Lecture 1 - Intro, Probability

Introduction - What is Thermo & Kinetics

Thermodynamics - "motion of heat"
classical science relating heat & work to energy, entropy, temperature
Originally Developed in 1800's before knew about atoms & molecules
thence "laws" of thermodynamics are empirical, but also not violated for sufficiently large systems
These ideas play key roles for understanding behavior of bulk molecular systems ("chemistry")

Already learned most concepts -
This class - formal understanding

of where rules come from, how/
when they apply

Topics include chemical eq,
phase transitions

Kinetics – motion of atoms & molecules

1) how motion of molecules connects
to temperature & pressure

2) Reaction "rates"

will use separate books for this
topic

Statistical Mechanics / Thermodynamics

Late 1800's – now

how do rules of thermo arise when
looking at large collections of molecules

Go from 3N dof → a few properties
(only need to know N, V, E eg)

some rules tell us about single molecules like how does a protein fold (and why / entropy-energy balance)

<u>Mathematics</u> - Language describing the rules. Calculus & probability are key to this topic and deeper understanding of chem & bio

will review this week & use throughout

[who took math for chem?]

<u>Data & programming</u> - Real research is done by using experimental equipment, recording data, and ascertaining trends

This is true for chem, bio, econ & anything else

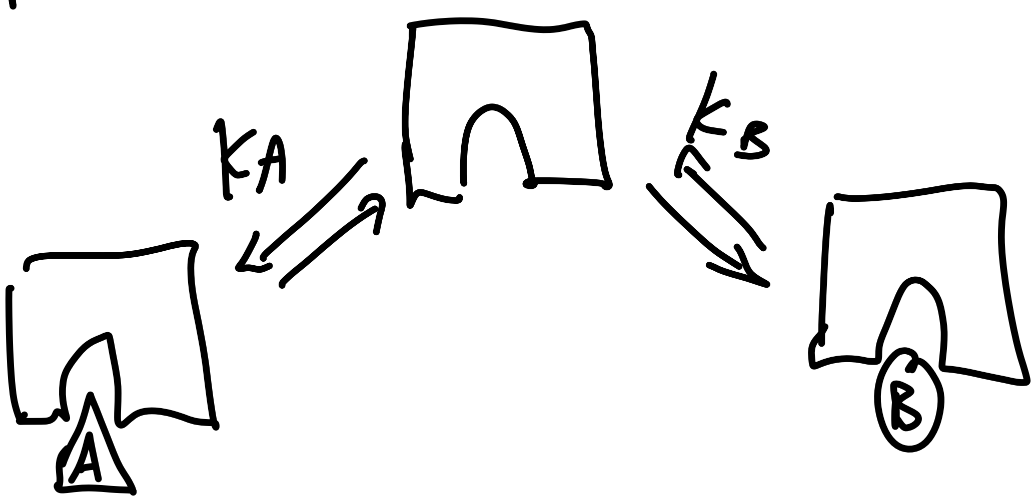
Simple programming lets us test ideas with "models"

Also "fit" data to "theory" to get parameters (recitation)

Probability Rd Page 1-19

Probability plays a major role in Stat. Mech. (end of course) but also in other areas of thermo & biochem Including properly analyzing data w/ Stats.

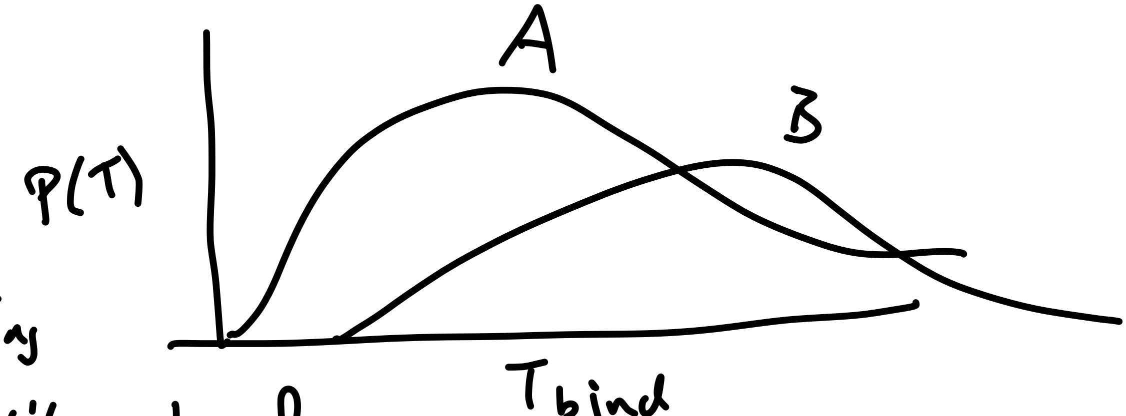
Example (1.2 in book) from chemical Eq



What fraction of molecules are unbound?
(later)

Example 2:

(made up)
time of binding



How long until unbound mc binds A or B on average?

Going to cover:

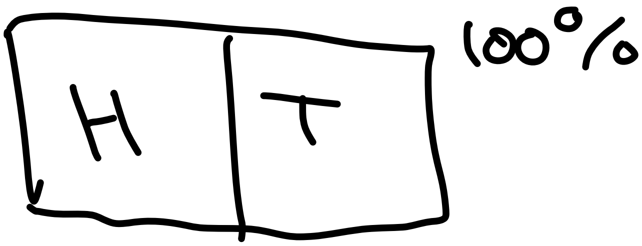
- <u>discrete</u> set of events
- <u>continuous</u> distributions (next time)
- do exercise work sheet

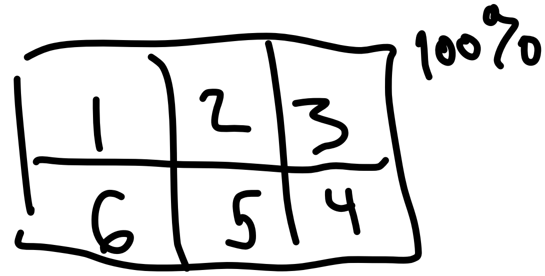
Independent events:

Probabilities don't effect one another

Flipping coin very important example (or rolling die, etc)

Exclusive outcomes for 1 event

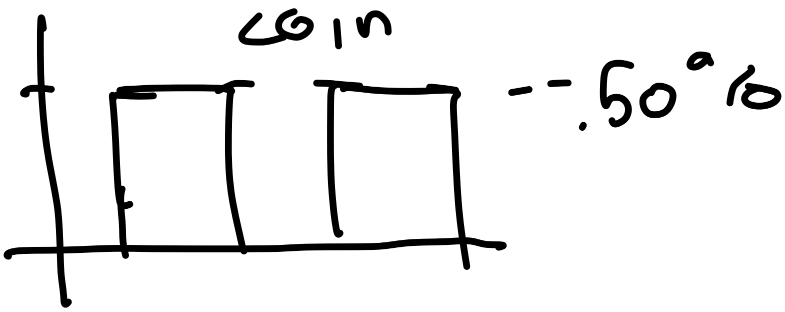


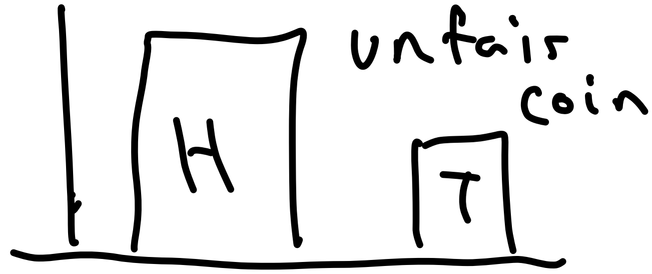


So for 1 event

$$1 = P_H + P_T \quad \text{or} \quad 1 = P_1 + P_2 + \dots + P_6$$

In general, discrete out comes plot as bar chart for probs



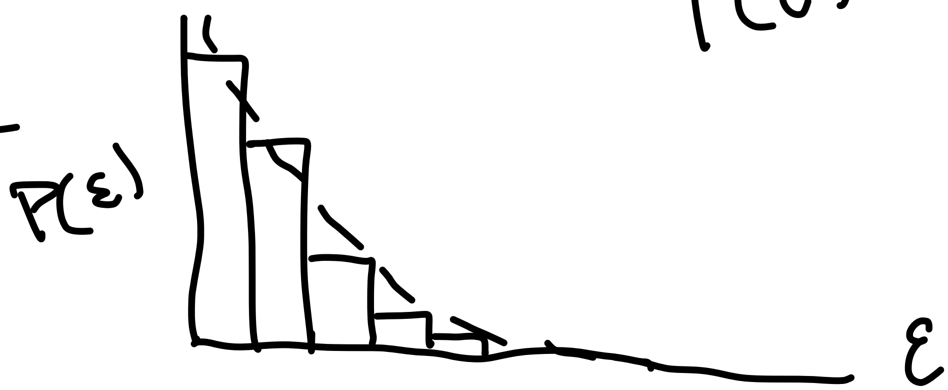


particle in a box

$$\varepsilon = \frac{h^2 n^2}{8mL^2}$$

$$P(\varepsilon) \propto e^{-\varepsilon/k_BT}$$

Can only be in 1 state

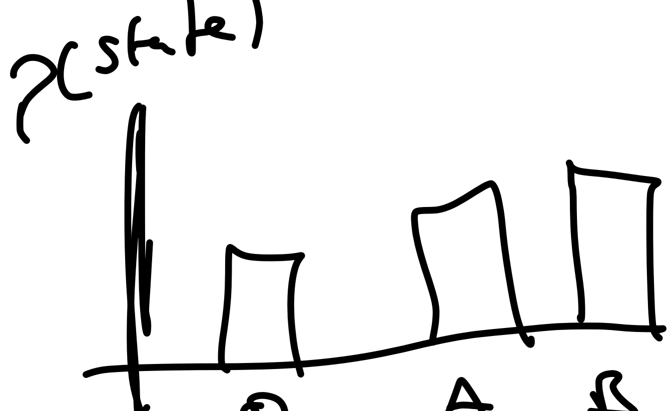


or

notation

$$1 = \sum_{n=1}^{\infty} P(n)$$

Prev example O, A, B



Probabilities combine with logical operations

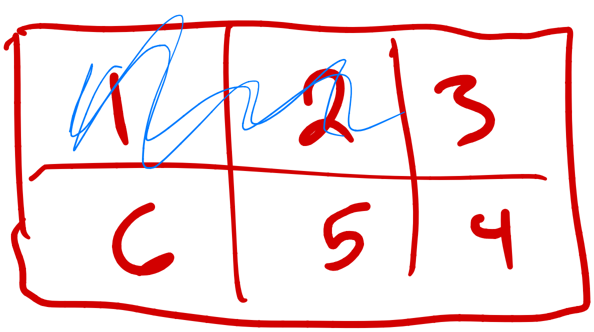
And "$\cap$"

Or "$\cup$" (in book <=> xor
Either A or B not both)

for dicrete states, what happens for and & or? [and multually exclusive outcomes]

$P_{n=1} \cap P_{n=2} = ?$ (0)

$P_{n=1} \cup P_{n=2} = ?$ $(P_{n=1} + P_{n=2})$

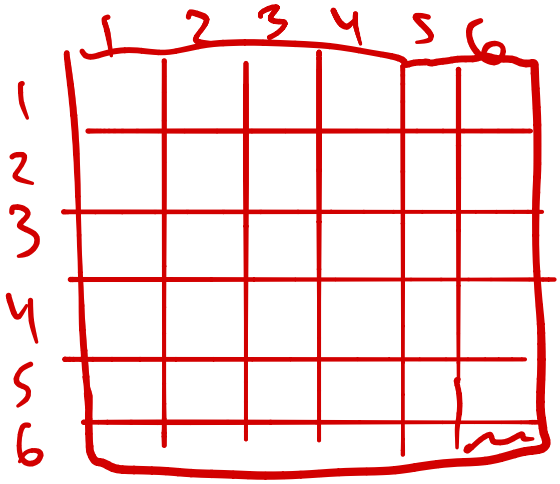


$2/6 = 1/3$

Probabilities of Independent Outcomes of separate events combine w/ these opperations too, but be careful, in a diff way

Example: 2 people each roll a die
what is prob of 2 sixes?

Combine into a single event to see rule



1/36 possible events

general rule for ind outcomes

$P_{A \cap B} = P_A \times P_B$