(4) <u>Specific heat at $h=0$</u> along 1^{st} order transition line

From above we can write

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

$$\equiv am^2 + bm^4$$

with $a = a_0(T-T_c)$ and $a_0 = \frac{k_B}{2}$

$b = \frac{k_B T}{12} \simeq \frac{k_B T_c}{12}$

Then for $T > T_c$ $m_0^2 = 0$

for $T < T_c$ $m_0^2 = -\frac{a}{2b}$ at minimum of $f(m,T)-f(0,T)$

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

so

$$g(h=0,T) = \min_m \left[f(m,T)\right] = f(m_0,T)$$

$T > T_c$ $g(h=0,T) = f(m_0,T) = f_0(T)$ as $m_0 = 0$

$T < T_c$ $g(h=0,T) = f(m_0,T) = f_0(T) + a m_0^2 + b m_0^4$

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

$$= f_0(T) - \frac{a^2}{2b} + \frac{a^2}{4b}$$

$$= f_0(T) - \frac{a^2}{4b}$$

with $a = a_0(T-T_c)$

and $b = \frac{k_B T_c}{12}$ <u>constant</u>

specific heat at $h=0$

specific heat per spin

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

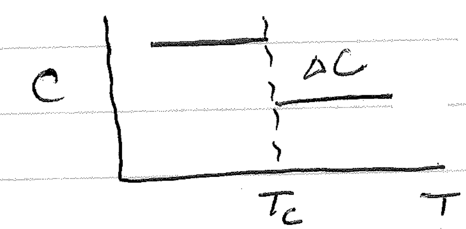
$$C = -T\,\frac{d^2 f(m_0(T), T)}{dT^2}$$

$$= -T\,\frac{d^2 f_0}{dT^2} \qquad T > T_c \quad \text{where } m_0 = 0$$

$$= -T\,\frac{d^2 f_0}{dT^2} + \frac{T a_0^2}{2b} \qquad T < T_c \quad \text{where } m_0^2 = \frac{-a}{2b}$$

since $\frac{da^2}{dT^2} = 2a_0^2$

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



Specific heat has a discontinuous jump at T_c

The piece $\frac{\partial^2 f_0}{\partial T^2}$ is the non-singular piece of the specific heat that is smooth and continuous as one passes through T_c.

We can define a critical exponent α for the specific heat by

$$C \propto |t|^{-\alpha} \quad \text{or}$$

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

For our mean field calculation this gives $\boxed{\alpha = 0}$.

<u>Summary</u>: Critical exponents for Ising model in mean-field theory

$T < T_c$, $h = 0$ $\quad m_0(T) \sim |t|^{\beta} \qquad \beta = 1/2$

$T = T_c$ $\quad h(m) \sim m^{\delta} \qquad \delta = 3$

$h = 0$ $\quad \chi(T) \sim \frac{1}{|t|^{\gamma}} \qquad \gamma = 1$

$$\lim_{t \to 0} \left(\frac{\chi^{+}}{\chi^{-}} \right) = 2 \quad \text{amplitude ratio}$$

$h = 0$ $\quad C(T) \sim |t|^{-\alpha} \qquad \alpha = 0$

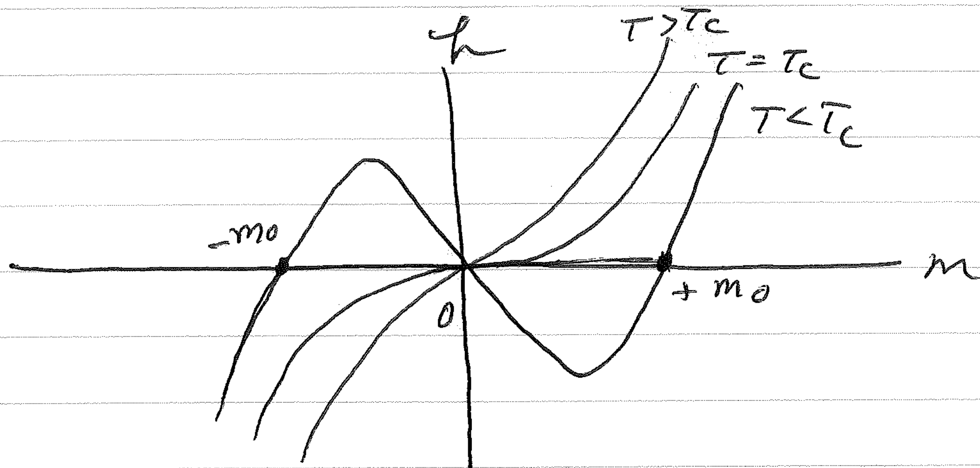
exponent values in mean field theory are independent of the dimension d of the system.

From exact Onsager solution of $d = 2$ Ising model

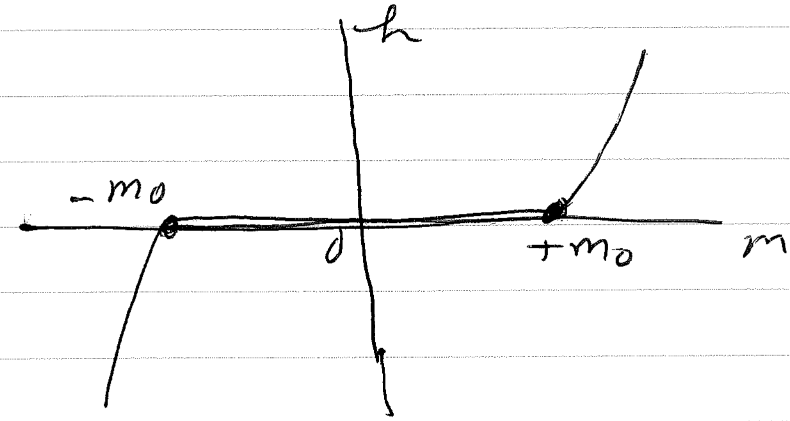
$\beta = 1/8$, $\delta = 15$, $\gamma = 7/4$, $\alpha = 0$ but C has logarithmic divergence $C \sim \ln|t|$

A closer look

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

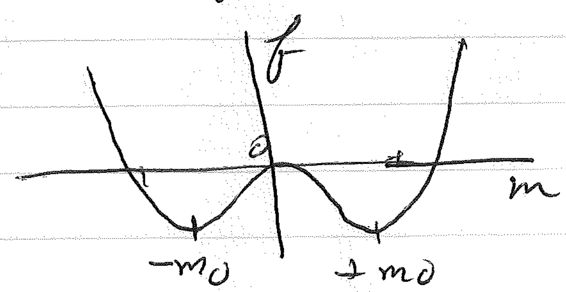


For $T < T_c$ we know that above $h(m)$ curve.
cannot be valid for $-m_0 \leq m \leq +m_0$
This is the coexistence region where $h = 0$
For $T < T_c$, the correct $h(m)$ curve is

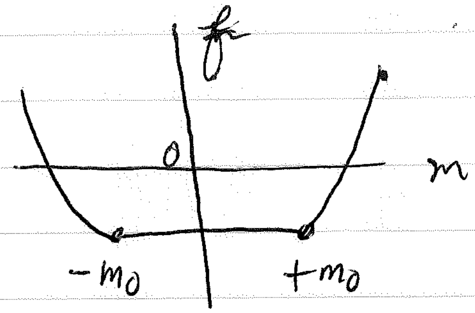


Such a "correction" based on our physical understanding is called the "Maxwell construction" (originally done in connection with the van der Waals theory of the liquid to gas phase transition.

If we use the above $h(m)$ for $T < T_c$, ~~then~~ to compute $f(m,T)$, then instead of



we get

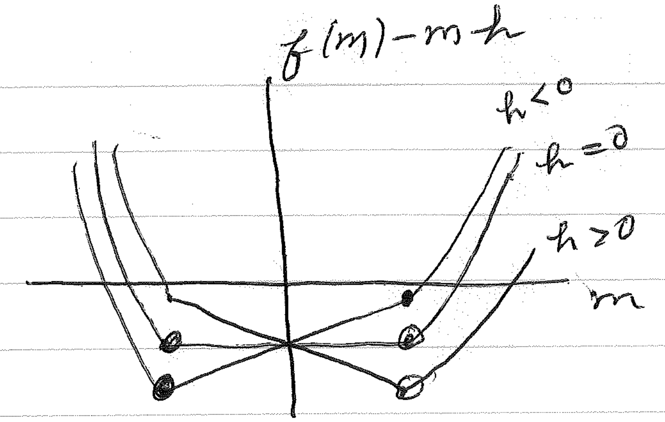


← $f(m)$ with Maxwell construction

Note: this can be thought of as if we take the top curve and replace it by its convex envelope. The top curve cannot be physically correct since $f(m)$ must be convex in m. Only the lower curve is convex.

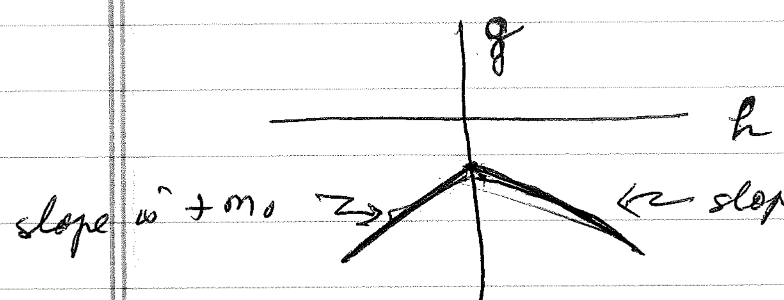
Using the above corrected $f(m)$, we can compute

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



$T < T_c$

$g(h) = \min_m [f(m) - mh]$ then results in



$T < T_c$

$\frac{dg}{dh} = -m$ is discontinuous at $h=0$

$\Rightarrow g(h)$ has a cusp-like maximum at $h=0$

Note: The mean field approx is *exact* in the limit that every spin interacts with every other spin (not just nearest neighbors). Then

$$\mathcal{H} = -\tilde{J} \sum_{i,j} s_i s_j - h \sum_i s_i$$

$$= -\tilde{J} \sum_i s_i \left(\sum_j s_j \right) - h \sum_i s_i$$

$$= -\tilde{J} \sum_i s_i \, N m - h \sum_i s_i$$

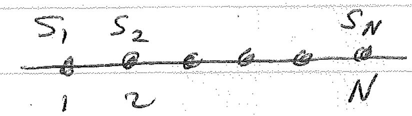
$$\mathcal{H} = -\left(\frac{z}{2} J m + h \right) \sum_i s_i$$

where we took $J \equiv \frac{2}{z} \tilde{J} N$. For infinite range coupling model, need to take coupling $J \propto \frac{1}{N}$ so that total energy scales with $E \propto N$ as desired.

In the above, $m[s_i] = \frac{1}{N} \sum_j s_j$ *depends* on the config $\{s_i\}$, however it is the same for every spin s_i

Ising model in 1-dimension

$h=0$ for simplicity



free boundary conditions

s_1 interacts only with s_2, s_N interacts only with s_{N-1}

$$\mathcal{H} = -J\sum_{i=1}^{N-1} s_i s_{i+1}$$

Define $\sigma_i = s_i s_{i+1}$, $i = 1, \ldots, N-1$

$$\sigma_i = \pm 1$$

$$\mathcal{H} = -J\sum_{i=1}^{N-1}\sigma_i \qquad s_1 s_j = \prod_{i=1}^{j-1}\sigma_i = (s_1 s_2)(s_2 s_3)\cdots(s_{j-1}s_j)$$
$$= s_1 s_2^2 s_3^2 \cdots s_{j-1}^2 s_j$$
$$= s_1 s_j$$

For every set of $\{\sigma_i\}_{i=1}^{N-1}$ there are 2 possible spin configurations depending on whether $s_1 = +1$ or -1

For a given value of s_1, then

$$s_j = \frac{1}{s_1}\prod_{i=1}^{j-1}\sigma_i$$

So

$$Z = \sum_{\{s_i\}} e^{\beta J\sum_{i=1}^{N} s_i s_{i+1}} = \underbrace{2}_{\text{two values for } s_1}\sum_{\{\sigma_i\}} e^{\beta J\sum_{j=1}^{N-1}\sigma_j} = 2\prod_{j=1}^{N-1}\sum_{\sigma_i=\pm1} e^{\beta J\sigma_i}$$

$$Z = 2\left[\sum_{\sigma=\pm1} e^{\beta J\sigma}\right]^{N-1} = 2\left[2\cosh\beta J\right]^{N-1}$$

Gibbs free energy

$$G(h=0,T) = -k_B T \ln Z = -k_B T \ln 2 - k_B T (N-1) \ln(2\cosh\beta J)$$

$$g = \lim_{N\to\infty} \frac{G}{N} = -k_B T \ln(2\cosh\beta J)$$

entropy $s = -\left(\frac{\partial g}{\partial T}\right)_{h=0}$ specific heat at const $h=0$ $C = T\left(\frac{\partial s}{\partial T}\right)_{h=0}$

$$= -T\left(\frac{\partial^2 g}{\partial T^2}\right)$$

$$s = k_B \ln(2\cosh\beta J) + \frac{k_B T}{2\cosh(\beta J)} 2 \frac{\partial}{\partial T}[\cosh(\beta J)]$$

$$= k_B \ln(2\cosh\beta J) + \frac{k_B T}{\cosh(\beta J)} \sinh(\beta J) J \frac{d\beta}{dT}$$

$$= k_B \ln(2\cosh\beta J) - \frac{J}{T}\tanh\beta J$$

$$s = k_B\left[\ln(2\cosh\beta J) - \beta J \tanh\beta J\right]$$

At $T\to\infty$, $\beta\to 0$,

$$\cosh\beta J \simeq 1 + \frac{1}{2}(\beta J)^2$$

$$\tanh(\beta J) \simeq \beta J$$

$$s \simeq k_B\left[\ln[2+(\beta J)^2] - (\beta J)^2\right]$$

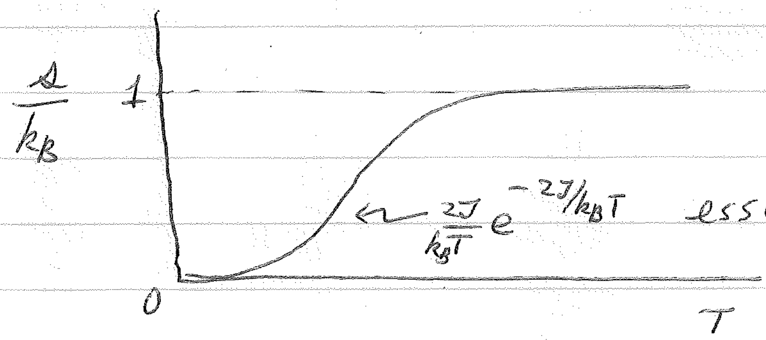
$$\simeq k_B \ln 2$$

At $T\to 0$, $\beta\to\infty$

$$\cosh\beta J \simeq e^{\beta J}$$

$$\tanh \simeq \frac{1-e^{-2\beta J}}{1+e^{-2\beta J}} \simeq 1 - 2e^{-2\beta J}$$

$$s \simeq k_B\left[\ln e^{\beta J} - \beta J(1-2e^{-2\beta J})\right] \simeq \frac{2J}{T} e^{-2J/k_B T}$$



essential singularity at $T=0$

$$C = T\left(\frac{\partial s}{\partial T}\right) = k_B T \left\{ \cancel{\frac{-2J\sinh\beta J}{2\cosh\beta J}\,\frac{1}{k_BT^2}} + \cancel{\frac{J}{k_BT^2}\tanh\beta J} + \frac{\beta J^2}{k_BT^2}\frac{\partial}{\partial(\beta J)}\tanh\beta J \right\}$$

$$= \frac{J^2}{k_BT^2}\frac{\partial}{\partial(\beta J)}(\tanh\beta J) = \frac{J^2}{k_BT^2}\frac{1}{(\cosh\beta J)^2}$$

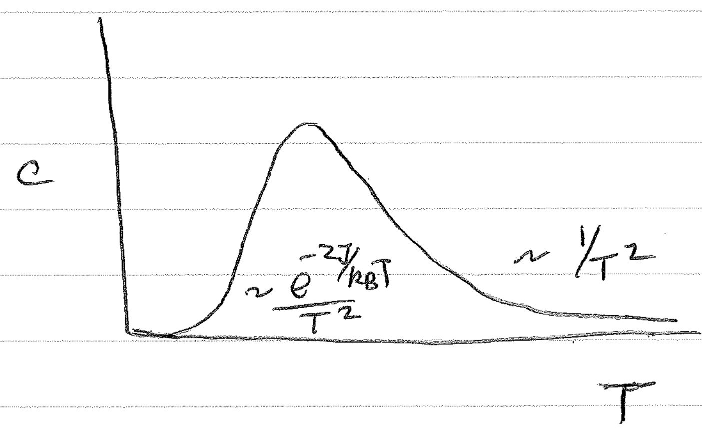
$$\boxed{C = k_B\left(\frac{\beta J}{\cosh\beta J}\right)^2}$$

as $T\to\infty$, $\beta\to 0$

$$C \simeq k_B\left(\frac{J}{k_BT}\right)^2$$

as $T\to 0$, $\beta\to\infty$

$$C \simeq k_B\left(\frac{J}{k_BT}\right)^2 e^{-2J/k_BT}$$



essential singularity at $T=0$

$\Rightarrow$ No singularity at any finite T.

$\Rightarrow$ No phase transition at any finite T