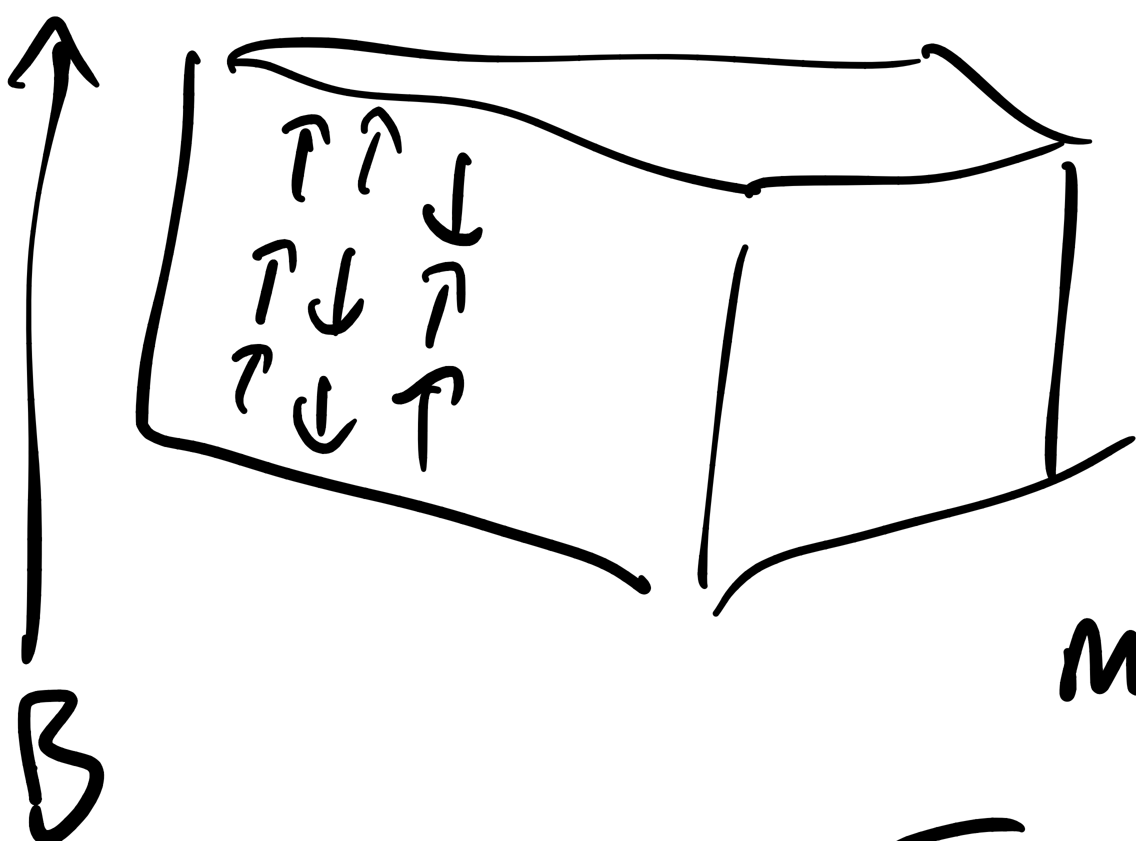
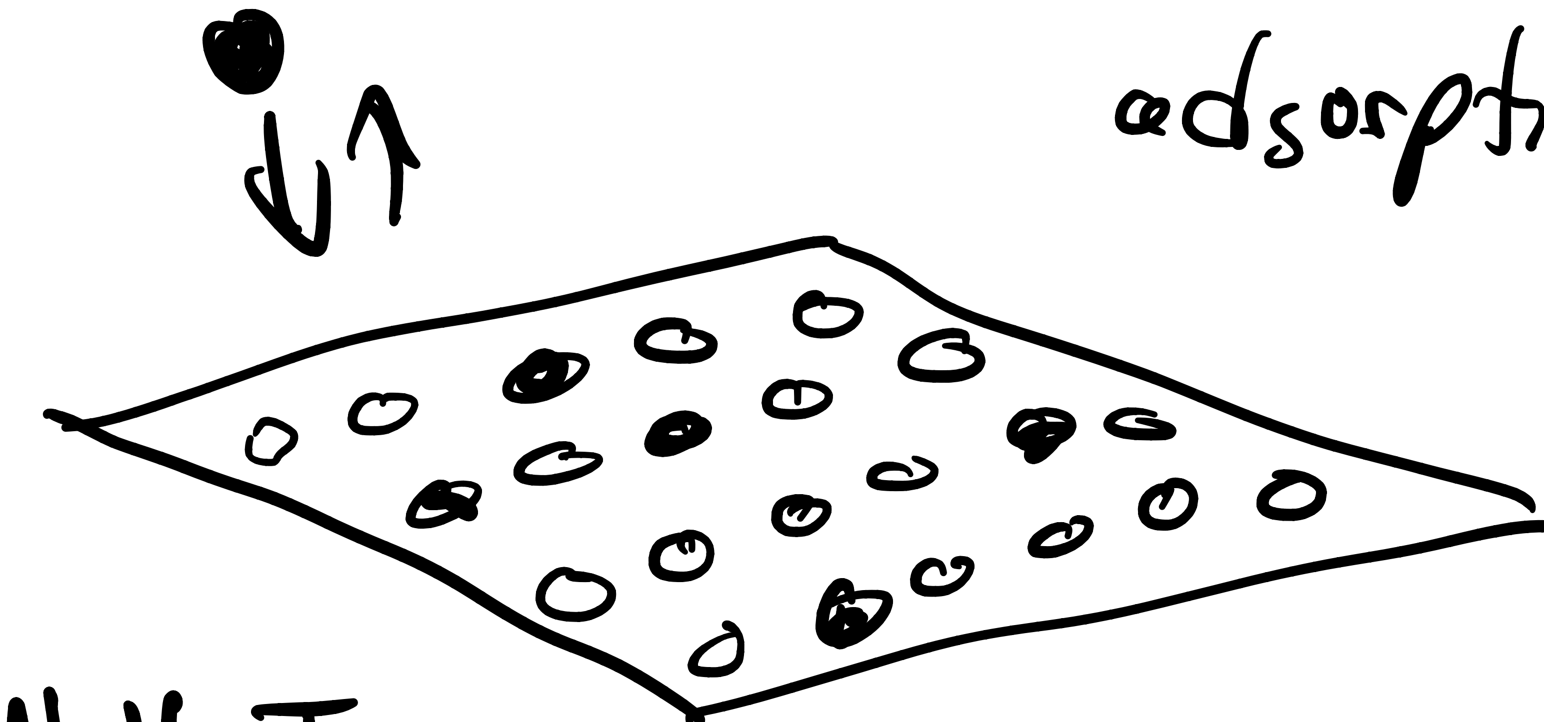
Lecture 22 – "Ising model"





Macro: N, V, T

$$E = \sum_{i \in \text{sites}} e_i \leftarrow \text{depends on neighbors}$$

microstates

State vector $\{\uparrow\downarrow\downarrow\uparrow \;\ldots\; \underbrace{\uparrow}_{N}\}$ 2^N possible states example ensemble average

avg magnitization $\Leftarrow$ what % are pointing up

$$m = \langle S_i \rangle = \frac{1}{N} \sum S_i$$

$\{+1, -1\}$

example observable O

$$P_{state} = \frac{e^{-\varepsilon_{state}/k_B T}}{Z}$$

$$\langle O \rangle = \sum_{\text{microstates}} O(\text{state})\, P(\text{state})$$

$$= \sum_{\#\text{pointing up}} \omega(\#)\, O(\#)\, P(\#)$$

Z partition function

$$Z = \sum_{\substack{\text{microstates} \\ i}} e^{-\beta \varepsilon_i} \qquad \beta = \frac{1}{k_B T}$$

What does Z tell us, connect to free energy & entropy

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

$$S_{Gibbs} = -k_B \sum_i P_i \ln(P_i) \qquad P_i = e^{-\beta\epsilon_i}/Z$$

Const N, U, T

$$= -k_B \sum_i P_i \ln\left[\frac{e^{-\beta\epsilon_i}}{Z}\right]$$

$$= -k_B \sum_i \left[P_i \ln\left(e^{-\beta\epsilon_i}\right) - P_i \ln Z\right]$$

$$= k_B \beta \underbrace{\sum_i P_i \epsilon_i}_{\langle \epsilon \rangle} + k_B \ln Z \overbrace{\cancel{\sum_i P_i}}^{1}$$

$$S = k_B \beta \langle \varepsilon \rangle + k_B \ln Z(N,V,T)$$

S.A.

$Z = \frac{1}{N!} V^N$

$$\frac{1}{T} = \frac{\partial S}{\partial U} = k_B \beta$$

$U = \langle \varepsilon \rangle$

from A, eg

$$P = -\left(\frac{\partial A}{\partial V}\right)_{N,T}$$

$$= + k_B T \left(\frac{\partial \ln Z}{\partial V}\right)_{N,T}$$

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

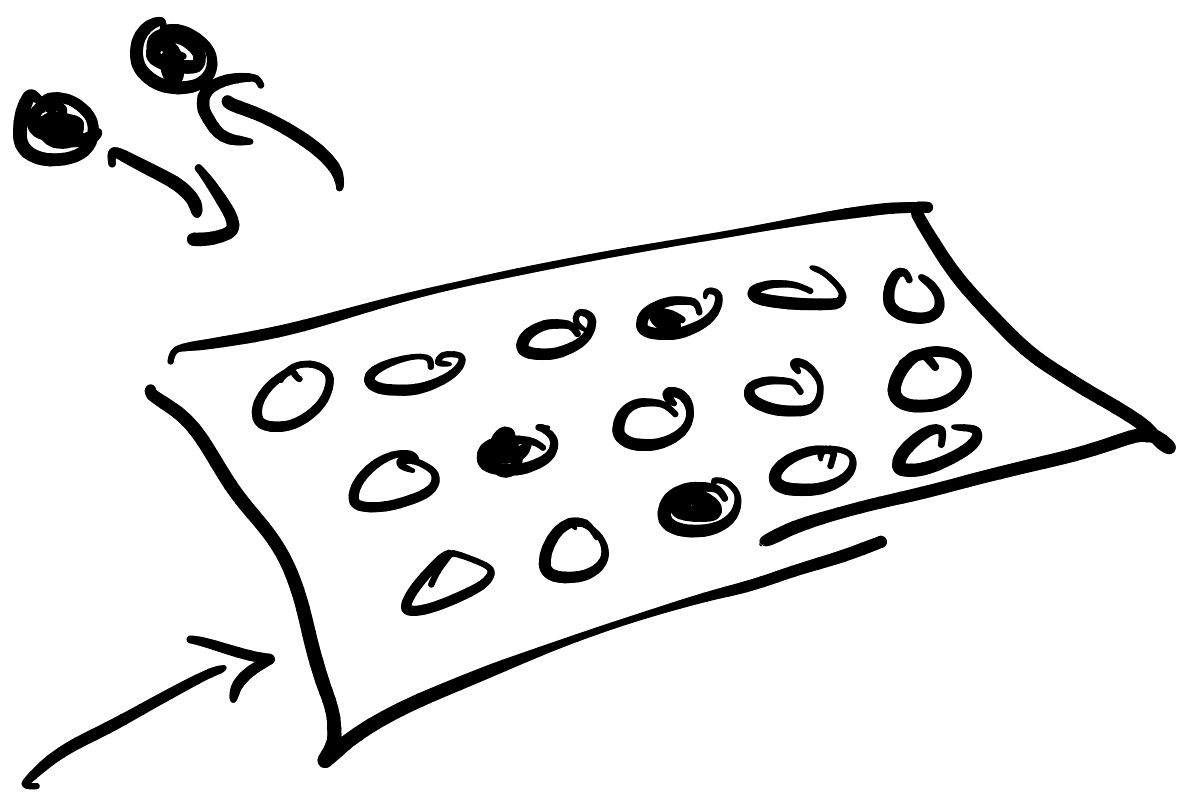
$$S = \frac{\langle \varepsilon \rangle}{T} + k_B \ln Z \rightarrow TS = \langle \varepsilon \rangle + T k_B \ln Z$$

$$\underline{A} = \langle \varepsilon \rangle - TS = \underline{-k_B T \ln Z}$$

Phase transitions, remember that the phase is the one with lower F.E.

Magnet: below some T $A(\text{aligned}) < A(\text{random})$

above some T opposite



N sites

can be black or white

alternative N molecules not const.

2 level system

$\uparrow \quad \downarrow$

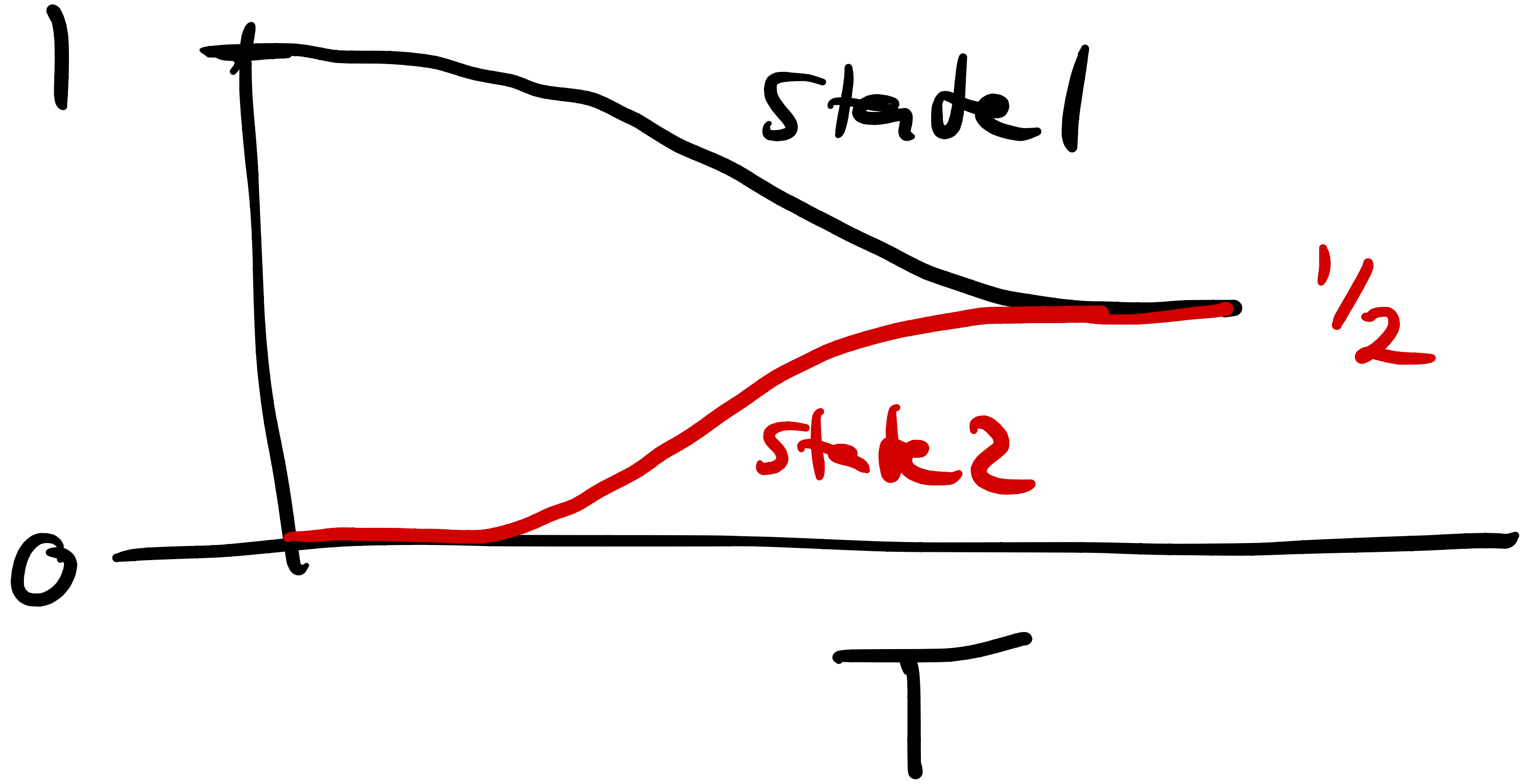
2 energies : $\varepsilon_1 \quad \varepsilon_2$

or $\quad 0 \quad + \epsilon$

$$Z = \underset{\text{up}}{e^{-\beta\epsilon_1}} + \underset{\text{down}}{e^{-\beta\epsilon_2}}$$

$$P_{up} = \frac{e^{-\beta\epsilon_1}}{Z} = \frac{e^{-\beta\epsilon_1}}{e^{-\beta\epsilon_1} + e^{-\beta\epsilon_2}} = \frac{1}{1 + e^{-\beta(\epsilon_2 - \epsilon_1)}}$$

$$P_{down} = e^{-\beta\epsilon_2}/Z \quad \ldots$$

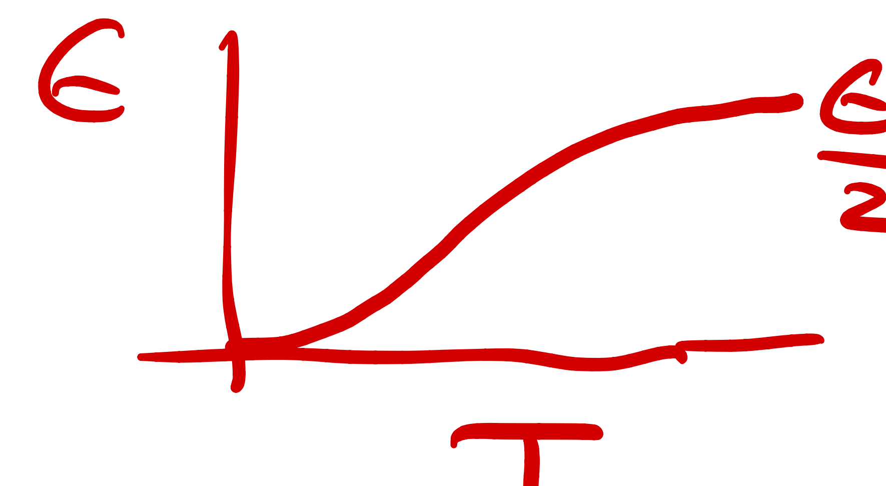


$$P_1 = \frac{1}{1+e^{-\beta(\epsilon_2-\epsilon_1)}}$$

$$\langle \varepsilon \rangle = \sum_{\substack{\text{state}\\ i}} \epsilon_i P_i = \frac{\epsilon_1 e^{-\beta\epsilon_1} + \epsilon_2 e^{-\beta\epsilon_2}}{e^{-\beta\epsilon_1} + e^{-\beta\epsilon_2}}$$

imagine $\epsilon_1 = 0$

$$= \frac{\epsilon\, e^{-\beta\epsilon}}{1+e^{-\beta\epsilon}} = \epsilon \frac{1}{1+e^{\beta\epsilon}}$$



$$\langle \varepsilon \rangle = -\frac{\partial \ln Z}{\partial \beta} \qquad Z = 1 + e^{-\beta\epsilon}$$

$$= \frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{-\epsilon e^{-\beta\epsilon}}{1+e^{-\beta\epsilon}} = \epsilon \cdot \frac{e^{-\beta\epsilon}}{1+e^{-\beta\epsilon}}$$

Heat capacity:

$$C_V = \left(\frac{\partial \langle \varepsilon \rangle}{\partial T}\right)_V = -\frac{\partial}{\partial T}\left(\frac{\partial}{\partial \beta}\ln Z\right) = k_B \beta^2 \frac{\partial^2}{\partial \beta^2}(\ln Z)$$

$$\frac{\partial}{\partial T} = \frac{\partial \beta}{\partial T}\frac{\partial}{\partial \beta} = \frac{\partial\left(\frac{1}{k_B T}\right)}{\partial T}\frac{\partial}{\partial \beta} = -\frac{1}{k_B T^2}\frac{\partial}{\partial \beta}$$

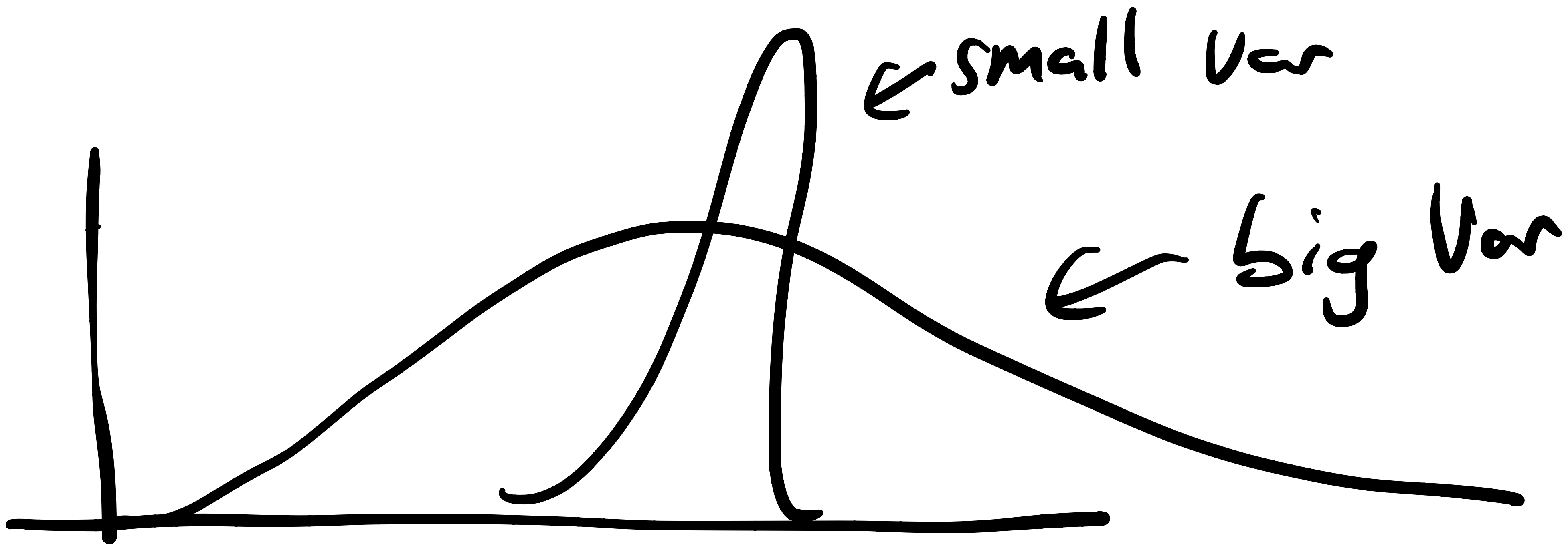
Turns out!

$$C_V \propto \mathrm{Var}(\varepsilon)$$

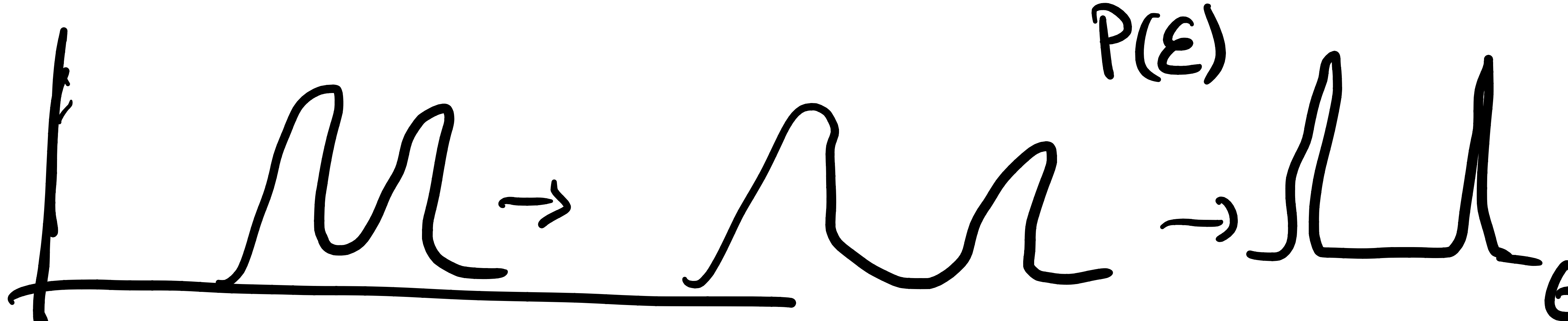
$$\frac{\partial \varepsilon}{\partial T} \quad '' \quad \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2$$

Fluctuation dissipation theorem

Onsager Regression Hypothesis



solid ↓ liq ↓



$\boxed{\uparrow}\boxed{\uparrow}$ - - - — $\boxed{\uparrow}$ N - TLS's

if independent

$$Z = \sum_{\substack{\text{states} \\ i=1}}^{2^N} P(i) = \sum_{\substack{\text{spin 1} \\ s_1}} P(s_1) \sum P(s_2) \sum P(s_3) \cdots$$

independent

$$= z_1 \cdot z_2 \cdot z_3 \cdots z_N$$

$$= z^N$$

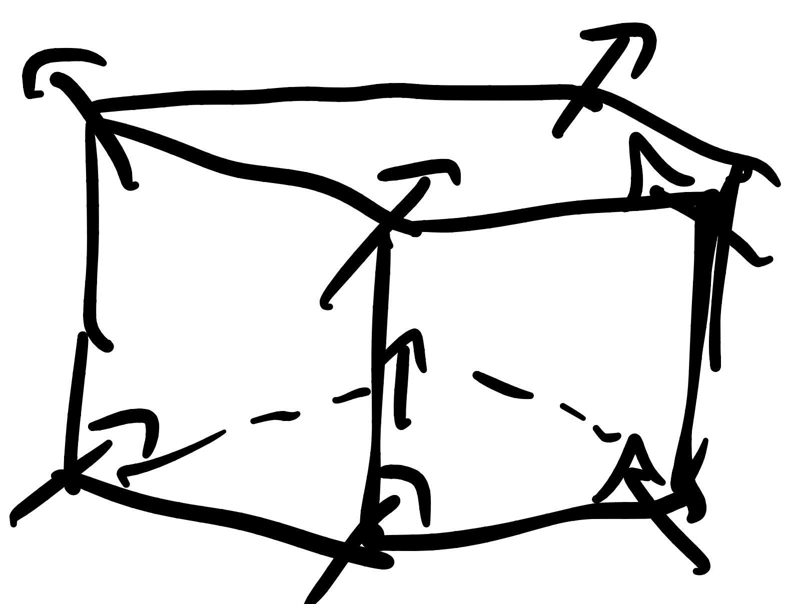
$$A = -k_B T \ln Z = -k_B T \ln(z^N) = -N k_B T \ln z$$

$$\langle E_{total} \rangle = N \langle \varepsilon \rangle_{TLS}$$

$$\left\langle \sum_{i=1}^{N} S_i \right\rangle = N \langle S_i \rangle \quad \text{if ind....}$$

Observation

spontaneous magnetization



3d system
3d spins

Suppose spins like to point in same direction

Classically $\quad \varepsilon = f(\vec{\mu}_i, \vec{\mu}_j)$ $\quad$ depend on distance

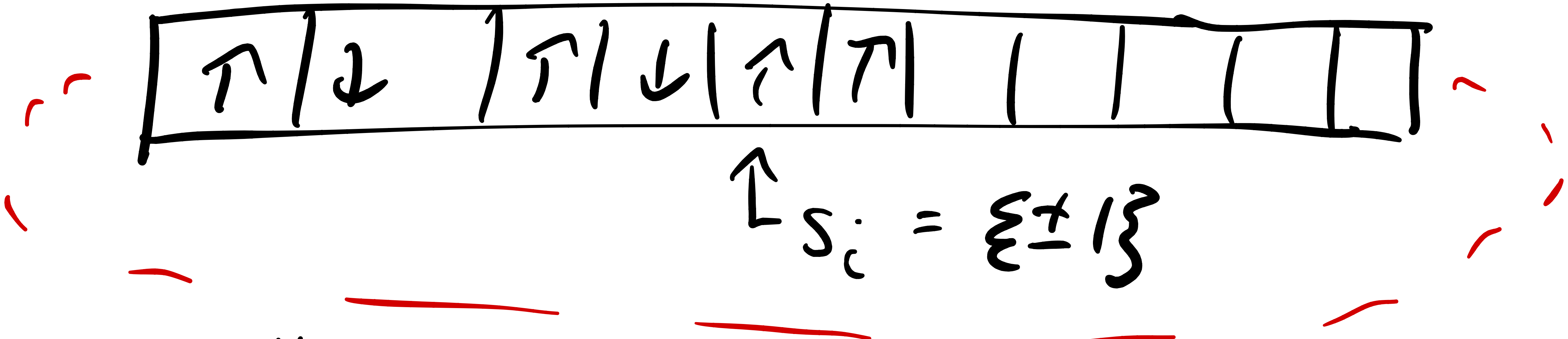
further apart | $= -\frac{\text{dot prod}}{r^6}$

weaker coupling

Ising: • consider only neighbors

• consider not vector spins, z direction

1d Ising model



1d

periodic?

$s_i = \{\pm 1\}$

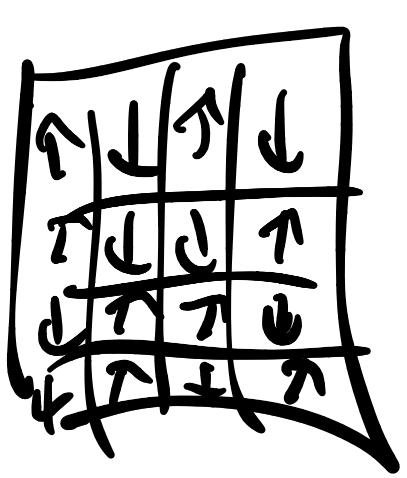
$$\varepsilon_i^{site} = -h s_i - J\left[s_i s_{(i+1)} + s_i s_{(i-1)}\right]$$

field

if like to align

$$\varepsilon_{total} = \sum_{i=1}^{N} \left(-h s_i - J s_i s_{i+1}\right)$$

1d Ising model



in dimension d, you have $2d$ neighbors

1d model — exact solution

we can write formula for

$T(\beta, h, J)$ $\quad N \to \infty$

$$m = -\frac{\partial \ln Z}{\partial h} \qquad h \to 0$$

No spontaneous mag...

2d! Onsager solution

is spont mag

$\shortparallel$