At equilibrium:

states $n = 1, \ldots, M$

energies $E_n(\vec{K})$

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

$\vec{K} = (K_1, K_2, \ldots)$ vector of parameters

equil. prob. $p_n^{eq} = \frac{e^{-\beta E_n}}{Z}$

$$Z = \sum_n e^{-\beta E_n}$$

physical observable O_n

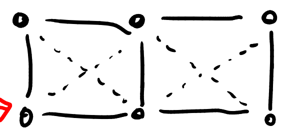
$$O(\vec{K}) = \langle O \rangle = \sum_n O_n p_n^{eq}$$

$\downarrow$

how do these change as a func. of $\vec{K}$

example: Ising model on a lattice

- - - - = nnn



states:

$n \longrightarrow \{s_1, s_2, \ldots\ldots\} = \vec{s}$

each site i: "spin" $s_i = \pm 1$ $\uparrow\downarrow$

$N = \#$ sites

$B = \#$ bonds

$\approx 2N$ for 2D square lattice as $N \to \infty$

$E_n(\vec{K}) \rightarrow \mathcal{H}_{\vec{s}}(j, h) =$

Hamiltonian $-j \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$

sum over all connected site pairs (i, j)

$\vec{K} = (j, h)$

$\#$ states $M = 2^N$

$j > 0$: ferromagnetic spin-spin interaction

$\Rightarrow$ tends to align nearest-neighbor (nn) spins

h: "magnetic field" term $\begin{cases} > 0 & \text{favors } \uparrow \\ < 0 & \text{favors } \downarrow \end{cases}$

rewrite: $-\beta \mathcal{H}_{\vec{s}} = J \sum_{\langle ij \rangle} s_i s_j + H \sum_i s_i$ $\qquad J \equiv \frac{j}{k_B T}$ $\quad H = \frac{h}{k_B T}$

$$p^{eq}_{\vec{s}} = \frac{e^{-\beta \mathcal{H}_{\vec{s}}}}{Z} \qquad Z = \sum_{\vec{s}} e^{-\beta \mathcal{H}_{\vec{s}}}$$

sum over $M = 2^N$ terms: hard to calculate when $N \to \infty$

note: $T = \frac{j}{k_B} J^{-1} \Rightarrow T \propto J^{-1}$

simple case: $N = 2$

$B = 1$

n	$\vec{s}$	$\exp(-\beta \mathcal{H}_{\vec{s}})$
1	$-1 \quad -1$	$\exp(J - 2H)$
2	$-1 \quad 1$	$\exp(-J)$
3	$1 \quad -1$	$\exp(-J)$
4	$1 \quad 1$	$\exp(J + 2H)$

$$Z(J, H) = e^{J-2H} + 2e^{-J} + e^{J+2H}$$

$$p^{eq}_{\vec{s}=(1,1)} = \frac{e^{J+2H}}{Z}$$

if $H > 0$ and $J^{-1} \to 0$ $(J \to \infty)$

$\longrightarrow 1$

if $H \to -\infty$ then $\to 0$

mean observables $\Rightarrow$ naturally calculate from derivatives of $\ln Z \propto$ free energy

i.e. $M(J, H) = \frac{1}{N} \left\langle \sum_i s_i \right\rangle =$ mean "magnetization" per spin

$$= \frac{1}{N} \sum_{\vec{s}} \frac{\left(\sum_i s_i \right) e^{-\beta \mathcal{H}_{\vec{s}}}}{Z}$$

$$= \frac{1}{N} \frac{\partial}{\partial H} \ln Z(J, H)$$

$$U(J,H) = -\frac{1}{B}\left\langle \sum_{\langle ij\rangle} s_i s_j \right\rangle$$

= mean spin-spin correlation per bond

$$= -\frac{1}{B}\frac{\partial}{\partial J}\ln Z(J,H)$$

= if $H=0$ this is just $\propto$ mean energy per bond

What about other observables? Add them to Hamiltonian, we take one (or more) derivatives of $\ln Z$, set prefactor to zero:

i.e. $$L(J,H) = \frac{1}{\underbrace{B_{nnn}}_{\#\text{ next nearest neighbor pairs}}}\left\langle \sum_{\langle ij\rangle_{nnn}} s_i s_j \right\rangle$$

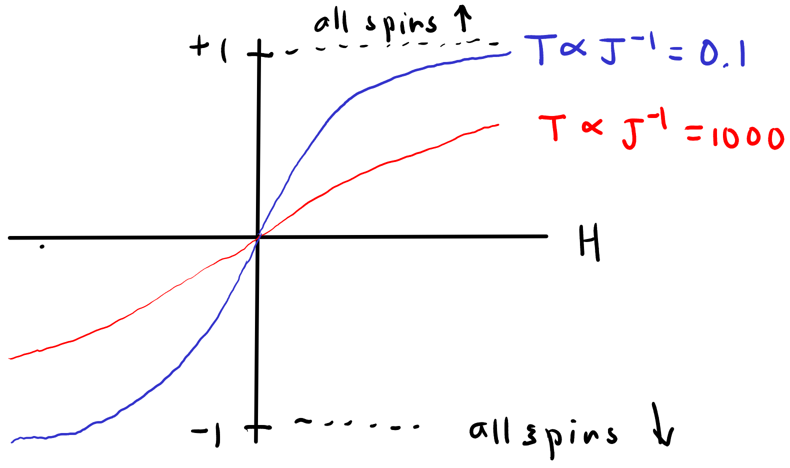
$$-\beta \mathcal{H}_{\vec{s}} = J\sum_{\langle ij\rangle} s_i s_j + H\sum_i s_i + X\sum_{\langle ij\rangle_{nnn}} s_i s_j$$

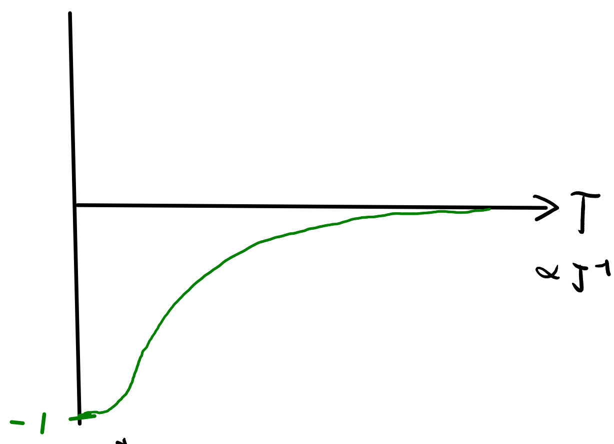
$$L(J,H) = \frac{1}{B_{nnn}}\frac{\partial}{\partial X}\ln Z(J,H,X)\Big|_{X=0}$$

we can imagine $\mathcal{H}_{\vec{s}}(J,H)$ to be a "surface" in an ∞ dim space of possible models:

$$\mathcal{H}_{\vec{s}}(J,H,\underbrace{X=0,\ K=0,\ \ldots}_{\text{other possible terms set to zero}})$$

$M=2$ example: $M(J,H)$ $\qquad$ $U(J, H=0)$





Interesting fact: for any finite N, $\ln Z$ & its derivatives are continuous in $J, H, \ldots$ $\Rightarrow$ $\ln Z$ is infinitely differentiable

$\Rightarrow$ when $N \to \infty$ (thermodynamic limit) no longer true: singularities are possible