Questions?

<u>LAST TIME</u>: traveling salesperson

→ NP problem ("exponentially hard")
→ minimize a function

<u>TRICK</u>: USE STATMECH TO FIND "APPROX." SOLUTION

↑ likely solution

<u>IDEA</u>: minimize $E(\vec{x})$

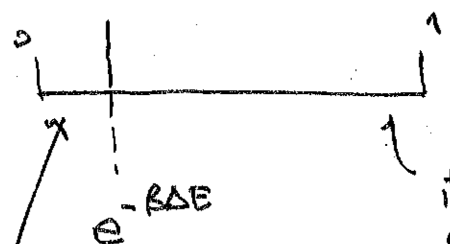
total distance

$$\vec{x} = [(x_1, y_1), (x_2, y_2), (x_3, y_3), \vdots, (x_N, y_N)]$$

LIST OF CITY COORDS <u>IN ORDER</u>

<u>MCMC</u>: start @ some random config (μ state)

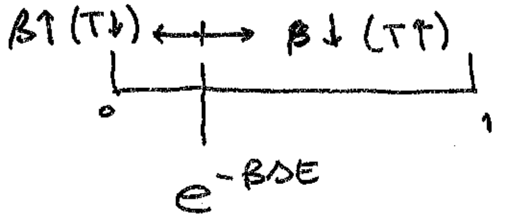
1. PICK A STEP TO A "NEIGHBORING" μSTATE
   ↳ SWAP i^{th} & j^{th} LOCATIONS in ORDERED LIST
2. IS it "energetically favorable"?
   Y: MAKE THE STEP
   N: ROLL DICE TO DECIDE TO STEP



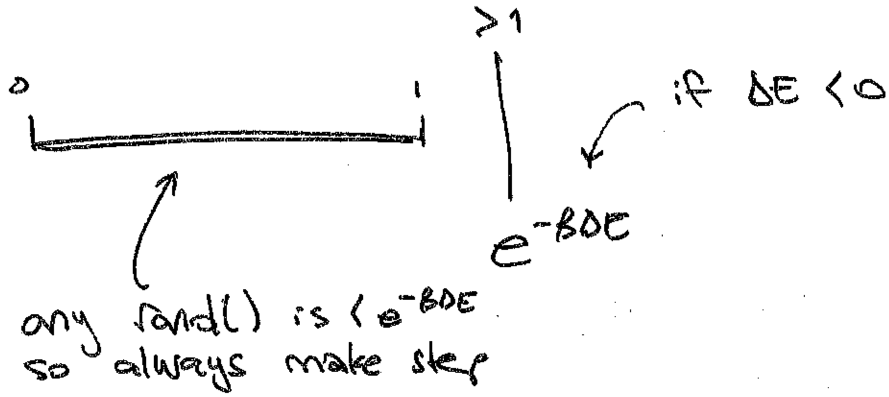
rand()

if rand() here, do <u>not</u> make step

if rand() here, <u>make step</u>



HOT: MORE LIKELY TO <u>CLIMB</u> POT. BARRIER



<u>reminder</u>: there is nothing <u>physical</u> about this random walk! We are not <u>simulating</u> an actual physical process.

WE ARE "SIMULATING" A WAY TO SAMPLE A PARAMETER SPACE.

IT DOES BETTER THAN

- GRADIENT DESCENT → stuck in local min.
- pure random sampling → opposite problem!

BTW: SIM. ANNEALING : KIRKPATRICK '83 ← long after "salesmen" were really a thing...

'94: QUANTUM ANNEALING (cond-mat/9402330)
Use QUANTUM TUNNELING w/ fake "kinetic E"

why? QM annealing more efficient than usual annealing for some materials

THE ISING MODEL : theory

FERROMAGNET : magnetism is quantum (Bohr)
CANNOT OCCUR IN CLASSICAL SYS.

MODEL : F.M. IS LATTICE OF SPINS $\longleftrightarrow$ $S = \frac{1}{2}$ MAG. MOMENTS

$$S_z = \pm 1/2$$

ENERGY IS GIVEN BY NEAREST NEIGHBOR INTERACTION

simple model

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

neg.

exchange constant

$S_i = \pm$

if i & j have opp orientation, ΔE is positive
" same " , ΔE is negative

ENERGY PREFERS ALIGNED SPINS (either ↑ or ↓)
TEMPERATURE ALLOWS MISALIGNMENT

$$P_\alpha = e^{-E_\alpha / k_B T} / Z$$

α state: config of ↑/↓ on each lattice site

FOR SIMPLICITY 2D LATTICE.

MAGNETIZATION : $M_\alpha = \sum_i S_i^{(\alpha)}$

α state

lattice site

$$M = \boxed{\langle M \rangle = \sum_\alpha M_\alpha P_\alpha}$$

<u>THEORY</u>: Mean field theory (from Giordano & Nakanishi CH. 8.2)

trick for estimating statmech systems:
REPLACE DIFFICULT QUANTITIES w/ THEIR AVG VALUES.

<u>PRETEND</u> $\exists$ BACKGROUND B field: H

$$E = -J \sum_{ij}^{N.N.} S_i S_j - \mu H \sum_i S_i$$

μ: mag moment of spin

H "biases" spin to align w/ it

SUPPOSE only one spin in this B field

↳ no J term... just some magnetic field (as if effect of all neighboring spins were condensed into H...)

<u>two state system</u>:

$$E = -\mu H \sum_i^{\pm} S_i \quad \longleftarrow \quad S_i = \pm$$

$$P_{\pm} = e^{-\beta(\mp \mu H)} / Z$$

$$Z = e^{+\mu H \beta} + e^{-\mu H \beta}$$

$$\boxed{\langle s \rangle = \sum_{S=\pm} S P_{\pm} = P_+ - P_- = \tanh(\mu H \beta)}$$

WE CAN USE THIS: BACK TO BIG SYSTEM

$$E = \sum_i \Big[-\underbrace{\Big(J \sum_j^{NN_i} S_j\Big)}_{\mu H_{eff}} - \mu H \Big] S_i$$

looks like

$$H_{eff} = \frac{J}{\mu} \sum_j^{NN_i} \langle s \rangle = \frac{J}{\mu} n \langle s \rangle$$

n: # of nearest nbrs

$\langle s \rangle$: MEAN FIELD APPROX

from single spin in fake H field:

$$\langle s \rangle = \tanh(\mu H \beta)$$

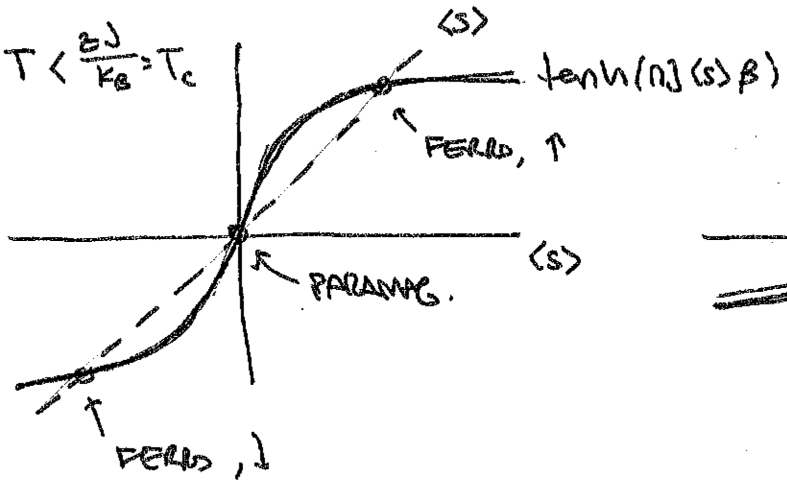
$$H \mapsto H_{eff} = \frac{nJ}{\mu}\langle s \rangle$$

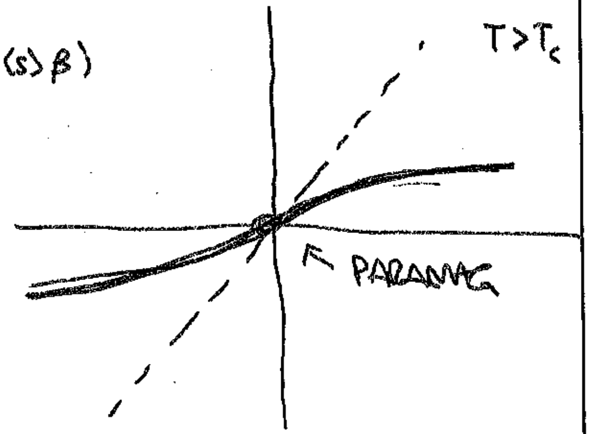
gives implicit relation for $\langle s \rangle$:

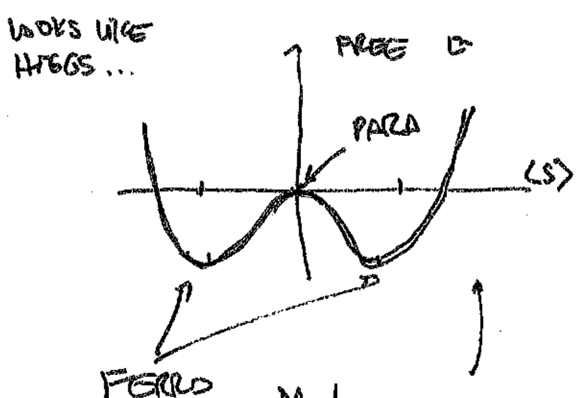
$$\boxed{\langle s \rangle = \tanh(nJ\langle s \rangle \beta)}$$

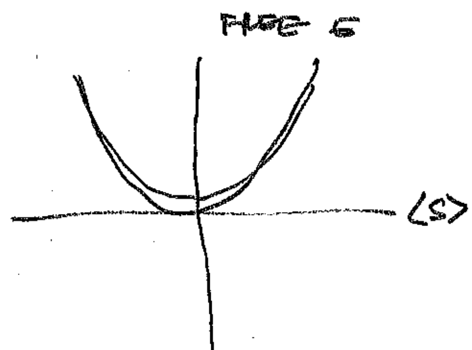
$n=4$ for 2D lat.

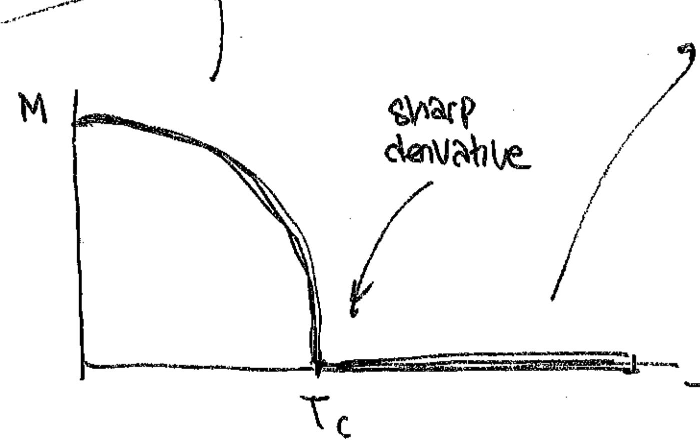
SOLUTION: PLOT IT. (both sides, look for i'sect)











2ND ORDER PHASE TRANSITION

CRITICAL PHENOMENA

can tune easily!

DIAGNOSING CRITICAL PHENOMENA:

Use: $\tanh(x) \approx x - \frac{1}{3}x^3$

$$\langle S \rangle \approx A\langle S \rangle \frac{1}{3}(A\langle S \rangle)^3 \longleftarrow A = nJ\beta = \frac{nJ}{T}$$

$$S = S\left(A - \frac{1}{3}A(AS)^2\right)$$

$$\frac{1}{3}A(AS)^2 = A - 1$$

$$S^2 = \frac{3}{A^3}(A - 1)$$

$$= \frac{3T^3}{n^3J^3}\left(\frac{nJ}{T} - 1\right)$$

$$= \frac{3T^2}{n^3J^3}(\underbrace{nJ}_{T_c} - T)$$

(setting $k_B = 1$)

$$\Rightarrow \langle S \rangle \sim \sqrt{\frac{3T^2}{n^3J^3}}\,(T_c - T)^{1/2} \text{ --- } \boxed{\beta = 1/2}$$

CRIT. EXPONENT

$$\frac{dM}{dT} = N\frac{d\langle S \rangle}{dT} \sim \frac{-1}{\sqrt{T_c - T}}$$

BLOWS UP @ $T = T_c$

$\beta = 1/2$ POWER LAW IS EXAMPLE OF UNIVERSALITY CLASS.