Physics 114 **Statistical Mechanics** **Spring 2018**

Seminar 1

Amy's presentation: Thermal Equilibrium

- Time has a natural direction for a large system. Thermodynamic systems *spontaneously approach equilibrium*, as long as they are not prevented from doing so. If already in equilibrium, as long as they are not perturbed, systems will remain there.
  Example:

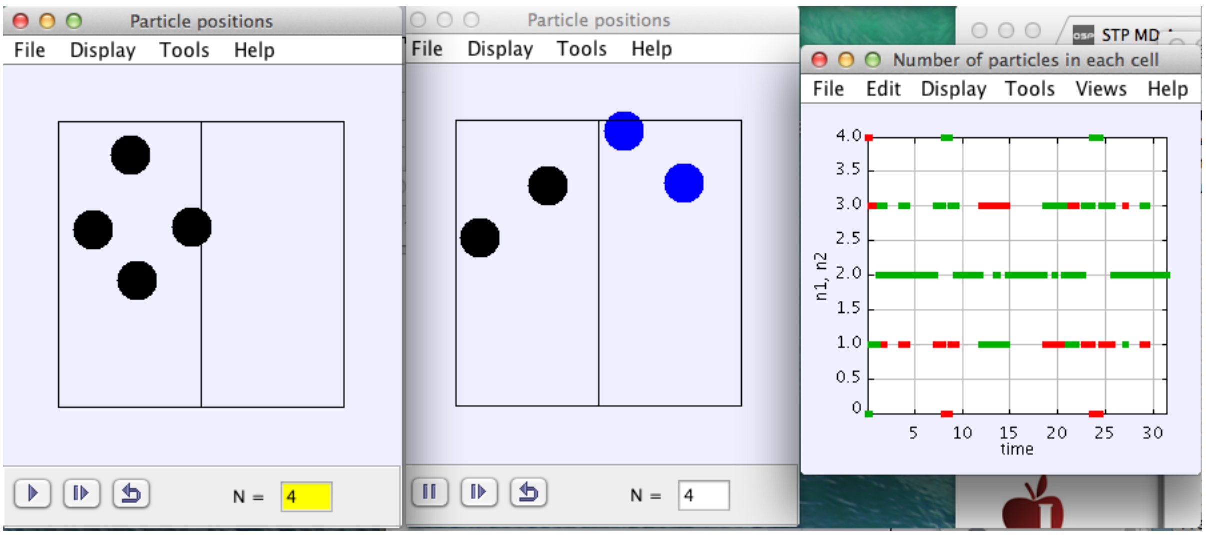


Figure 1: Starting configuration shown on left, snapshot during evolution shown on right. For a tiny system, there really is no "arrow of time". Collisions are individually time-reversible. With such a tiny system, there is no evolution toward a type of state involving all particles that is more dramatically likely than another. Further, hitting "reverse" which reverses time in the sense that all velocity vectors reverse their direction, will bring us back to an initial state. (This code is stp_MDApproachToEquilibriumTwoParitions.jar)

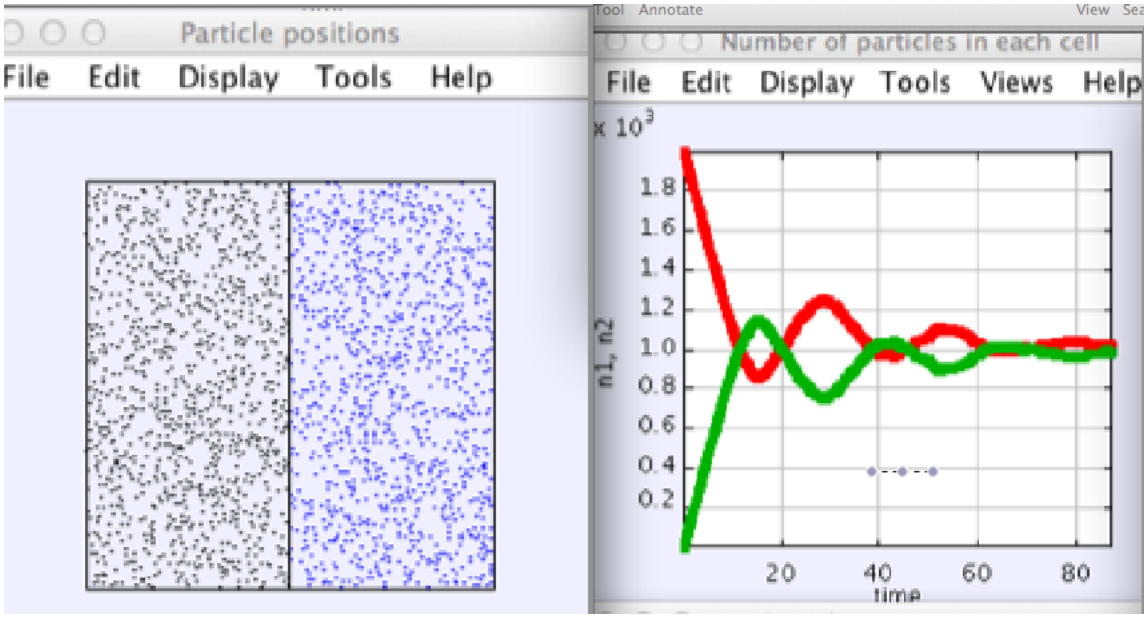


Figure 2: For a large system, there really is an "arrow of time". Collisions are individually time-reversible, but the trend toward more probable macro states - the ones with more microstates contributing to them - makes the system flow to a set of configurations representative of equilibrium. There is no way to reverse this arrow of time, due to inevitable uncertainties. These are due to quantum mechanics in the real world, and due to finite numerical precision in the digital world.

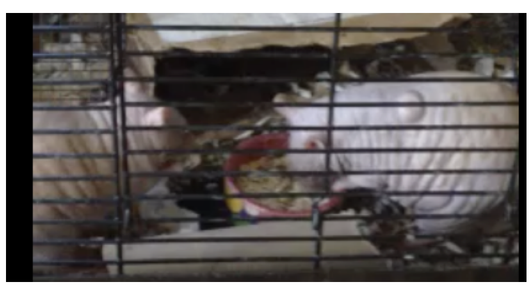


Figure 3: Here are two rats sharing a bowl of oatmeal. Can we detect whether a video of these rats is run forward or backward ... which way is the arrow of time is pointing? If you know some rat psychology, you can tell that indeed, the arrow of time points so that each rat pulls the bowl toward himself, not pushes it toward the other rat. Sharing is caring! ;-P

- There are multiple kinds of equilibria. Energy, volume, number of particles in a certain part of the system, and more ... are macroscopic properties that can equilibrate.

- In equilibrium we observe a mean, or average, value of macroscopic properties that we don't constrain to have precise values.
  Example:

  - If we have a box of volume V containing N particles of an idealized gas at temperature T, then the *expected* or *average* value of the pressure is $\bar{P} = NkT/V$.
  - If we have a cylinder under pressure P containing N particles of an idealized gas at temperature T, then expected value of the volume is $\bar{V} = NkT/P$.
  - If we have a box of volume V containing photons at a temperature T then the average number of photons *and* the average pressure are set by thermal equilibrium conditions. It turns out that $\bar{P} = \frac{\zeta(4)}{\zeta(3)}\bar{N}kT/V$. Approximately: $\bar{P} = 0.9\ \bar{N}kT/V$.

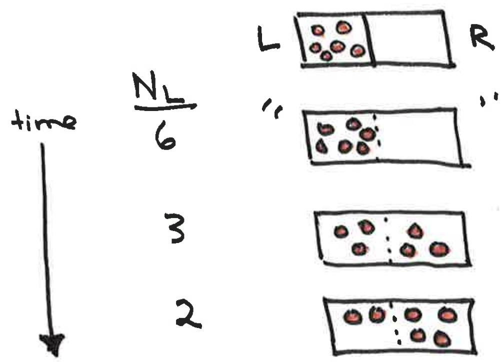
- Equilibrium is a situation in which disorder is maximized, subject to constraints. **see Example on next page**

- If two systems are in thermodynamic equilibrium with each other, there are no net macroscopic flows of matter or of energy between them. For a single system in equilibrium, no such flows exist between the parts of that system.

- *Entropy* is a quantity that correlates with disorder ... is larger for macrostates that correspond to larger numbers of microstates ... and is maximized in equilibrium, subject to constraints. *Example: Beans (next page)*

Example: Distinguishable red beans

Say have $N = 6$ beans.
Say macrostate is N_L, the number on left side of box once partition is removed. Box is shaken ...



With partition in place...

in equilibrium? No

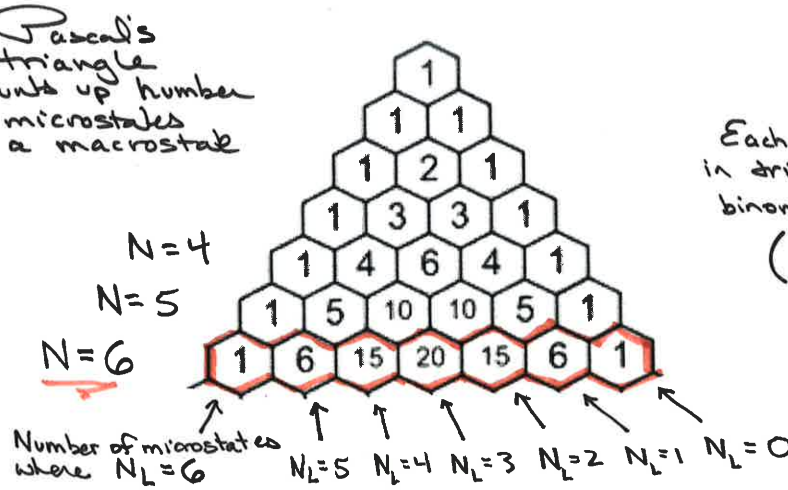
Yes

Yes

The "arrow of time" involves transfer of energy, particles, information, ... from fewer degrees of freedom to more degrees of freedom. (Here, there are just two degrees of freedom, L and R.)

Microstate is which beans of #1, #2, #3, #4, #5, #6 are on L side of box.

Pascal's triangle counts up number of microstates in a macrostate



Each entry in triangle is binomial coefficient

$$\binom{N}{N_L} = \frac{N!}{N_L!\,(N-N_L)!}$$

Entropy of beans

Entropy S, is larger for a macrostate with more associated microstates. Call the number of micro's in a macro Ω. Here $\Omega = 20$ is the largest; it corresponds to the largest S and thus the associated macrostate with $N_L = 3$ is the average: $\overline{N_L} = 3$. There will be fluctuations around this average however.

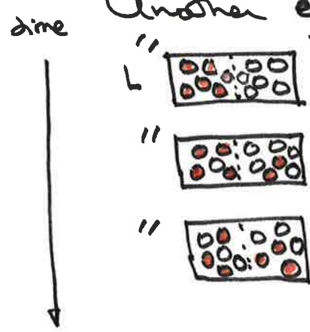
Another example: Red and White beans

here $N^R = 6$

$N^W = 6$

Macrostate: (N^R_L, N^W_L)

time



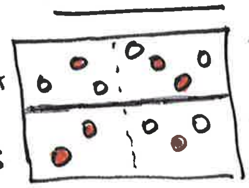
Entropy S is a measure of disorder

S is

→ Extensive: eg. double the total number of red beans & white beans ⇒ you double S

→ Additive: Macrostate: $(N^R_{LA}, N^R_{LB}, N^W_{LA}, N^W_{LB})$

Box A L_A R_A



Box B L_B R_B

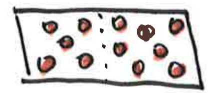
← boxes are separated by partition

$$S_{TOT} = S_A + S_B$$

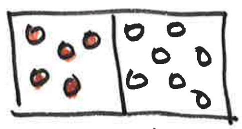
macrostate (N^R_{LA}, N^W_{LA}) (N^R_{LB}, N^W_{LB})

→ for indistinguishable beans *

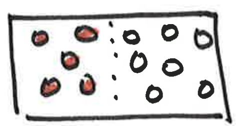
time

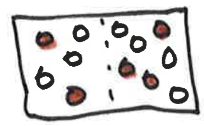
L:  R has same microstate (as well as same macrostate) as "  "

But

L  R

and

L  R

have a different microstate from "  "

$S_{unmixed} < S_{mixed}$

There is an entropy of mixing

* red & white are two different species of bosons