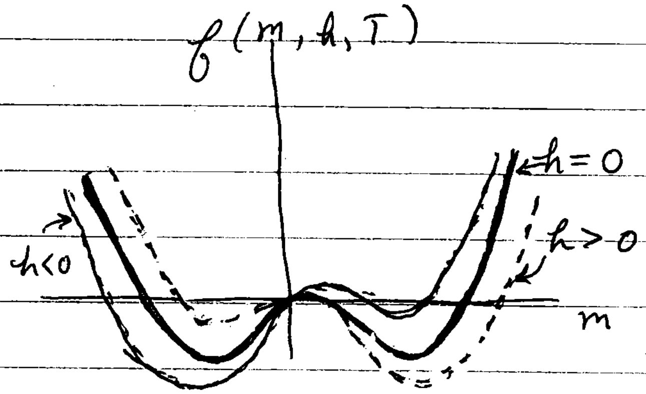
$$\left. \begin{array}{lll} h = 0, & m_0(T) \sim |t|^\beta & \underline{\beta = 1/2} \\ & & \\ T = T_c, & h(m) \propto m^\delta & \underline{\delta = 3} \\ & & \\ h = 0, & \chi(T) \propto \frac{1}{|t|^\gamma} & \underline{\gamma = 1} \\ & \lim_{t \to 0} \frac{\chi^+}{\chi^-} = 2 & \end{array} \right\} \text{mean field critical exponents}$$

$$h = 0, \quad C(T) \propto |t|^\alpha \quad \underline{\alpha = 1}$$

Landau theory of 1st order transition

For $T < T_c$, $h \neq 0$

$$g(h,T) = \min_m \left[f(m,T) - hm \right] \equiv \min_m \left[f(m,h,T) \right]$$



as h goes smoothly through zero, the value of m that minimizes f(m, h, T) jumps discontinuously from $+m_0$ to $-m_0$.

2nd order transition – order parameter goes continuously to zero

1st order transition – order parameter jumps discontinuously

<u>Note</u>: Landau theory ≡ mean field theory
gives the same values of the critical exponents
<u>independent</u> of dimension d, and number of
components of spin n.

For n-component spins with $\vec{m} = \frac{1}{N}\sum_i \vec{S}_i$

$$f(\vec{m},T) = f_0 + a|\vec{m}|^2 + b|\vec{m}|^4 + \cdots$$

everything comes out the same!

But can get some interesting new behaviors by doing other thin

① $f(m,T) = f_0 + a\,m^2 - b\,m^4 + c\,m^6$

$b>0$ ⇒ quartic term is negative,
need m^6 term to give stability

This describes a <u>tricritical point</u> where a <u>line</u> of
1st order transitions becomes a <u>line</u> of 2nd order
transitions

② put in spatially varying terms: ex: a superconductor
in an applied magnetic field. Order parameter is
condensate wavefunction $\psi(\vec{r})$.

$$f(\psi,T) = f_0 + \underset{\text{minimize wrt } \psi \text{ to get Abrikosov vortex lattice}}{a|\psi|^2 + b|\psi|^4} + \underset{\substack{\uparrow \\ \text{kinetic energy of supercurrents}}}{c\,|(\vec{\nabla} + i\overset{\substack{\text{magnetic vector potential} \\ \downarrow}}{\vec{A}})\psi|^2}$$

$\vec{\nabla}\times\vec{A} = \vec{B}$ magnetic field