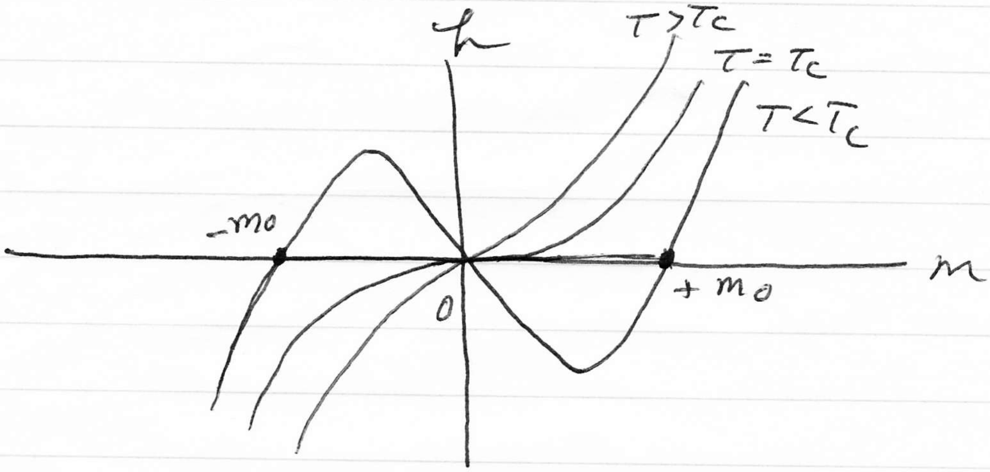
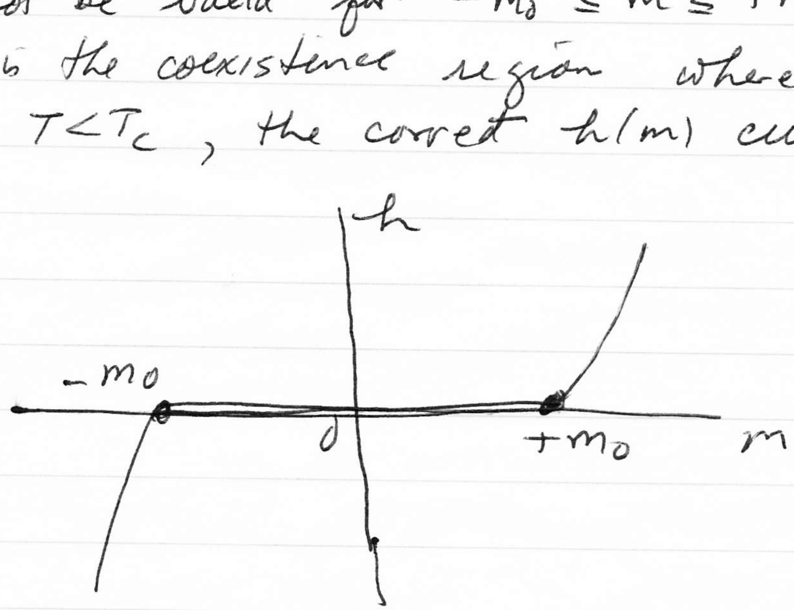
A closer look at the mean-field solution near T_c

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

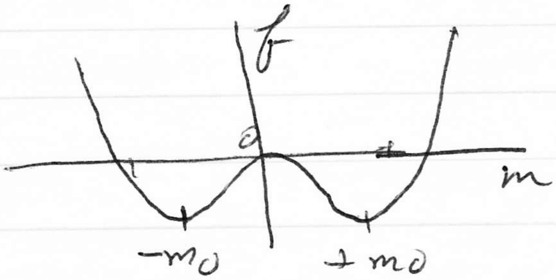


For $T < T_c$ we know that above $h(m)$ curve cannot be valid for $-m_0 \le m \le +m_0$
This is the coexistence region where $h = 0$
For $T < T_c$, the correct $h(m)$ curve is

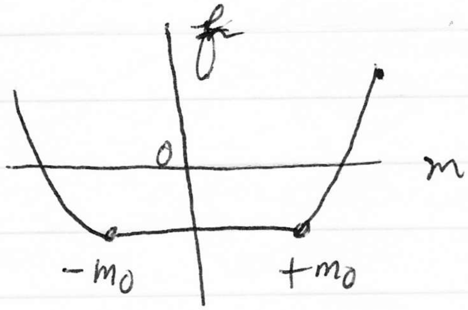


Such a "correction" based on our physical understanding is called the "Maxwell construction" (originally done in connection with the van der Waals theory of the liquid to gas phase transition).

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



we get

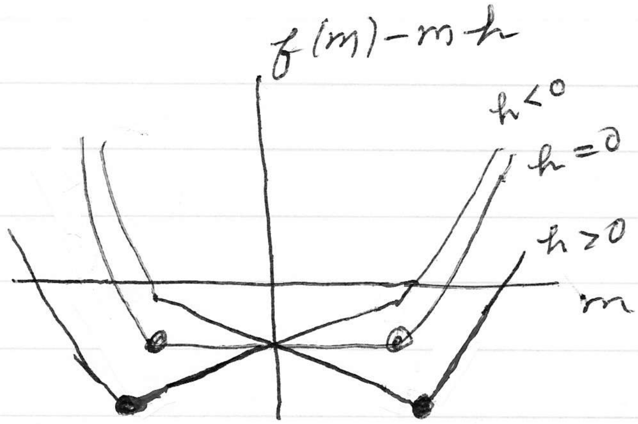


← $f(m)$ with Maxwell construction

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

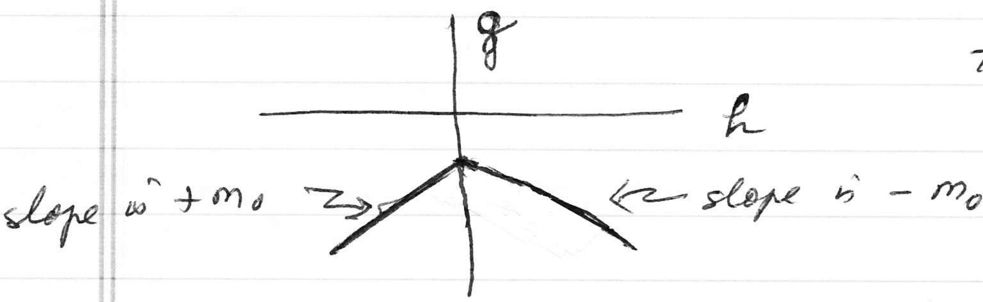
Using the above corrected $f(m)$, we can compute

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



$T < T_c$

$g(h) = \min\limits_{m} \left[f(m) - mh \right]$ then results in



$T < T_c$

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

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

Lattice-Gas model

sites i, $n_i = 1$ or 0

1 if site occupied by a particle

0 if site unoccupied

$$\mathcal{H} = -J\sum_{\langle ij\rangle} n_i n_j - \mu \sum_i n_i$$

μ ← chemical potential

J ↑ attractive interaction between particles on neighboring sites

Map to Ising model: $s_i = 2n_i - 1 = \pm 1$

$$n_i = \frac{s_i+1}{2}$$

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\left(\frac{s_i+1}{2}\right)\left(\frac{s_j+1}{2}\right) - \mu\sum_i\left(\frac{s_i+1}{2}\right)$$

$$= -J\sum_{\langle ij\rangle}\left(\frac{s_i s_j}{4} + \frac{s_i}{2} + \frac{s_j}{2} + \frac{1}{4}\right) - \frac{\mu}{2}\sum_i s_i - \mu\frac{N}{2}$$

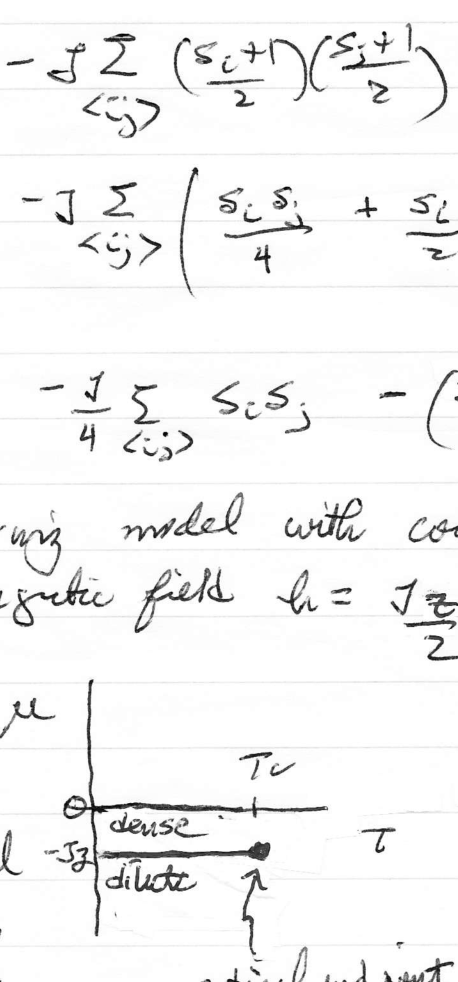
N ← # sites

$$= -\frac{J}{4}\sum_{\langle ij\rangle} s_i s_j - \left(\frac{Jz}{2} + \frac{\mu}{2}\right)\sum_i s_i - \underbrace{\left(\frac{Jz}{8} + \frac{\mu}{2}\right)N}_{\text{constant so ignore}}$$

Ising model with coupling $J/4$ and magnetic field $h = \frac{Jz}{2} + \frac{\mu}{2}$

$\mu = (2h - Jz)$

coexistence line is at $h=0$ or $\mu = -Jz$



liquid-gas critical point has same critical exponents as the Ising model!

$k_B T_c = \frac{zJ}{8}$

discontinuous jump in M of Ising model becomes discontinuous jump in density $\frac{1}{N}\sum_i n_i$ as cross from dense to dilute phase

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

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

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

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

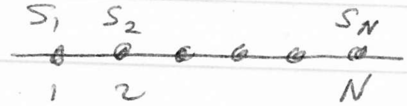
$$\mathcal{H} = -\left(\frac{z}{2} J m + h \right) \sum_i s_i$$

where we took $J \equiv \frac{2}{z} \tilde{J} N$. In 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, $m[s_i] = \frac{1}{N} \sum_j s_j$ <u>depends</u> 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 $\sigma_i = S_i S_{i+1}$, $i = 1, \cdots, N-1$

$$\sigma_i = \pm 1$$

$$\mathcal{H} = -J \sum_{i=1}^{N-1} \sigma_i \qquad S_1 S_j = \prod_{i=1}^{j-1} \sigma_i = (S_1 S_2)(S_2 S_3) \cdots (S_{j-1} S_j)$$

$$= S_1 S_2^2 S_3^2 \cdots S_{j-1}^2 S_j$$

$$= S_1 S_j$$

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

$$Z = \sum_{\{S_i\}} e^{\beta J \sum_{i=1}^{N} S_i S_{i+1}} = 2 \sum_{\{\sigma_i\}} e^{\beta J \sum_{j=1}^{N-1} \sigma_j} = 2 \prod_{j=1}^{N-1} \sum_{\sigma_i = \pm 1} e^{\beta J \sigma_i}$$

two values for S_1

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

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 $h=0$ $C = T\left(\frac{\partial s}{\partial T}\right)_{h=0}$

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

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

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

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

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

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

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

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

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

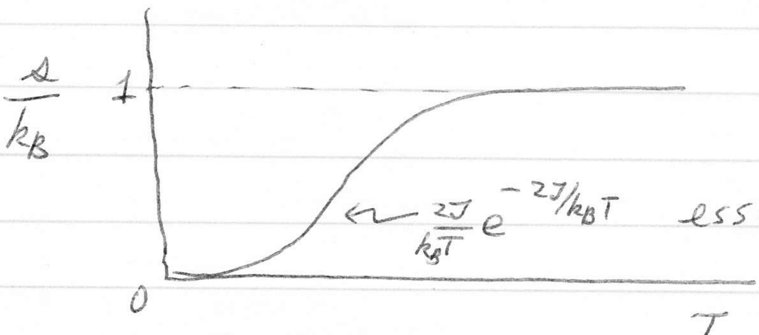
$$\simeq k_B \ln 2$$ ← each spin equally likely up or down

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

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

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

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



essential singularity at $T = 0$

(essential singularity means no Taylor series exists with finite radius of convergence)

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

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

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

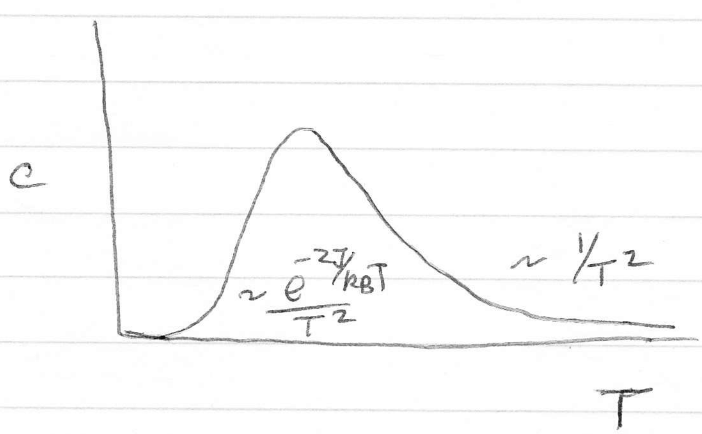
$$\boxed{C = k_B\left(\frac{\beta J}{\cosh\beta J}\right)^2}$$

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

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

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

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



essential singularity at $T = 0$

$\Rightarrow$ No singularity at any finite T.

$\Rightarrow$ No phase transition at any finite T