Mean field Theory

$$E = \mathcal{H} = -\frac{1}{2} J \sum_{ij} J_{ij} \sigma_i \sigma_j - H \sum_i \sigma_i$$

with

$$J_{ij} = \begin{cases} J & \text{if } i,j \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

A force exerted on a particular spin σ_i due to everything else:

$$-\left(\frac{\partial E}{\partial \sigma_i}\right) = H + \sum_j J_{ij} \sigma_j$$

$\boxed{\text{where did the 2 go?}}$

(each $\sigma_i \sigma_j$ pair appears twice)

We'll call this the "instantaneous" field for spin σ_i:

$$H_i' = H + \sum_j J_{ij} \sigma_j$$

$\therefore$

$$E = -\sum_i H_i' \sigma_i$$

energy is a single sum over the instantaneous fields

H_i' has an average or mean value as the rest of the σ_j spins fluctuate

$$\langle H_i' \rangle = H + \sum_j J_{ij} \langle \sigma_j \rangle$$

average value of spin σ_j

Now, suppose all the spins are fluctuating in exactly the same way. That is, they all have the same average:

$$\langle \sigma_j \rangle = \langle \sigma_1 \rangle = \langle \sigma_i \rangle$$

This means:

$$\langle H_i' \rangle = H + \sum_j J_{ij} \langle \sigma_i \rangle$$

$$= H + \underbrace{2d}_{\text{number of nearest neighbors}} J \langle \sigma_i \rangle$$

We can now write an approximate Hamiltonian:

$$\underbrace{\mathcal{H}}_{\text{exact}} = -\sum_i \underbrace{H_i'}_{\text{instantaneous field}}$$

$$\mathcal{H}_0 = -\sum_i \underbrace{\langle H_i' \rangle}_{\text{mean field}} \sigma_i$$

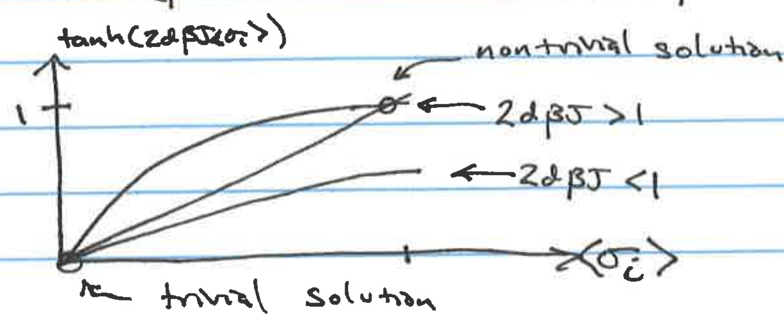
But how do we know what $\langle H_i' \rangle$ is? We need $\langle \sigma_i \rangle$

$$\langle \sigma_i \rangle \approx \frac{\sum_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_0} \sigma_i}{\sum_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_0}}$$

All spins are identical, so

$$\langle \sigma_i \rangle = \frac{\sum_{\sigma_i = \pm 1} e^{+\beta \langle H_i' \rangle \sigma_i} \sigma_i}{\sum_{\sigma_i = \pm 1} e^{+\beta \langle H_i' \rangle \sigma_i}} = \frac{e^{\beta \langle H_i' \rangle} - e^{-\beta \langle H_i' \rangle}}{e^{\beta \langle H_i' \rangle} + e^{-\beta \langle H_i' \rangle}}$$

$$\langle \sigma_i \rangle = \tanh(\beta \langle H_i' \rangle) = \tanh(2d\beta J \langle \sigma_i \rangle)$$



What is the magnetization of the lattice?

$$\langle m \rangle = \frac{1}{N} \sum_i \langle \sigma_i \rangle = \langle \sigma_i \rangle$$

$$= \frac{e^{\beta 2 J d m} - e^{-\beta 2 J d m}}{e^{\beta 2 J d m} + e^{-\beta 2 J d m}}$$

$$m = \frac{e^{4 \beta J d m} - 1}{e^{4 \beta J d m} + 1}$$

$$m \left(e^{4 \beta J d m} + 1\right) = e^{4 \beta J d m} - 1$$

$$e^{4 \beta J d m} (m - 1) = -1 - m$$

$$e^{4 \beta J d m} = \frac{-1-m}{m-1} = \frac{m+1}{1-m}$$

$$4 \beta J d m = \ln \frac{m+1}{1-m}$$

$$\beta = \frac{1}{4 J d m} \ln\left(\frac{m+1}{1-m}\right) \approx \frac{1}{4 d J} \frac{1}{m} \left(2m + \frac{2m^3}{3}\right)$$

Near T_c, m is very small, so we can Taylor expand in small m to get β

$$\beta_c \approx \frac{1}{2 d J} = \frac{1}{k_B T_c}$$

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

d	MFT	real
1	$2J/k_B$	0
2	$4J/k_B$	$2.269\, J/k_B$
3	$6J/k_B$	$4J/k_B$

MFT overestimates T_c predicting one for 1-D where there is none.

MFT neglects correlations!

Can we do better?

$$Q = \sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}} \quad \leftarrow \text{true partition function}$$

Suppose $\mathcal{H}$ is close to a reference Hamiltonian $\mathcal{H}_0$

$$\mathcal{H} = (\mathcal{H} - \mathcal{H}_0) + \mathcal{H}_0$$

$$Q = \sum_{\{\sigma_n\}} e^{-\beta(\mathcal{H} - \mathcal{H}_0)} e^{-\beta \mathcal{H}_0}$$

Also suppose that the reference hamiltonian has an easily solved partition function:

$$Q_0 = \sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}_0}$$

If we compare Q & Q_0 we can recognize Q as a thermal average in the states of $\mathcal{H}_0$:

$$Q = Q_0 \langle e^{-\beta(\mathcal{H} - \mathcal{H}_0)} \rangle_0 \quad \leftarrow \text{averaged over state probabilities set by } \mathcal{H}_0$$

We can invoke Jensen's Inequality

$$\langle e^x \rangle \geq e^{\langle x \rangle} \quad \text{or} \quad \int e^{f(x)} dx \geq e^{\int f(x) dx}$$

$$Q = Q_0 \langle e^{-\beta(\mathcal{H} - \mathcal{H}_0)} \rangle_0 \geq \underbrace{Q_0 e^{-\beta \langle \mathcal{H} - \mathcal{H}_0 \rangle_0}}_{\text{call this } Q_T}$$

So we have

$$Q_T \leq Q_{exact}$$

We can convert both Q_{exact} & Q_T to free energies

$$A_T = -k_B T \ln Q_T = -k_B T \ln Q_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \geq A_{exact}$$

$$\boxed{-k_B T \ln Q_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \geq A_{exact}}$$

This is called the Gibbs-Bogoliubov inequality. It is a <u>variational</u> principle. It means we can choose better & better approximate $\mathcal{H}_0$ Hamiltonians and we will always have an upper bound on A_{exact}!

Once we have a variational principle, we can choose $\mathcal{H}_0$ with <u>variational parameters</u> and minimize A_T with respect to these parameters.

For example, if we choose:

$$\mathcal{H}_0 = -\sum_n h_n \sigma_n$$

each spin has a unique field, but spins are decoupled.

$$Q_0 = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} e^{\beta h_1 \sigma_1} e^{\beta h_2 \sigma_2} e^{\beta h_3 \sigma_3} \cdots e^{\beta h_N \sigma_N}$$

$$= \left(\sum_{\sigma_1=\pm 1} e^{\beta h_1 \sigma_1}\right)\left(\sum_{\sigma_2=\pm 1} e^{\beta h_2 \sigma_2}\right) \cdots \left(\sum_{\sigma_N=\pm 1} e^{\beta h_N \sigma_n}\right)$$

$$= (2\cosh \beta h_1)(2\cosh \beta h_2) \cdots (2\cosh \beta h_N)$$

$$= \prod_{i=1}^{N} (2\cosh \beta h_i)$$

$$A_0 = -k_B T \ln Q_0 = -k_B T \sum_{n=1}^{N} \ln\left[2\cosh(\beta h_n)\right]$$

To use the G-B inequality, we also need $\langle \mathcal{H} - \mathcal{H}_0 \rangle_0$:

$$\begin{aligned} \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 &= \langle \mathcal{H} \rangle_0 - \langle \mathcal{H}_0 \rangle_0 \\ &= \langle \mathcal{H} \rangle_0 + \sum_n h_n \langle \sigma_n \rangle_0 \\ &= -\frac{1}{2}\sum_{n,n'} J_{n,n'} \langle \sigma_n \sigma_{n'} \rangle_0 - h \sum_n \langle \sigma_n \rangle_0 + \sum_n h_n \langle \sigma_n \rangle_0 \end{aligned}$$

Too many $\langle \sigma_n \rangle_0$. Call them $S_n = \langle \sigma_n \rangle_0$

$$\langle \mathcal{H} - \mathcal{H}_0 \rangle_0 = -\frac{1}{2}\sum_{n,n'} \langle \sigma_n \sigma_{n'} \rangle_0 - h \sum_n S_n + \sum_n h_n S_n$$

If these are uncorrelated $\langle \sigma_n \sigma_{n'} \rangle = \langle \sigma_n \rangle \langle \sigma_{n'} \rangle$

Now, Let's plug things in to get A_T :

$$A_T = -k_B T \ln Q_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0$$

$$= \underbrace{-k_B T \sum_{n=1}^{N} \ln 2\cosh \beta h_n - \frac{1}{2}\sum_{n,n'} J_{nn'} S_n S_{n'} - h \sum_n S_n + \sum_n h_n S_n}_{\text{all of this } \geq A_{exact}}$$

We can minimize A_T with respect to the parameters h_n & S_n

$$\frac{\partial A_T}{\partial h_n} = -\tanh(\beta h_n) + S_n = 0 \quad \Rightarrow \quad \boxed{h_n = k_B T \tanh^{-1} S_n}$$

$$\frac{\partial A_T}{\partial S_n} = -1 \sum_{n'} J_{nn'} S_{n'} - h + h_n = 0$$

So if we solve for h_n in terms of s_n a bit of identity gymnastics gives us

$$\ln\left[2\cosh(\beta h_n)\right] = -\frac{1}{2}\ln(1+s_n) - \frac{1}{2}\ln(1-s_n) + \ln 2$$

We can put all of this into A_T and arrive at:

$$A_T = N\left\{\left[-\frac{J\nu}{2} + \frac{k_B T}{2}\right]s^2 + \frac{k_B T}{12}s^4 - hs - k_B T\ln 2\right\}$$

+ terms of $O(s^6)$

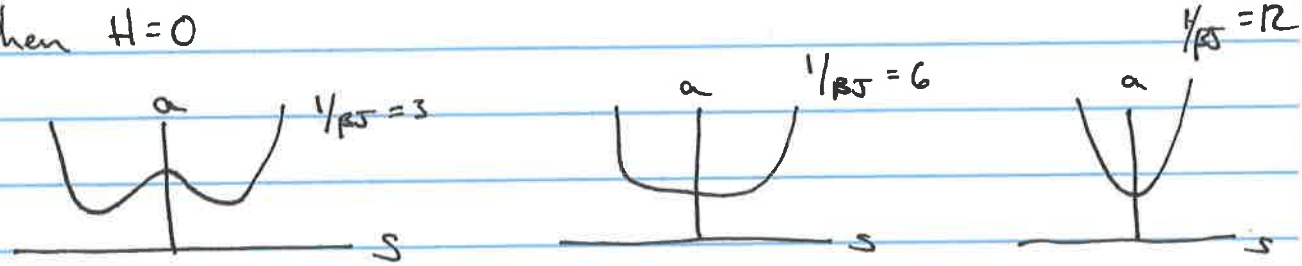
The free energy per spin is:

$$a = \left[-\frac{J\underbrace{\nu}_{\text{coordination \# of lattice}}}{2} + \frac{k_B T}{2}\right]\underbrace{s}_{\text{mean spin: } s=\langle\sigma\rangle_0}{}^2 + \frac{k_B T}{12}s^4 - hs - k_B T\ln 2$$

free energy per spin

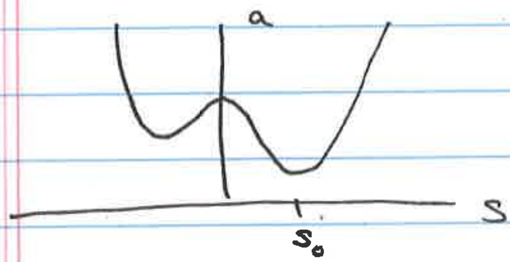
This function is an interesting result.

When $H=0$



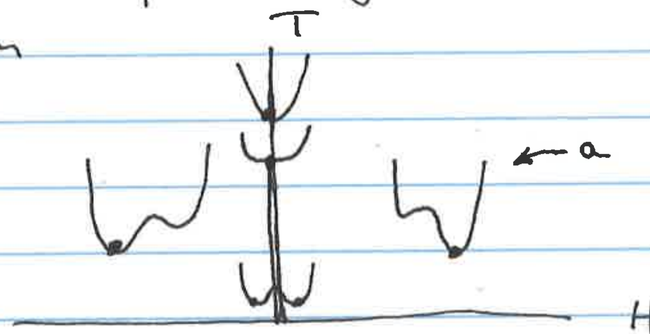
$T < T_c$ $\qquad$ $T = T_c$ $\qquad$ $T > T_c$

If $H \neq 0$

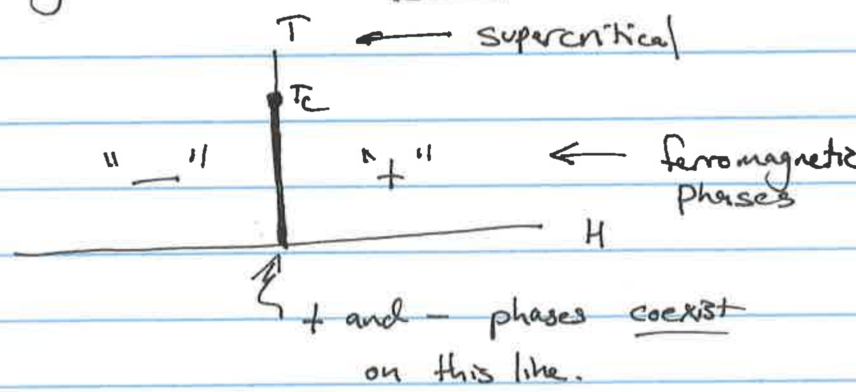


ferromagnetic when $J > 0$

We can make a T-H phase diagram with this free energy expression



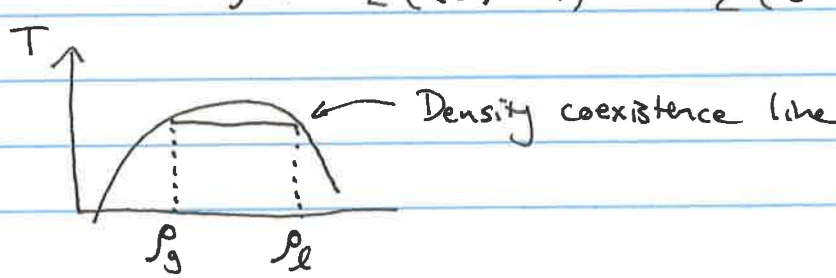
Lowest free energy governs the phase



We can also use this result to find critical exponents for the lattice gas:

Remember: $\rho_n = \frac{1}{2}(\sigma_n + 1)$ with $\rho_n = 0, 1$

$$\therefore \quad \langle \rho \rangle = \frac{1}{2}(\langle \sigma \rangle + 1) = \frac{1}{2}(s + 1)$$

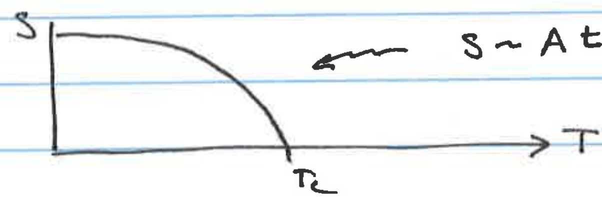


How do we determine critical exponents?

First: T_c is where the s^2 term disappears

$$\frac{k_B T_c}{2} - \frac{J\nu}{2} = 0$$

$$\boxed{T_c = \frac{J\nu}{k_B} = \frac{2dJ}{k_B} = \frac{6J}{k_B} \text{ in 3D}}$$



$s \sim A t^{\beta}$ below T_c where

$t = |T - T_c|$

Second: We also derived in MFT $2dJs = kT \tanh^{-1} s$

For small s,

$$\tanh^{-1} s = s + \frac{s^3}{3} + \frac{s^5}{5} + \frac{s^7}{7} + O(s^9)$$

Therefore:

$$2dJs \approx k_B T \left(s + s^3/3\right)$$

We want to calculate s in terms of a small parameter

$$\epsilon = \frac{T_c - T}{T_c} = 1 - \frac{T}{T_c}$$

So:

$$2dJs = kT\left(s + \frac{s^3}{3}\right)$$

$$kT_c s = kT\left(s + \frac{s^3}{3}\right)$$

$$s = \frac{kT}{kT_c}\left(s + \frac{s^3}{3}\right) = \frac{T}{T_c}\left(s + \frac{s^3}{3}\right)$$

$$s = (1-\epsilon)\left(s + \frac{s^3}{3}\right)$$

$$S = s + \frac{s^3}{3} - \epsilon s - \frac{\epsilon s^3}{3}$$

$$1 = 1 + \frac{s^2}{3} - \epsilon - \frac{\epsilon s^2}{3}$$

$$\epsilon = \frac{s^2}{3} - \frac{\epsilon s^2}{3}$$ ← both ϵ & s are small

so:

$$\epsilon \doteq \frac{s^2}{3} \Rightarrow s = \sqrt{3\epsilon}$$

So: $$s = \sqrt{3\,\frac{T_c - T}{T_c}}$$ and $\beta = 1/2$

One more sneaky way to get correlation functions

$$\langle \sigma_1 \sigma_n \rangle = \frac{1}{Q} \sum_{\{\}} \sigma_1 \sigma_n \, e^{-\beta \mathcal{H}}$$

with $\mathcal{H} = \frac{-J}{2} \sum_{ij} \sigma_i \sigma_j$ or $-\sum_n J_n \sigma_n \sigma_{n+1}$

$$e^{-\beta \mathcal{H}} = e^{\beta \sum_n J_n \sigma_n \sigma_{n+1}} = e^{\sum_n j_n \sigma_n \sigma_{n+1}}$$

with $j_n = \frac{J_n}{k_B T}$

$$\therefore \quad Q = \sum_{\{\}} e^{\sum_n j_n \sigma_n \sigma_{n+1}}$$

$$\frac{\partial Q}{\partial j_1} = \sum_{\{\}} \sigma_1 \sigma_2 \, e^{\sum_n j_n \sigma_n \sigma_{n+1}}$$

$$\frac{\partial^{n-1} Q}{\partial j_1 \partial j_2 \partial j_3 \cdots \partial j_{n-1}} = \sum_{\{\}} (\sigma_1 \sigma_2)(\sigma_2 \sigma_3) \cdots (\sigma_{n-1} \sigma_n) \, e^{\sum_n j_n \sigma_n \sigma_{n+1}}$$

$$\frac{\partial^{n-1} Q}{\partial j_1 \partial j_2 \partial j_3 \cdots \partial j_{n-1}} = \sum_{\{\}} \sigma_1 \sigma_2^2 \sigma_3^2 \sigma_4^2 \cdots \sigma_{n-1}^2 \sigma_n \, e^{\sum_n j_n \sigma_n \sigma_{n+1}}$$

$$= \sum_{\{\}} \sigma_1 \sigma_n \, e^{\sum_n j_n \sigma_n \sigma_{n+1}}$$

$$Q = 2 \prod_{i=1}^{N-1} (2 \cosh j_i)$$

$$\langle \sigma_1 \sigma_n \rangle = \prod_{p=1}^{n} \tanh j_p = (\tanh j)^n$$

$$= e^{-|\ln \tanh j| n}$$

$$= e^{-n/\xi} \qquad \text{where } \xi = \frac{1}{|\ln \tanh j|}$$

exponentially decaying correlations!