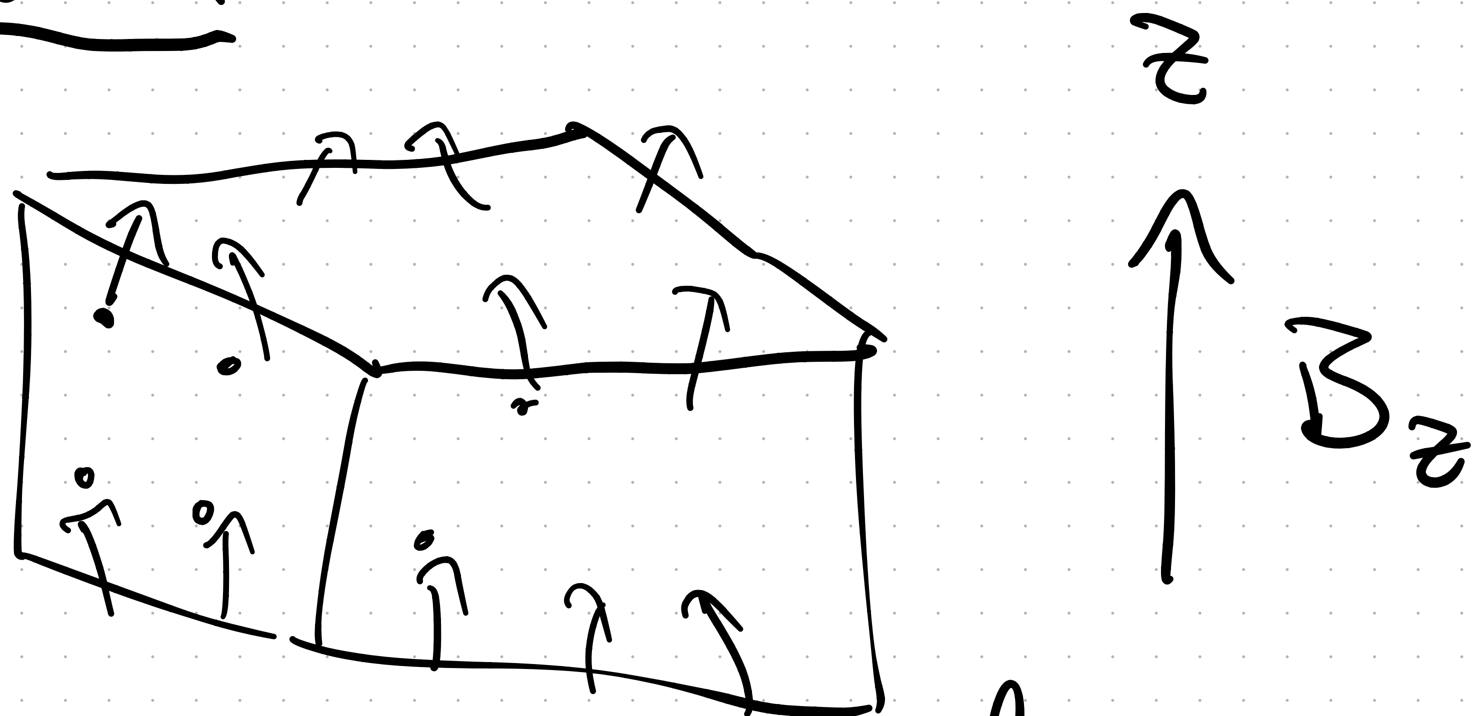
Ising Model



align in a magnetic field

Some materials, where the spins align w/o a field

"Sponeous magnetization"

Spins like to point in the same direction

Spins like to point in the same direction means $\uparrow\uparrow$ is good

$\downarrow\uparrow$ or $\uparrow\downarrow$ is bad

"ferromagnetic" $\downarrow\downarrow$ is good

M total magnetization in z direction

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

if all are up

$\vec{\mu} = (0, 0, \mu)$

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

$M(\text{all up}) = N\mu$

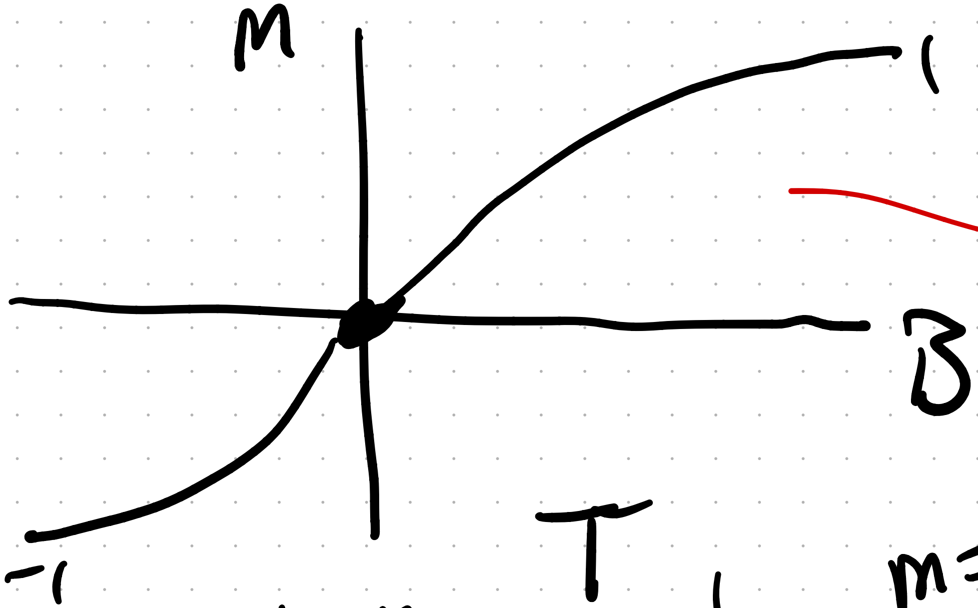
$M(\text{all down}) = -N\mu$

m magnetization per spin

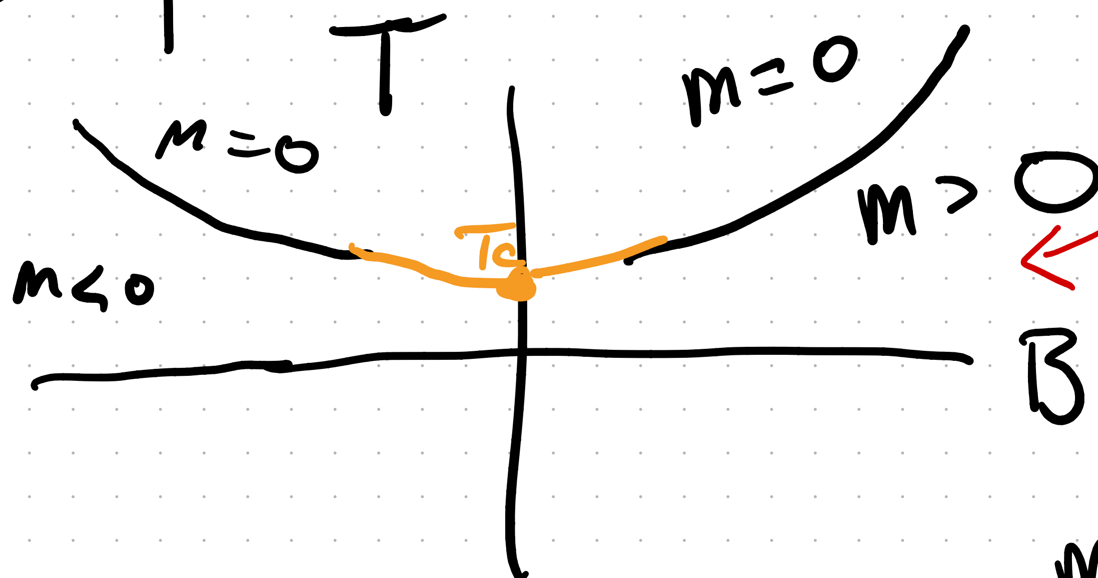
as $M/N \in$ from -1 to 1

"order parameter"

phase transition $\rightarrow$ change in order param.

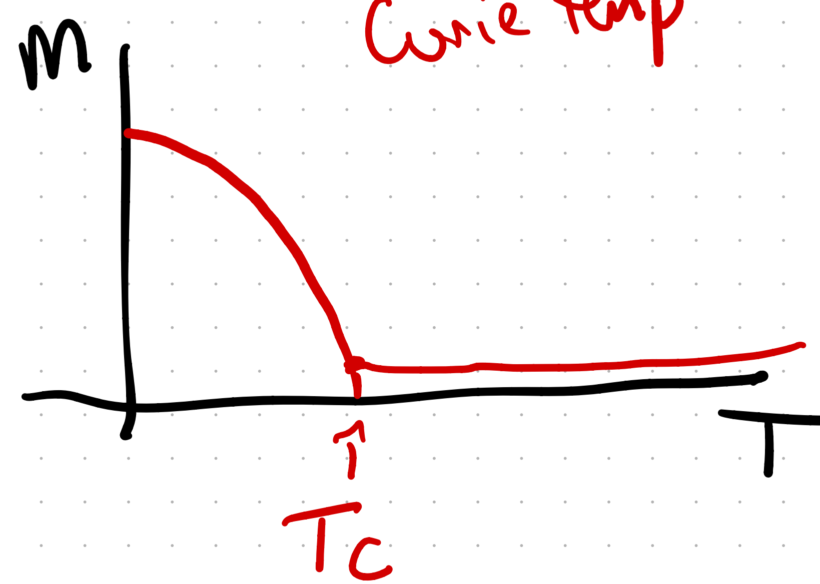


at some temp



T_c critical temp

Curie temp

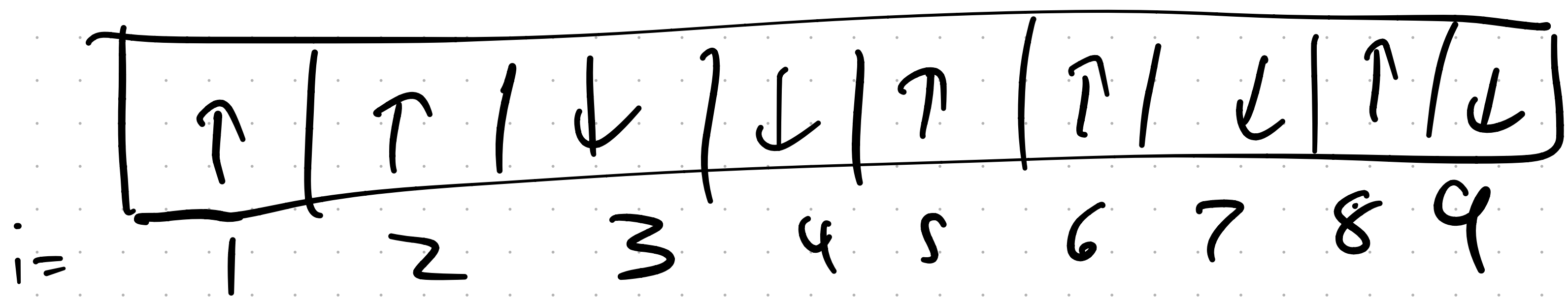


What should happen at $B=0$?

Ising model

before 3d spins on
a 3d crystal

simplest model
1d spins on a 1d lattice



$$S_i = \pm 1/2$$

1) like to align w/ field

$$\varepsilon_i^{field} = -hS_i \begin{cases} -h/2 & \text{if spin up} \\ h/2 & \text{if spin down} \end{cases}$$

2) Spins like to align with neighbors

just look at nearest neighors

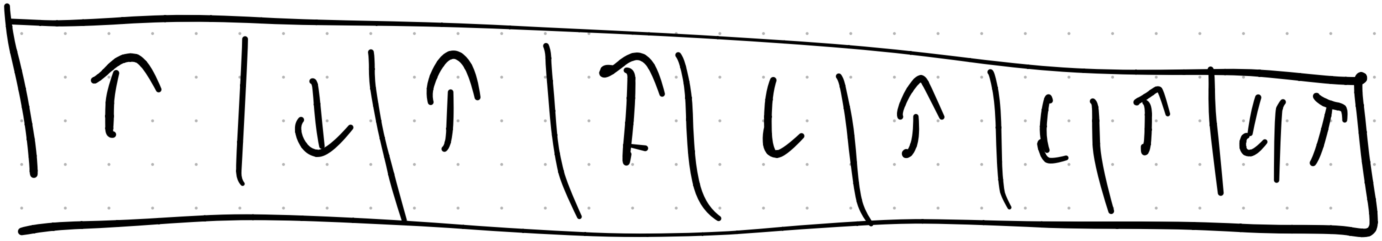
$+\,+$ $\underbrace{\uparrow\uparrow}_{\text{"good"}}$ $\qquad$ $\underbrace{\uparrow\downarrow \quad \downarrow\uparrow}_{\text{"bad}}$ or $\underbrace{\downarrow\downarrow}_{\text{"good"}}$ $\ldots$

$$E_{neighbor} = -J S_i S_{i+1}$$

$$= \begin{cases} -J/4 & \text{aligned} \\ +J/4 & \text{not aligned} \end{cases}$$

$J > 0$ ferro magnetic

$J < 0$ anti ferro magnetic



N sites

$\{s_i\}$ a particular configuration

$$\mathcal{E}_{total} = \sum_{i=1}^{N-1} -J s_i s_{i+1} - h s_i \qquad - h s_N$$

for a particular arrangement

Make this "infinite" by

$$s_{N+1} = s_1 \Rightarrow \boxed{\mathcal{E}(\{s_i\}) = \sum_{i=1}^{N} -J s_i s_{i+1} - h s_i}$$

Want to know is $M(T, h)$

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

$$\beta = \frac{1}{k_B T}$$

What is a state?

particular set of S_i's

string $S_1 S_2 \cdots S_N$

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

$$= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} e^{-\beta E(\vec{s})}$$

total number of states

2 for first site

$\times 2$ for second site

⋮

total # $= 2^N$

Example — take $J=0$

$$Q(\beta, h, J=0) = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \cdots \sum_{s_N=\pm1} e^{-\beta\mathcal{E}(\vec{s})}$$

$$\mathcal{E} = \sum_{i=1}^{N} -h s_i$$

$N=2$
$$\sum_{s_1=\pm 1/2} \sum_{s_2=\pm 1/2} e^{-\beta[-h(s_1+s_2)]}$$

$$e^{+\beta h(s_1+s_2)} \to \sum_{s_1=\pm 1/2} \left[e^{\beta h(s_1+\frac{1}{2})} + e^{\beta h(s_1-\frac{1}{2})} \right]$$

$$[e^{\beta h} + e^{0}] + [e^{0} + e^{-\beta h}]$$

$$Q = \sum_{s_1, s_2, \ldots s_N} \exp\left(-\beta\left(\sum_{i=1}^{N} -J s_i s_{i+1} - h s_i\right)\right)$$

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

$$Q(\beta = 0) = \sum_{s_1 s_2 \cdots s_N} (1) = 2^N$$

what is $\langle m \rangle = 2 \langle s_i \rangle$

$$\langle s_i \rangle = \frac{1}{N} \left\langle \sum_{i=1}^{N} s_i \right\rangle_{\text{thermal}} = \frac{1}{N} \sum_{\text{states}} \left(\sum_{i=1}^{N} s_i \right) P_{\text{state}}$$

$$P_{\text{state}} = e^{-\beta E_{\text{state}}} / Q$$

$$\langle s_i \rangle = \frac{1}{N}\left\langle \sum_{i=1}^{N} s_i \right\rangle$$

$$\beta \sum J s_i s_{i+1} + \beta h \sum_{i=1}^{N} s_i$$

$$= \frac{1}{N} \sum_{s_1, s_2, \dots s_N = \pm 1} \frac{\left(\sum_{i=1}^{N} s_i\right) \exp\left(\beta\left(\sum_{i=1}^{N} J s_i s_{i+1} + h s_i\right)\right)}{Q}$$

$$= \frac{1}{N}\left(\frac{\partial \ln Q}{\partial h}\right) \cdot \frac{1}{\beta}$$

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

$$\frac{\partial \ln Q}{\partial h} = \frac{1}{Q} \frac{\partial Q}{\partial h}$$

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

$T \to \infty \quad Q = 2^N \Leftarrow$ constant

$$\langle s \rangle_{T \to \infty} = 0$$

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

each sik is independent

$$Q = \sum_{s_1, s_2 \ldots, s_N = \pm 1/2} e^{\beta h \sum_{i=1}^{N} s_i} = \sum_{s_1, s_2 \ldots s_N} e^{\beta h s_1} e^{\beta h s_2} e^{\beta h s_3} \cdots e^{\beta h s_N}$$

$$Q = \left(\sum_{s_1=\pm 1/2} e^{\beta h s_1}\right)\left(\sum_{s_2=\pm 1/2} e^{\beta h s_2} \cdots\right)\left(\quad\right)\cdots\left(\sum_{s_N} e^{\beta h s_N}\right)$$

$$= q^N \quad \leftarrow \text{independent sites } \underline{\text{distinguishable}}$$

$$q_i = \sum_{s_i=\pm 1/2} e^{\beta h s_i} = e^{\beta h/2} + e^{-\beta h/2}$$

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

$$Q = q^N$$

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

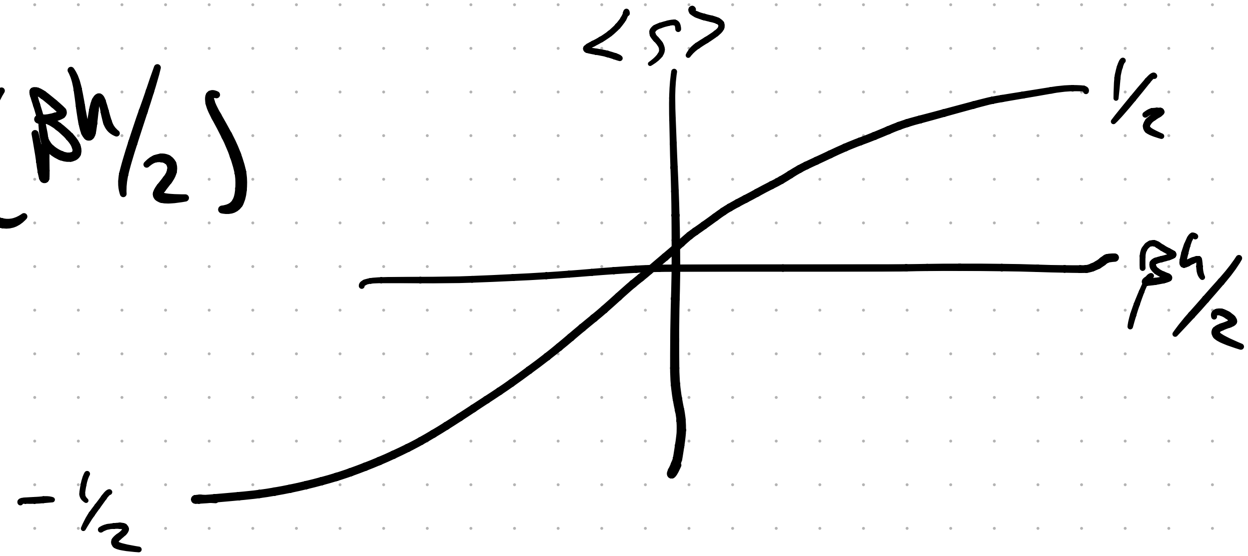
$$= k_B T \frac{\partial \ln q}{\partial h} = k_B T \cdot \frac{1}{q} \frac{\partial q}{\partial h}$$

$$= k_B T \cdot \frac{1}{e^{\beta h/2} + e^{-\beta h/2}} \cdot \beta/2\, e^{\beta h/2} - \frac{\beta}{2} e^{-\beta h/2}$$

$$\langle s \rangle = k_B T \cdot \frac{1}{e^{\beta h/2} + e^{-\beta h/2}} \cdot \frac{\beta}{2} e^{\beta h/2} - \frac{\beta}{2} e^{-\beta h/2}$$

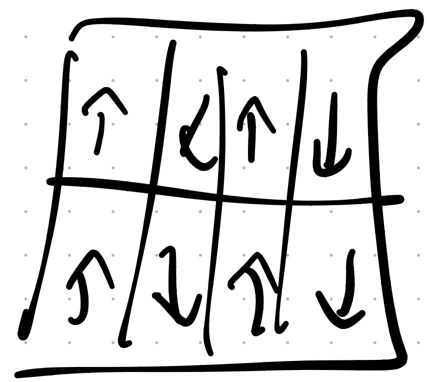
$$= \frac{1}{2} \cdot \underbrace{\frac{e^{\beta h/2} - e^{-\beta h/2}}{e^{\beta h/2} + e^{-\beta h/2}}}_{\tanh(\beta h/2)}$$

$$= \frac{1}{2} \tanh(\beta h/2)$$



What about $J > 0$

- problem is exactly soluable in 1d
  w/ matrices

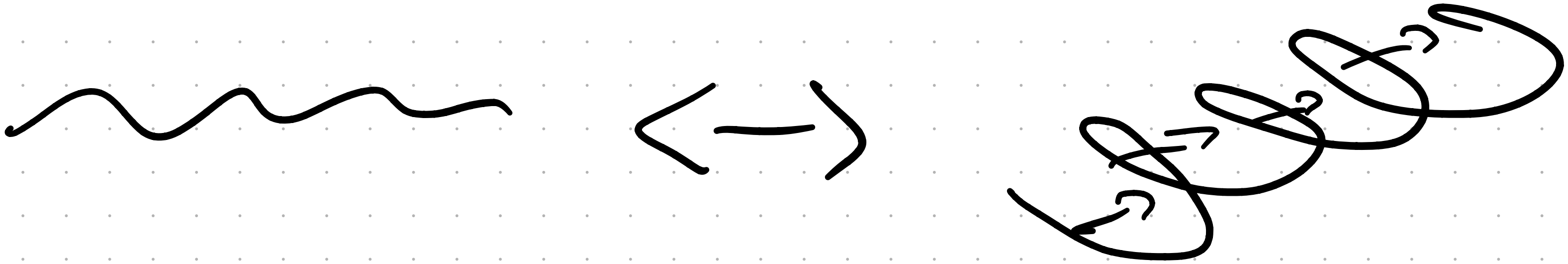


- exactly soluable in 2d

3d and higher $(d < \infty)$

In 2d & higher, there is a
spontaneous magnetization transition

In 1d, there isn't / can't be



gain H-bond energy

lose entropy

H	C	H	C	C	H
↑	↓	↑	↓	↓	↑