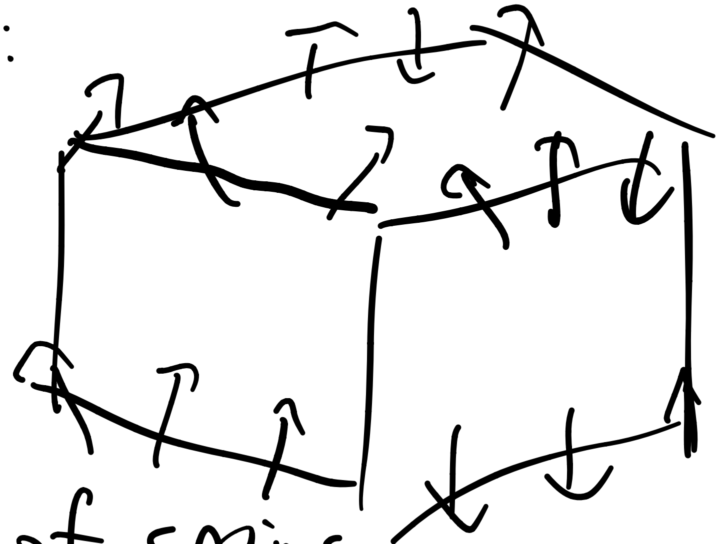
Ising Model:

represents



alignment of spins

in a material - magnetization

w/ or w/o magnetic field

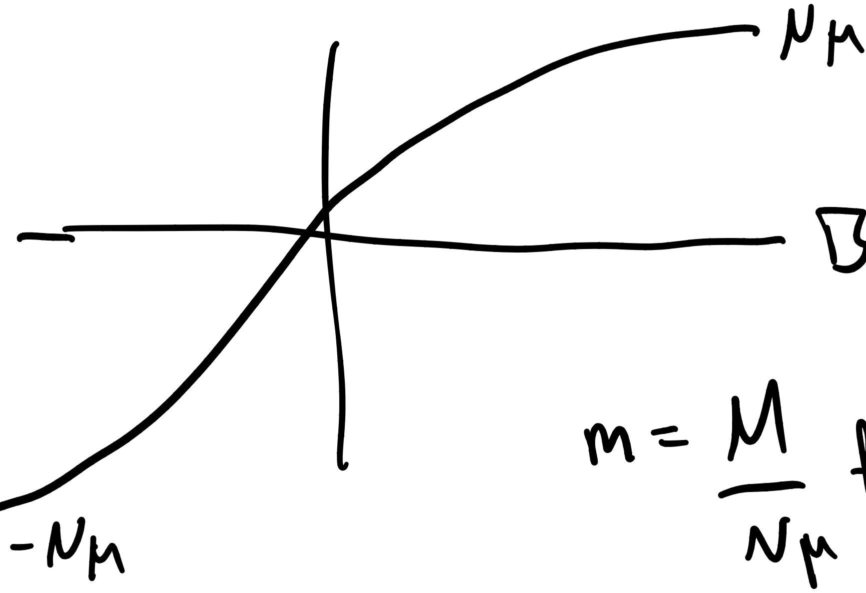
suppose spins like to align

Observed behavior

$$M = \sum_{i=1}^{N} \vec{\mu} \cdot \hat{z}$$

max is $N\mu$, all up

min is $-N\mu$ all down



B field along $\hat{z}$

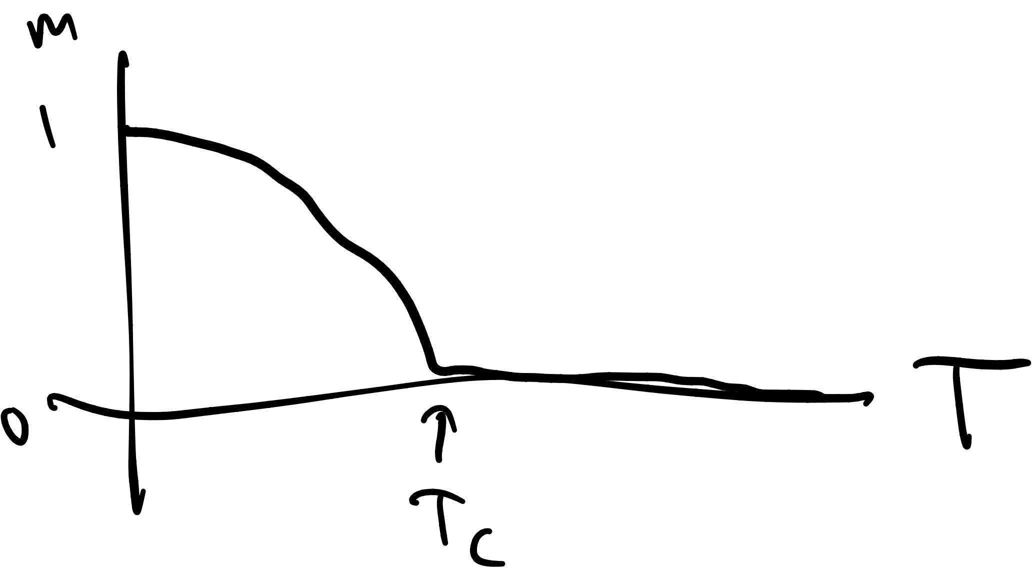
$m = \dfrac{M}{N\mu}$ from + 1 to y

But what about 0 field
"spontaneous magnetization"

@ high T $\langle \vec{\mu} \rangle = 0$ random

So $M = 0$

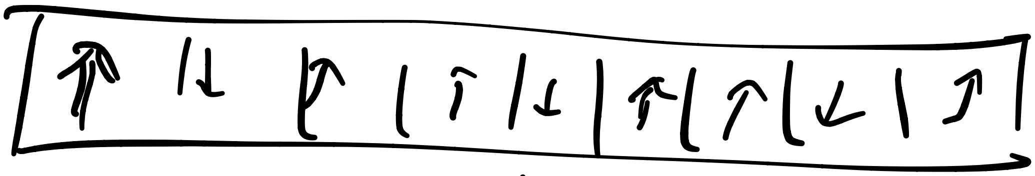
What about at low T → if spins like to align



phase transition

First studied statistical thermo by ising using simplified model

first midterm



can also be A/B (chem reaction or HC helix coil)

$$S_i = \pm \frac{1}{2}$$

like to align with field

$\varepsilon_{field} = -hs_i$ good to face up

like to align (feromagnetic)

← energy neg if $J>0$ & same dir

$$\varepsilon_{neighbor} = -Js_is_{i-1} - Js_is_{i+1}$$

$$\varepsilon_i^{site} = -hs_i - \underbrace{J}_{2} s_i(s_{i-1}+s_{i+1})$$

← double count

$$\varepsilon_{tot} = \sum_{i=2}^{N-1} -s_i\left[h+\frac{J}{2}(s_{i-1}+s_{i+1})\right] + \text{end terms}$$

$\mathcal{E}$ is a function of N

can make pseudo infinite by saying $S_{N+1} = S_1$ and $S_0 = S_N$

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

question is, what is $\langle s_i \rangle \Leftarrow$ mag per site $(/2)$

Have to consider partition function

what is partition func? Sum over all states.

$$Q = \sum_{\text{states}} e^{-\beta \mathcal{E}(\text{state})}$$

but what is a state?

particular set $s_1 = -\frac{1}{2}$ $s_2 = +\frac{1}{2}$ etc

$$Q = \sum_{s_1=\pm 1/2} \sum_{s_2=\pm 1/2} \cdots \sum_{s_N=\pm 1/2} e^{-\beta \mathcal{E}(s_1, s_2, \ldots s_N)}$$

suppose $\beta \to \infty \gg h$ or J
(energy units)

then $Q = \sum \sum \sum \cdots \sum (1)$

$= \text{counting states} = 2^N$

what is $\langle s \rangle$

$$Q = \sum_{\{s_i\}} e^{-\beta \sum(-J s_i s_{i+1} - h s_i)}$$

$$\langle s \rangle = \left\langle \frac{\sum s_i}{N} \right\rangle = \frac{1}{N} \langle \sum s_i \rangle = \frac{1}{N} \cdot \frac{\sum_{\{s_i\}} (\sum s_i) e^{-\beta \mathcal{E}(s_i)}}{Q}$$

$$\frac{\partial \ln Q}{\partial h} = \frac{1}{Q} \frac{\partial Q}{\partial h} = \frac{\sum_{\{s_i\}} \beta \sum_{i=1}^{N} s_i \, e^{-\beta \mathcal{E}(s_i)}}{Q} = \frac{N}{k_B T} \cdot \langle s \rangle$$

so $\langle s \rangle = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial h}$

$$\langle s \rangle_{T=\infty} = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial h} = 0 \,!$$ ← constant

Another solvable case

$J = 0$, this means $\mathcal{E} = -\sum_{i=1}^{N} h s_i$

$$Q = \sum_{\{s_i\}} e^{\sum \beta h s_i} = \sum_{\{s_i\}} e^{\beta h s_1} e^{\beta h s_2} \ldots$$ ← do sums separately

$$= \sum_{s_1 = \pm 1} e^{\beta h s_1} \sum e^{\beta h s_2} \cdots \sum_{s_N = \pm 1} e^{\beta h s_N}$$

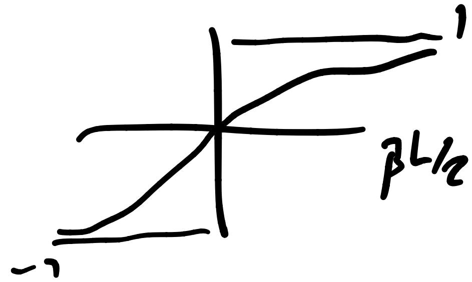
$$= \left(\sum_{s_i = \pm 1} e^{\beta h s_i} \right)^N = q^N \qquad \text{(sites disting)}$$

$$q = e^{\beta h/2} + e^{-\beta h/2}$$

$$\langle s \rangle = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial h} = k_B T \frac{\partial \ln q}{\partial h}$$

$$= \frac{\left(\beta/2 \, e^{\beta h/2} - \beta/2 \, e^{-\beta h/2} \right) k_B T}{q}$$

$$= \frac{1}{2} \left[\frac{e^{\beta h/2} - e^{-\beta h/2}}{e^{\beta h/2} + e^{-\beta h/2}} \right] = \frac{1}{2} \tanh(\beta h/2)$$



$$\sinh(x) = \frac{1}{2}\left[e^{x} - e^{-x} \right]$$

$$\cosh(x) = \frac{1}{2}\left[e^{x} + e^{-x} \right]$$

$$\varepsilon = \sum_{i=1}^{N} -h s_i \quad \Rightarrow \quad \langle \varepsilon \rangle = \sum_{i=1}^{N} -h \langle s_i \rangle$$

$$= -Nh \langle s_i \rangle$$

Question now is what happens if

$J \neq 0$

Turns out problem is soluable in
1d & 2d, 3d or more no exact solution!

In 2d and higher, spontaneous magnetization even at zero field in thermodynamic limit

Will talk about how to solve 1d in context of helix-coil model

What is H-C model?

α-Helix is a common SS-element in proteins

consider each residue as H or C conformation