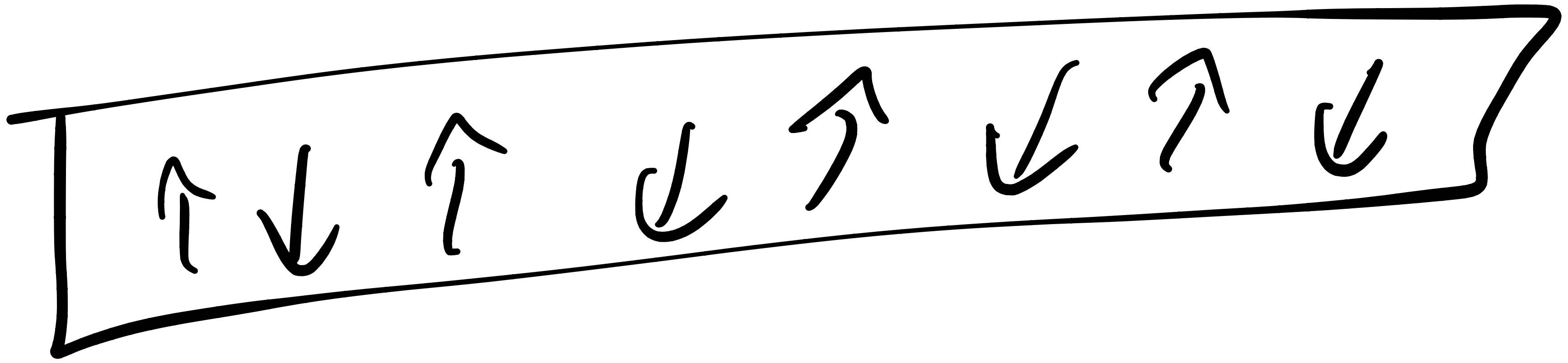
Lecture 23 Helix coil model & ising model



Ferromagnetic ~ want to align

$$\mathcal{E} = \sum_i -J s_i s_{i+1} - h s_i \qquad -\frac{\partial \mathcal{E}}{\partial h} = \sum_i s_i$$

$J > 0$, ferromagnetic

higher dimensions

$$\sum_{\langle ij \rangle} -J s_i s_j - h s_i$$

$\langle ij \rangle$ ← neighbors

want to "solve" Ising model

$\rightarrow A = -k_B T \ln Z(\beta, N)$ $\Leftarrow$ for some J, h

$$Z = \sum_{\text{states } i} e^{-\beta \varepsilon_i} = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} e^{-\beta E(s_1, s_2 \ldots s_N)}$$

$$\left(\sum_i -J s_i s_{i+1} - h s_i \right)$$

2 limits:

$T \to \infty$

$$Z = \sum_{s_1} \cdots \sum_{s_N} (1) = 2^N$$

other situation, $J=0$

$$Z = \sum_{S_1}\sum_{S_2}\cdots\sum_{S_N} \underbrace{e^{-\beta\sum_i -hS_i}}_{e^{\beta S_1} e^{\beta S_2} \cdots e^{\beta S_N}}$$

$$= \sum_{S_1} e^{\beta S_1 h} \sum_{S_2} e^{\beta S_2 h} \cdots \underbrace{\sum_{S_N} e^{\beta S_N h}}_{z}$$

$$= z^N = (e^{\beta h} + e^{-\beta h})^N$$

$$A = -k_B T N \ln(e^{\beta h} + e^{-\beta h})$$

$\beta \to 0 \qquad A = -k_B T N \ln(2)$

$J \to 0 \qquad A = -k_B T N \ln\left(e^{\beta h} + e^{-\beta h}\right)$

$$m = \langle s_i \rangle = \frac{1}{N} \langle \sum_i s_i \rangle$$

$\uparrow N_{up} - N_{down}$

$$\underbrace{\langle \sum_i s_i \rangle}_{O} = \underbrace{\sum_x X P(x)}_{\text{in general}} = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} O(s_1 \ldots s_N) \frac{e^{-\beta E(s_1 \ldots s_N)}}{Z}$$

$$\frac{\partial Z}{\partial h} = \sum_{s_1} \cdots \sum_{s_N} \beta\left(\sum_i s_i\right) e^{-\beta \mathcal{E}(s_1 \ldots s_N)}$$

$$\frac{\partial \ln Z}{\partial h} = \frac{1}{Z}\frac{\partial Z}{\partial h} = \beta \langle \sum s_i \rangle$$

$$m = \frac{1}{N}\langle \sum s_i \rangle = \underbrace{\frac{k_B T}{N}\frac{\partial \ln Z}{\partial h}}_{\text{use this}} = -\frac{1}{N}\frac{\partial A}{\partial h}$$

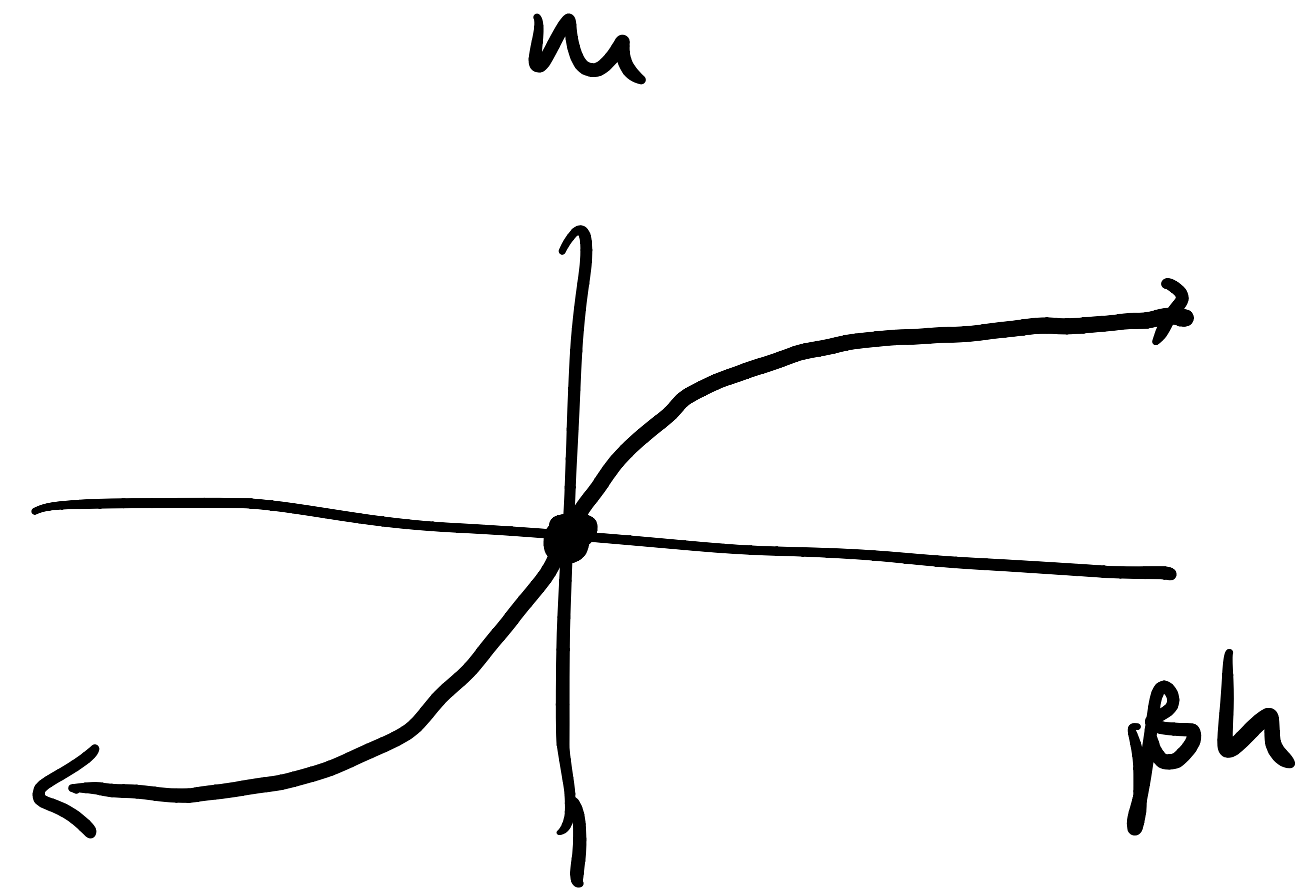
① $m = k_B T \dfrac{\partial \ln(2)}{\partial h} = 0$ @ $T \to \infty$

② $Z = (e^{\beta h} + e^{-\beta h})^N$

$m = k_B T \dfrac{\partial \ln(\;)}{\partial h}$

$$Z = \left(e^{\beta h} + e^{-\beta h}\right)^N$$

$$\frac{\partial \ln Z}{\partial h} = N \underbrace{\frac{\beta e^{\beta h} - \beta e^{-\beta h}}{e^{\beta h} + e^{-\beta h}}}$$

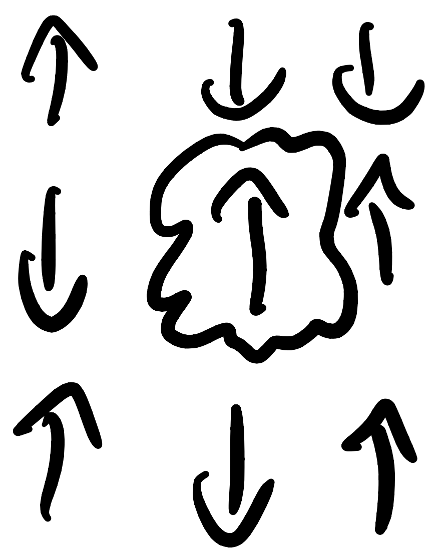


$$m = \tanh(\beta h)$$

, with $J = 0$

Can get $A(\beta, h)$, can come back to it later is $m(J>0, h=0) \to 1$?

Approximate solution: mean field theory



what direction is 1 spin in average environment

$$\mathcal{E} = \sum_i -J s_i s_{i+1} - h s_i \approx \sum_i -J s_i m - h s_i$$

$$= \sum_i s_i(-Jm - h)$$

effective local field

independent

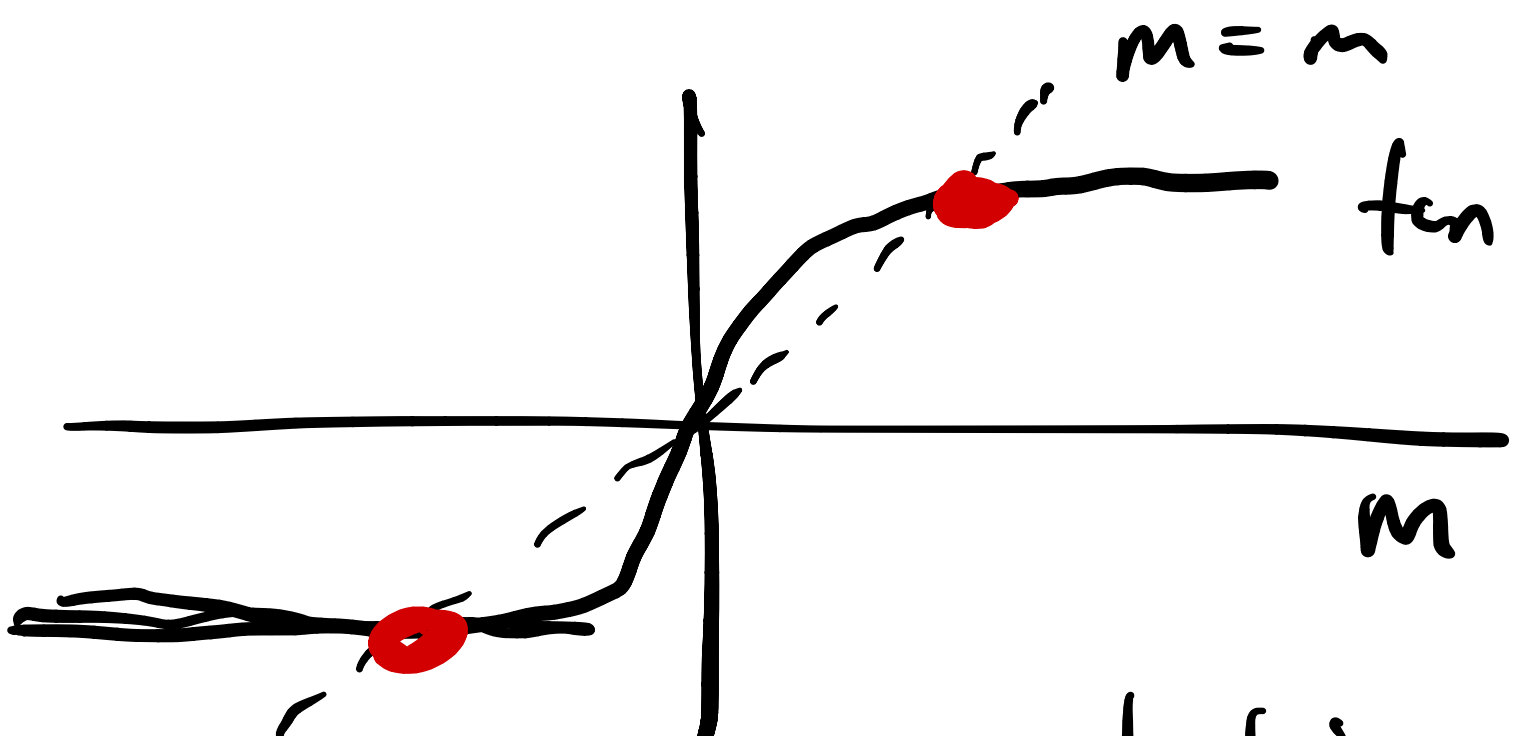
MFT prediction is

more dimensions

$$m = \tanh(\beta[h + Jmd])$$

is this true?

solve graphically



$\tanh(\cancel{\beta h} + Jmd)$ β

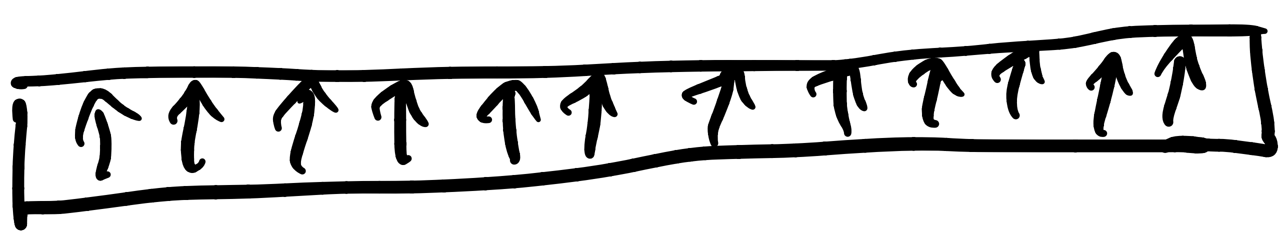
no external field

what is J/k_BT

MFT is physically wrong in 1d

but only quantitatively wrong in $d \geq 2$
and qualitatively right

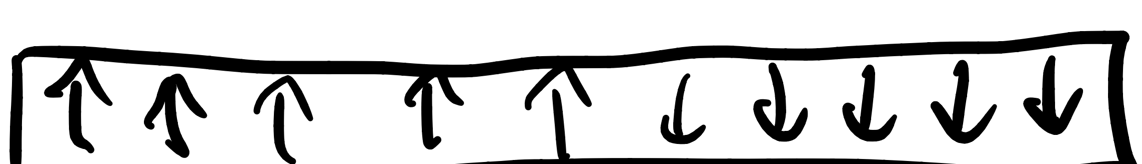
Why no spontaneous magnetization in 1d but there is in higher dimensions



$J > 0, \; h = 0$

$\mathcal{E} = \mathcal{E}_{min} = -JN \;, \quad m = 1$

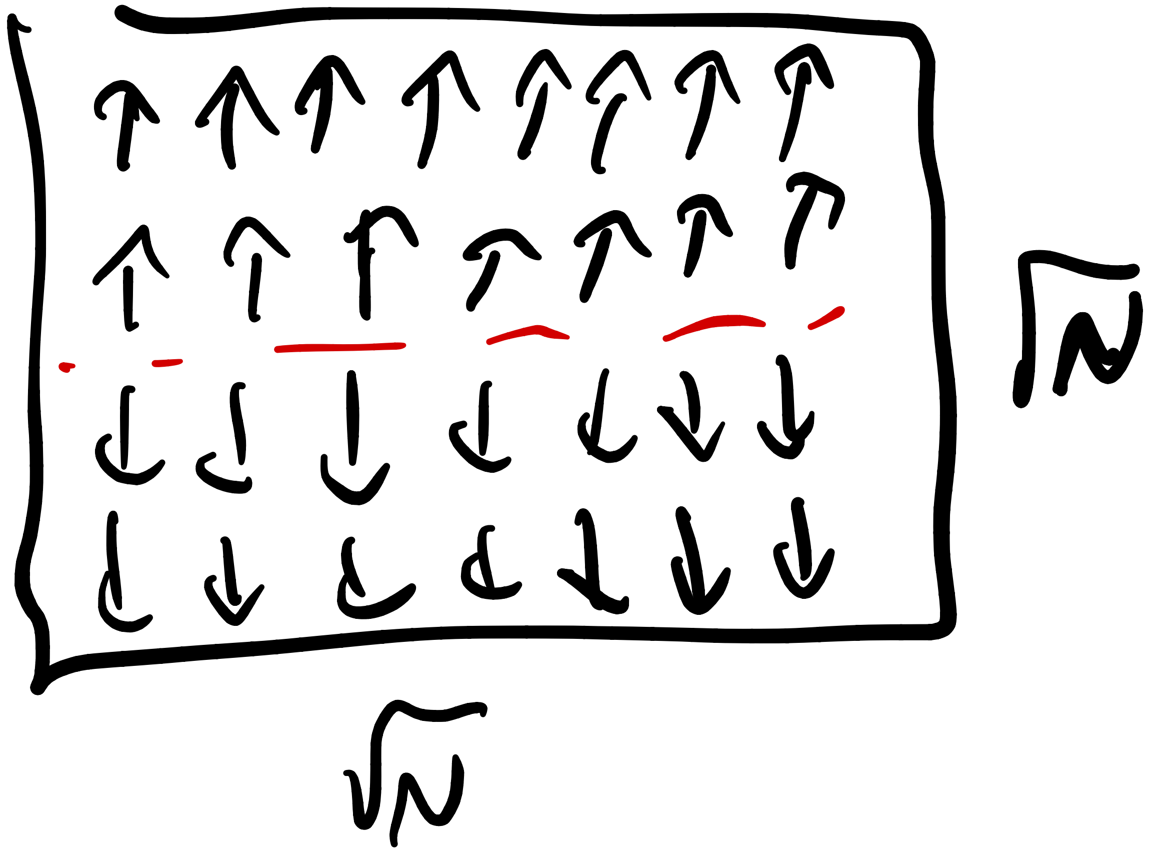
interfaces almost 0 energy



$\mathcal{E} = -JN + 2J \qquad m = 0$

In 2d

N spin system



$m = 0$

$$\mathcal{E} = \mathcal{E}_{min} + 2J\sqrt{N}$$

interface is $\sqrt{\text{system size}}$

area vs volume

as $d \uparrow$ surface area/volume ratio $\uparrow$

Zimm - Bragg model / Helix-coil model

N amino acids $\qquad\qquad$ α - helix

C	C	C	C	C	C	C	C	$\leftrightarrow$	H	H	H	H	H	H	H	H	H

which is preferred

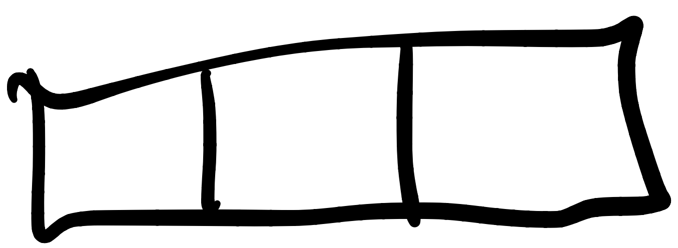
C has energy 0, H has an energy $-h$

$-J$ for neighbors

think about 1 amino acid

$$P_H / P_C \sim e^{\beta h} = K \qquad C \rightleftharpoons H$$

Independent model



$C \leftarrow 1$

$$C\cdot C\cdot C + K\cdot K\cdot C + K\cdot C\cdot C + K\cdot C\cdot K + C\cdot K\cdot C + K\cdot K\cdot K + C\cdot C\cdot K + C\cdot K\cdot K$$

$$2^N = 8$$

Z

$$Z = z^N = \underbrace{(1+k)}_{\text{like } e^{\beta h} + e^{-\beta h}}{}^N = \sum_{n=0}^{N} \binom{N}{n} K^n (1)^{N-n}$$

$$= \sum_{n=0}^{N} \binom{N}{n} K^n \qquad \text{independent}$$

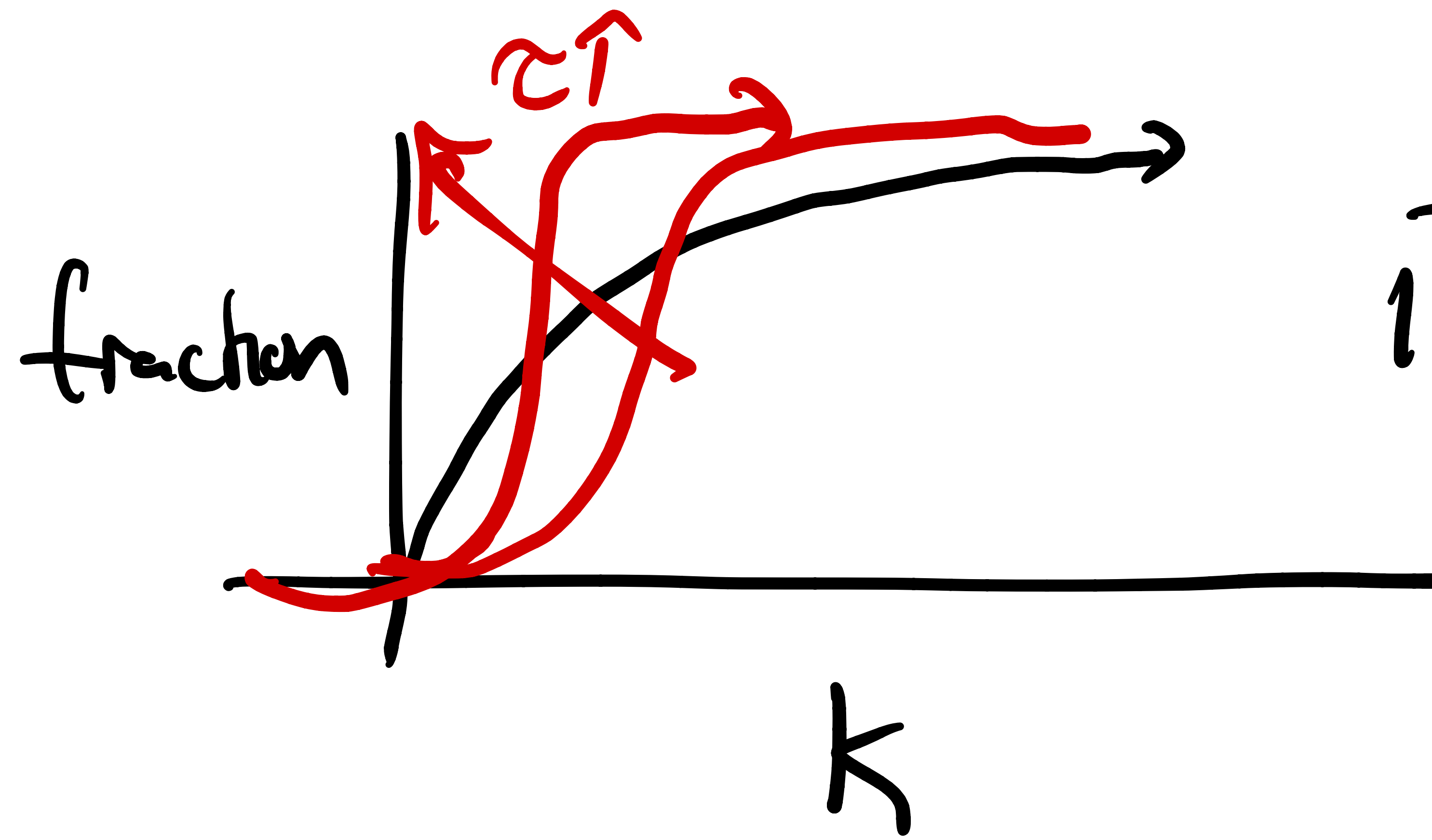
Scenario - zipper model, z coupling is big

$$\boxed{\text{CCHHHCCC}} \qquad Z = \sum_{n=0}^{N} (N-n+1) K^n z^{n-1}$$

fraction of residues that are helical

$$\langle n \rangle = \sum_{n=0}^{N} n\, P(n) = \sum_{n=0}^{N} n\, \frac{BF(n)}{Z}$$

$$= k\, \frac{\partial \ln Z}{\partial k}$$



$$\frac{K}{1+K}$$