Lecture 1: Overview of the Class, & Introduction to Statistical Mechanics

Today:

1. Self introduction
2. Survey on background
3. Go through syllabus
4. What is Stat Mech
5. First example

Ask about technology
Random numbers

What is Statistical Mechanics?

Chemists care about atoms, molecules, materials
can compute properties of a (small) molecule using QM
Most chemistry experiments have much more (think 10^{23})
Many properties of system can be measured without knowing exact position of all atoms [eg heat capacity, T_m, ...]

Guess: these are averages of some quantity over the possible positions of the atoms/molecules in the system
(assume no reactions for now)

In this class:

look at how measurable quantities arise for systems of molecules. Connect Classical Mech w/

① Thermodynamics (entropy, free-energies, heat capacities, etc)

② Look at Kinetic properties, eg. rates of changing between states, spectroscopies

③ Understand how computer simulations generate solutions for problems with no exact solution.

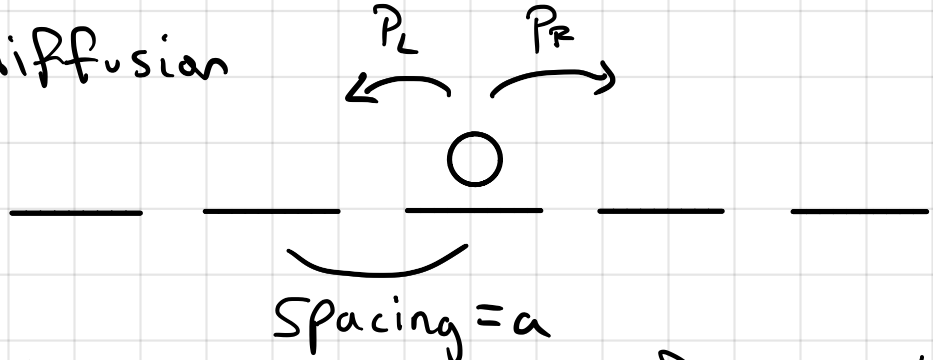
Q: (w/ neighbor): What are current research problems you've heard about that might connect with SM?

My examples: structure of a liquid & how is it measured, how to polymers behave in solution, how do proteins fold, how do molecules behave at interfaces
how do systems: melt, freeze, self-assemble?
does this depend on dimension? (eg confinement)

"Statistical" mechanics means we need to understand some simple ideas from Stat

Eg: Diffusion, will consider 1d on lattice, later 3D diffusion, theory of Brownian motion, Einstein 1905

1-d diffusion



moves distance a w/ prob P_R to right or P_L to the left, imagine $P_L = P_R = 0.5$ to start

How far does it get in N steps?

The "dynamics" are the same as flipping a coin N times

moves: $\{\overset{m_1}{L}, \overset{m_2}{R}, \overset{m_3}{L}, \overset{\dots}{L}, R, L\} = \{m_i\}$

"trajectory": $\{\underset{x_0}{0}, \underset{x_1}{-a}, \underset{\dots}{0}, -a, -2a, -a, -2a\} = \{x_i\}$

Let's generate our own data and see what happens: rand $\in (0,1)$, if $< .5$, left

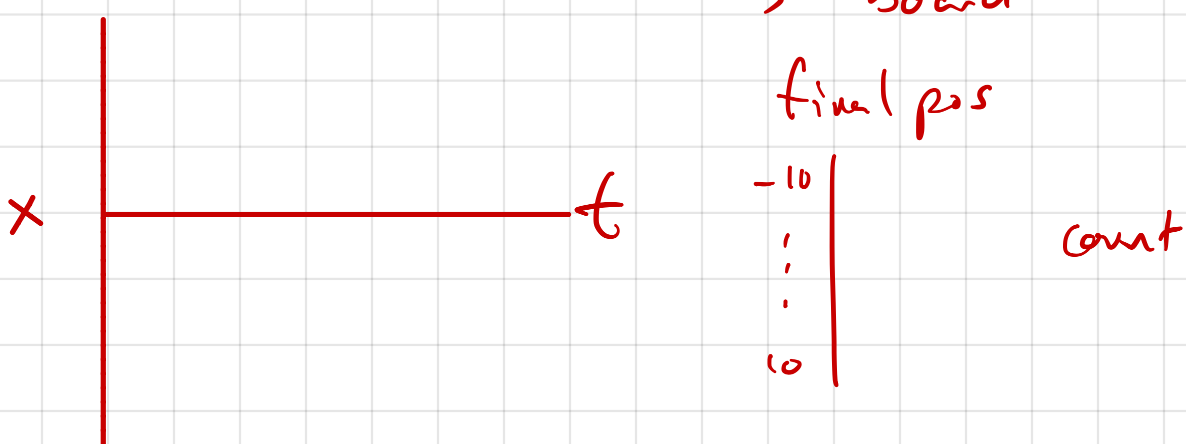
Draw table: w/ partner

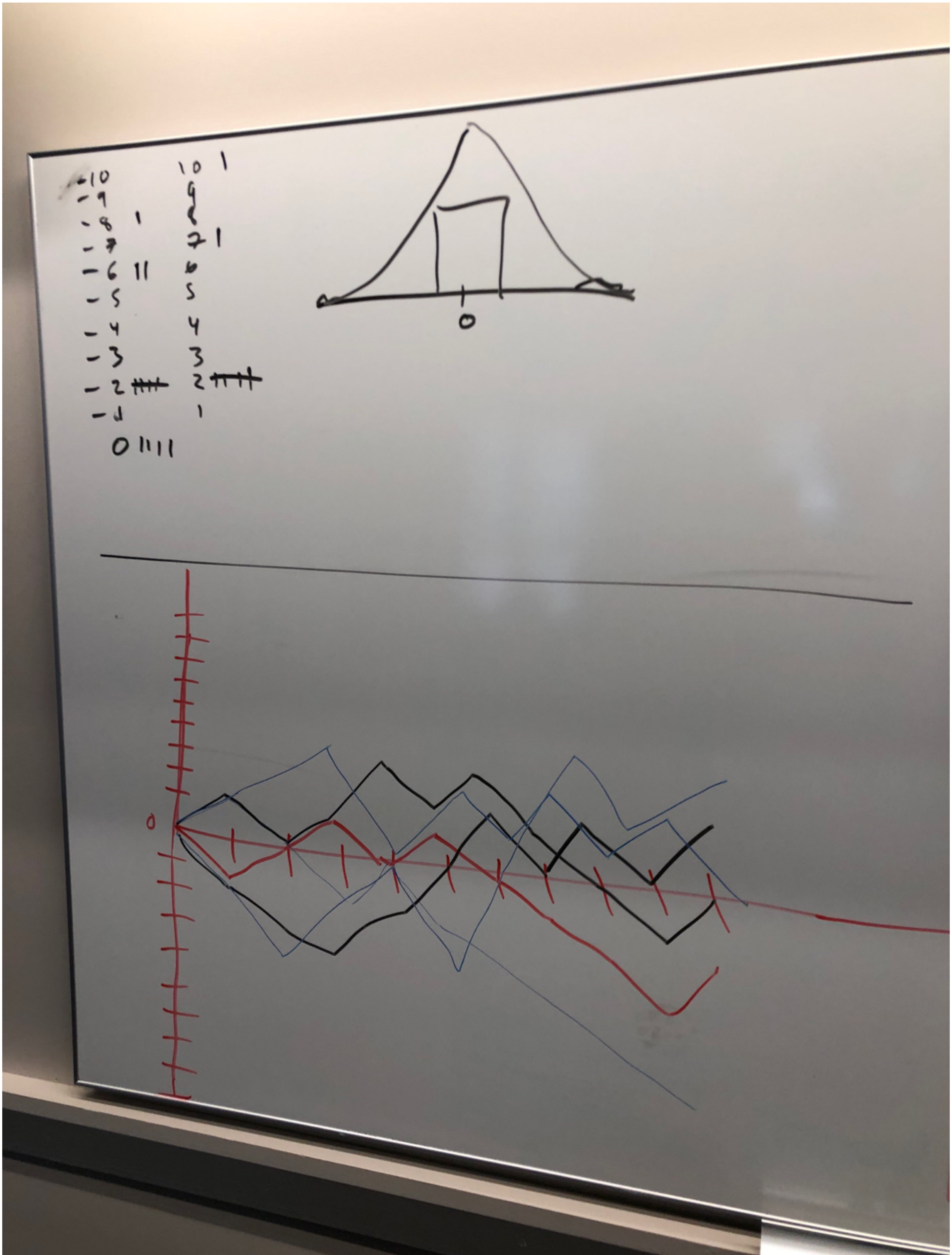
r: .1, 1, .2, .2, .7, 1, .8, .2, .7, .6
m: L, R, L, L, R, R, R, L, R, R
t: 0, $-a$, 0, $-a$, $-2a$, $-a$, 0, a, 0, a, $2a$

do 2x

$\rightarrow$ board

Plot




-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
10
9
8
7
6
5
4
3
2
1
0
0

How should we analyze this kind of data?

Want to consider average of quantities we can measure for the particle.

Average over time means we watch for a long time and average "observables"

$$\langle A \rangle = \lim_{M \to \infty} \sum_{i=1}^{N} A(X_i)$$

For this system, what is the average position?

$$\langle x \rangle = \lim_{M \to \infty} \frac{1}{M} \sum_{i=0}^{M} x_i = \lim_{M \to \infty} \frac{1}{M}\Big(\cancelto{0}{x_0} + \underbrace{\sum_{i=1}^{M} m_i}_{aN_+ - aN_-}\Big) = \lim_{M \to \infty} a\left(\frac{N_+}{M} - \frac{N_-}{M}\right)$$

$$= a(p_+ - p_-) = a(p_+ - (1 - p_+)) = 2a(p_+ - \tfrac{1}{2})$$

If $p_+ = 1/2$, stays in place on average, otherwise "drift" L or R

$\langle x \rangle = \langle disp \rangle = 0$, but we see final positions are spread how can we quantify this?

Need to consider "Ensemble quantities", ie what would happen for many independent copies of a system

Def^n:
$$\langle A \rangle_{ensemble} = \sum_{\substack{n \\ \text{states}}} P_n A_n$$

In many cases we assume

$$\langle A \rangle_{ensemble} = \langle A \rangle_{time}$$

(Say system is "ergodic")

But easier to compute most things as ensemble average on paper (and time/trj avg on computer)

How can we do it for this system?

Call $d_M = a\sum_{i=1}^{M} m_i$, displacement @ M

$$= a(N_+ - N_-) = a(2N_+ - M)$$

$d_M \in \{-M, \dots, M\}$ but what is $P(\hat{N}_+)$?

Q: What is probability of choosing N_+ in M trials?

$$P(\hat{N}_+) = \binom{M}{N_+} p_+^{N_+} (1-p_+)^{M-N^+},$$

$$\langle N_+ \rangle = Mp_+$$

$$Var(N_+) = Mp_+(1-p_+)$$

Will finish in more details next time