A review of what we know:

$$\mathcal{H} = -H \sum_{i=1}^{N} \sigma_i - \frac{J}{2} \sum_{i=1}^{N} \sum_{j \in NN_i} \sigma_i \sigma_j$$

nearest neighbor sum

0°K states with $H=0$:

$J > 0 \longrightarrow$ degenerate ferroelectric states
all up, $\langle m \rangle = +1$
all down, $\langle m \rangle = -1$

$J < 0 \longrightarrow$ degenerate anti-ferroelectric states
$+-+-$ and $-+-+$
both with $\langle m \rangle = 0$

At any temperature in 1D, we've shown that

no field

$$Q_N = 2(2\cosh \beta J)^N$$

field

$$Q_N \cong \left(e^{\beta J}(\cosh \beta H + \sqrt{\sinh^2 \beta H - e^{-4\beta J}}\right)^N$$

we got here using a transfer matrix diagonalization & the cyclic invariance of the trace

More derivative tricks:

$$\langle m \rangle = \frac{1}{Q} \sum_{\{\sigma_i = \pm 1\}} \left(\left(\sum_{i=1}^{N} \sigma_i\right) \frac{1}{N} e^{\beta(H \sum \sigma_i + \frac{J}{2} \sum \sum \sigma_i \sigma_j)} \right)$$

you should be able to look at this and see

$$\langle m \rangle = \frac{\partial \ln Q}{\partial (\beta H)} \cdot \frac{1}{N} = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial H}$$

$$\langle m \rangle = \frac{\sinh(\beta H)}{\sqrt{\sinh^2 \beta H + e^{-4\beta J}}} \longleftarrow \text{always } 0 \text{ when } H = 0$$

The other first derivative property of interest

$$\frac{\langle E \rangle}{N} = \frac{1}{N} \frac{-\partial \ln Q}{\partial \beta} = -J \tanh \beta J$$

has no discontinuities

The second derivative properties

susceptibility

$$\chi = \frac{\partial \langle m \rangle}{\partial H}$$

$$= \frac{\beta \cosh(\beta H)}{\left(1 + e^{4\beta J} \sinh^2(\beta H)\right)^{3/2}}$$

$$\lim_{H \to 0} \chi = \frac{\beta}{\sqrt{e^{-4\beta J}}} \longleftarrow \text{only diverges at } T = 0$$

heat capacity

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

$$= \frac{+J^2}{kT^2} \operatorname{sech}^2(\beta J)$$

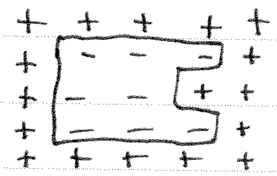
no divergences!

Conclusions: there are no phase transitions in the 1-D Ising model!!

Peierls Theorem

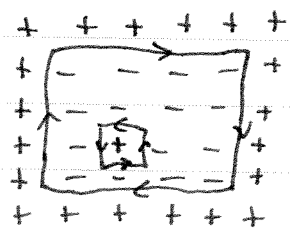
For 2D Ising model, $\exists$ a temperature T_c at which the probability of "+" spins $\neq$ the probability of "−" spins. (i.e $\langle \sigma_n \rangle \neq 0$ below T_c)

Consider an array of spins:



$\leftarrow$ energy = J × length of perimeter

N spins on an array, with all spins on outside set to "+"



a "contour" passes through the midpoint of every +− bond

a "closed" contour meets itsel

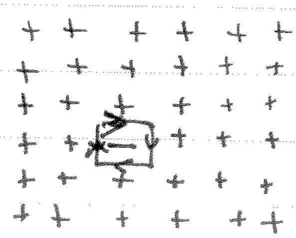
$$\underbrace{C(l, i)}_{}$$

l: length, i: label

Energy of closed contour = $E(C) = Jl$

Direction: RHS of path has "—" spins

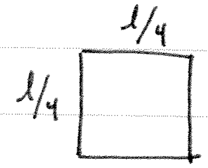
Conjugate: Reverse all spins to RHS of contour



$$\tilde{C}(l, i)$$

$$E(\tilde{C}) = E(C) - 2lJ$$

the contour with the maximal # of enclosed spins for a given length is a regular polygon:



$$A = N_{max} = \frac{l^2}{16}$$

$\mathcal{M}(l) =$ total # of contours of length l

$\mathcal{M}(l) \leq$ total # of contours we can draw

$$\mathcal{M}(l) \leq \underbrace{N}_{\text{places to start}} \times \underbrace{4}_{\text{choices of direction on step 1}} \times \underbrace{3^{l-1}}_{\text{choices of direction on following steps}} \times \underbrace{\frac{1}{2l}}_{\text{required to close loop}}$$

$$X(l,i) = \begin{cases} 1 & \text{if configuration contains contour } c(l,i) \\ 0 & \text{otherwise} \end{cases}$$

# of negative spins ↓ ; maximal # of contours of length l ; does configuration contain this contour

$$N_- \leq \sum_l \underbrace{\left(\frac{l^2}{16}\right)}_{\text{maximal enclosed spins}} \sum_{i=1}^{\mathcal{M}(l)} X(l,i) = \underline{\text{overestimate}} \text{ of } N_-$$

$$\langle X(l,i) \rangle = \frac{\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})} X(l;i)}{\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})}}$$

we can do this as a "constrained" sum over only those configurations containing $c(l,i)$

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$$\langle X(l,i)\rangle = \frac{\displaystyle\sum_{\substack{\text{constrained}\\ \text{configs}}} e^{-\beta E(C(l,i))}}{\displaystyle\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})}}$$

← we can underestimate the denominator as the same constrained configs but without the contour

$$\langle X(l,i)\rangle \leq \frac{\displaystyle\sum_{\text{configs}} e^{-\beta E(C(l,i))}}{\displaystyle\sum_{\text{configs}} e^{-\beta E(\tilde{C}(l,i))}}$$

← since $E(\tilde{C}) = E(C) - Jl$

$$\langle X(l,i)\rangle \leq e^{-\beta J l}$$

$$\frac{\langle N_-\rangle}{N} \leq \frac{1}{N}\sum_{l}\left(\frac{l^2}{16}\right)\sum_{i=1}^{M(l)}\langle X(l,i)\rangle$$

$$\leq \sum_{l=4}^{\infty}\left(\frac{l^2}{16}\right)3^{l-1}e^{-J\beta l}\;\frac{4}{2l}$$

$$\frac{\langle N_-\rangle}{N} < \frac{\frac{5}{24}e^{-4\alpha}}{1-e^{-\alpha}} \qquad \text{where } \alpha = \frac{J}{T} - \ln 3$$

$$\frac{\langle N_-\rangle}{N} \ll \frac{1}{2} \quad \text{as } T \to 0$$

$\therefore$ there must be a T_c below which

$$\frac{\langle N_-\rangle}{N} < \frac{1}{2}$$

2D exact solution:

Lars Onsager 1940's Phys. Rev. 65, 117-149 (1944)

$$Q(\beta, N) = \left[2\cosh(\beta J)\, e^{I}\right]^{N}$$

$$I = \frac{1}{2\pi}\int_0^{\pi} d\phi \,\ln\left\{\frac{1}{2}\left[1 + (1-\mathcal{K}^2\sin^2\phi)^{1/2}\right]\right\}$$

$$\mathcal{K} = \frac{2\sinh(2\beta J)}{\cosh^2(2\beta J)}$$

Critical Temperature: $T_c = \dfrac{2.269\,J}{k_B}$

$$\frac{C_v}{N} \approx \frac{8k_B}{\pi}(\beta J)^2 \ln\left|\frac{1}{T-T_c}\right| \qquad \alpha = 0$$

$$\frac{M}{N} \approx (\text{const})\,(T_c - T)^{1/8} \longleftarrow T < T_c$$

$$\beta = \frac{1}{8}$$

3D : No exact solution yet!

Numerically :

$$\frac{C_v}{N} \propto |T - T_c|^{-0.125}$$

$$\frac{M}{N} \propto (T_c - T)^{0.313} \qquad T < T_c$$

$$T_c \sim \frac{4J}{k_B}$$

Next time : Approximate theories for 2 & 3D!

Mean-field theory

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

$$J_{i,j} = \begin{cases} J & \text{if } i,j = NN \\ 0 & \text{otherwise} \end{cases}$$

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

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

where's the $\frac{1}{2}$? ($\sigma_i\sigma_j$ appears twice)

We'll call this the instantaneous ~~fie~~ field for spin i

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

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

energy is a single sum over instantaneous fields

H_i' has an average value as the rest of the spins fluctuate:

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

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

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

$$\langle H_i'\rangle = H + \sum_j J_{i,j}\langle\sigma_i\rangle$$

$$\langle H_i'\rangle = H + 2dJ\langle\sigma_i\rangle$$

# of nearest neighbors

We can now write an approximate Hamiltonian:

$$\mathcal{H} = -\sum_i H_i' \sigma_i$$

exact — instantaneous field

mean field

$$\mathcal{H}_0 = -\sum_i' \langle H_i' \rangle \sigma_i$$

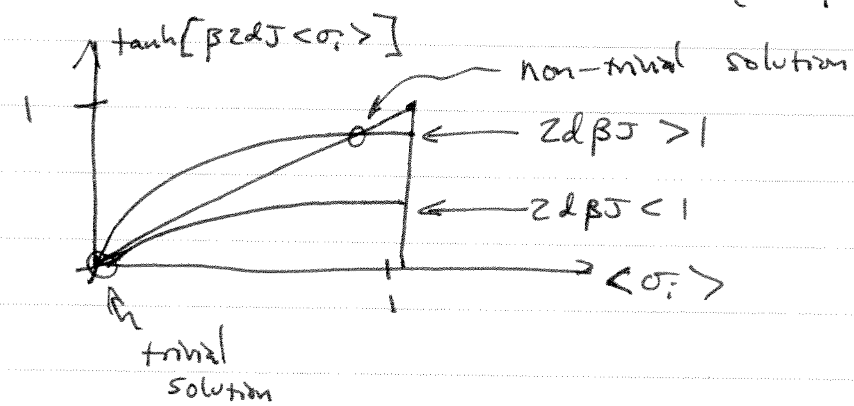
But how do we know what $\langle H_i' \rangle$ is? We need $\langle \sigma_i \rangle$

$$\langle \sigma_i \rangle \cong \left[\frac{\sum'_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_0} \sigma_i}{\sum'_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_0}} \right]$$

All spins are identical, so:

$$\langle \sigma_i \rangle \approx \left[\frac{\sum_{\sigma_i = \pm 1} e^{-\beta \langle H_i' \rangle \sigma_i} \sigma_i}{\sum_{\sigma_i = \pm 1} e^{-\beta \langle H_i' \rangle \sigma_i}} \right] = \frac{e^{\beta \langle H_i' \rangle} - e^{-\beta \langle H_i' \rangle}}{e^{\beta \langle H_i' \rangle} + e^{-\beta \langle H_i' \rangle}}$$

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



What is the magnetization of the lattice?

$$\langle M \rangle = \sum_i \langle \sigma_i \rangle = N \langle \sigma_i \rangle; \quad m = \frac{\langle M \rangle}{N} = \langle \sigma_i \rangle$$

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

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

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

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

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

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

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

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

$$\beta_c \approx \frac{1}{2dJ}$$

$$\frac{1}{k_B T_c} = \frac{1}{2dJ}$$

$$\boxed{T_c = \frac{2dJ}{k_B}}$$

So there is a critical T_c in Mean Field Theory

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

MFT over estimates T_c, predicting one for 1-D where there is none

MFT neglects correlations!