

February 1, 2013

Physics 132

Prof. E. F. Redish

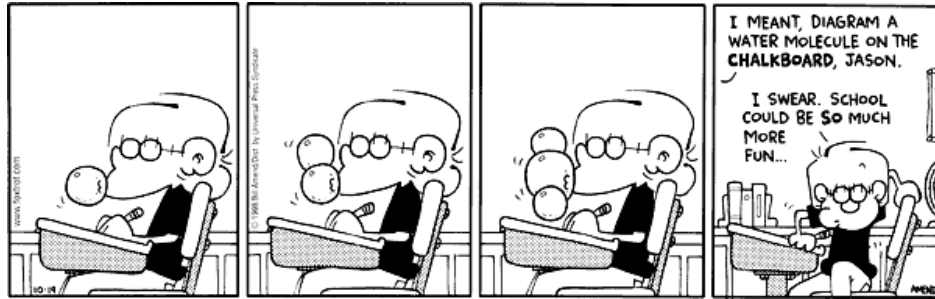
■ Theme Music: Robert Alda

Luck be a lady

From "Guys & Dolls"
original cast recording

■ Cartoon: Bill Amend

FoxTrot



Foothold ideas: Inter-atomic interactions



- The interaction between atoms arises from the combination of the electrical forces of its components (electrons and nuclei).
 - It can be quite complex and involve electron sharing and chemical bonds.
 - The complexity arises from the quantum character of electrons.
- Despite this complexity, a simple potential model summarizes many features of a two-atom interaction.

2/1/13

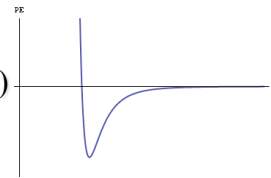
3

Physics 132

Foothold ideas: Inter-atomic potentials



- The interaction between neutral atoms includes an attraction at long-range that arises from the fluctuating charge distribution in each atom; the PE behaves like $1/r^6$.
- When the atoms are pressed close, they repel each other strongly; both because the +nuclei repel and because of the Pauli principle (two electrons cannot be in the same state).
- Two commonly used models are:
 - The Lennard-Jones potential ($A/r^{12}-B/r^6$)
 - The Morse potential (exponentials)



2/1/13

4

Physics 132

Emergence

- Emergence means that a phenomenon that is essentially invisible or undetectable when looked at “in the small” builds up in a coherent fashion as the system you look at gets larger.
- At the large scale, the result is of great (even dominant) importance.

2/1/13

Physics 132

6

Example of Emergence

■ Evolution

- If a single species of birds on an isolated island have a range of bill thicknesses, they may all survive and interbreed well under normal circumstances.
- If the climate shifts so that the birds at the two extremes are more likely to survive than those in the middle – by only a little bit! – after a few decades the population may consist only of birds with only the smallest and largest bills.
- If the climate now stays shifted, after a few millenia, genetic drift can take the two populations apart so that they can no longer interbreed and would be identified as different species.
- The shift may not be visible over a few generations.

2/1/13

Jonathan Weiner, *The Beak of the Finch*

8

Foothold principles: Randomness

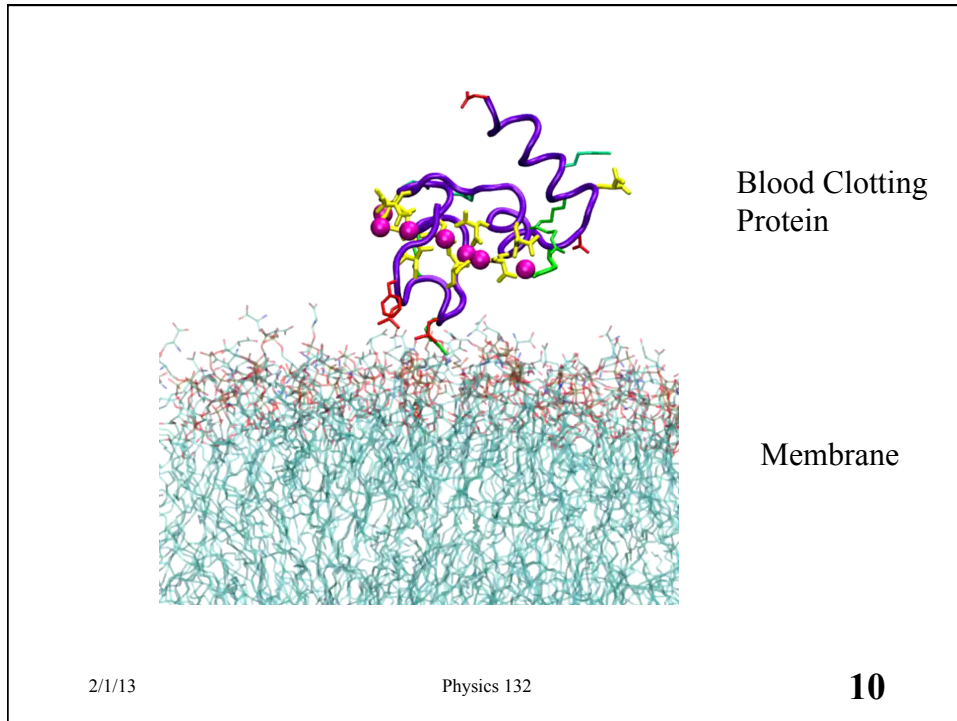


- Matter is made of of molecules in constant motion and interaction. This motion moves stuff around.
- If the distribution of a chemical is non-uniform, the randomness of molecular motion will tend to result in molecules moving from more dense regions to less.
- This is not directed but is an emergent phenomenon arising from the combination of random motion and non-uniform concentration.

2/1/13

Physics 132

9




Fick's law: a simplified model of diffusion

- The red molecules do a random walk (as a result of collisions with fluid molecules)
- Assume
 - Uniform density in each bin
 - Ignore up/down motions
 - Move with uniform (average) velocity
 - Choose bin width to be average distance red molecule travels before colliding.
 - Ask net amount going through a surface of area A in a time

2/1/13 Physics 132 11

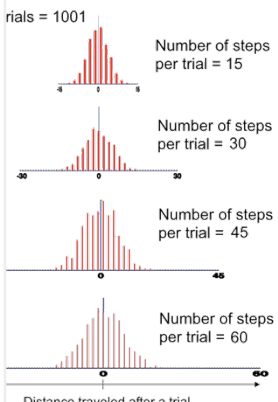
Foothold ideas: Random walk in 1D



- As a result of random motion, an initially localized distribution will spread out, getting wider and wider. This phenomenon is called *diffusion*
- The width of the distribution will grow like

$$\langle (\Delta x)^2 \rangle = 2Dt$$

- D is called *the diffusion constant* and has dimensionality $[D] = L^2/T$



trials = 1001

Number of steps per trial = 15

Number of steps per trial = 30


Number of steps per trial = 45

Number of steps per trial = 60

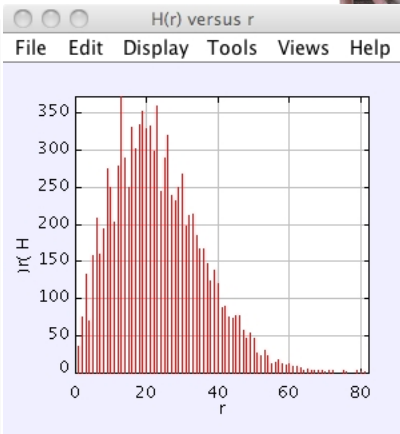
Distance traveled after a trial

12

Foothold ideas: Random walk in 2D



- The density of walkers decreases uniformly as you get farther from the source.
- The total number within a given radius peaks – since the area within a radius r decreases to 0 as r gets small. (“phase space”)
- The width of the peak grows with the square root of time.



- In 2D: $\langle (\Delta r)^2 \rangle = \langle (\Delta x)^2 \rangle + \langle (\Delta y)^2 \rangle = 4Dt$

2/1/13 Physics 132

13

Key idea for the 2nd Law

- The critical idea for the second law of thermodynamics is that in a thermal system (lots of things moving randomly) energy can be in various places and moves around through interactions.
- If more is in one place than another, the random motion will tend to spread it around – even it out. This is just like the diffusion of particles.

2/1/13

Physics 132

14

Foothold ideas: Thermal Equilibrium & Equipartition



- Degrees of freedom – where energy can reside in a system.
- Thermodynamic equilibrium is dynamic. Changes keep happening, but equal amounts in both directions.
- Equipartition – At equilibrium, the same energy density in all space and in all DoFs.

2/1/13

Physics 132

15

Foothold ideas: Microstate and macrostates



- A *microstate* is a specific distribution of energy telling how much is in each DoF.
- A *macrostate* is a statement about some average properties of a state (pressure, temperature, density,...).
 - A given macrostate corresponds to many microstates.
- If the system is sufficiently random, each microstate is equally probable. As a result, the probability of seeing a given macrostate depends on how many microstates it corresponds to.

2/1/13

Physics 132

16

Reading questions

- I learned this [microstates] in general chemistry, but I do not quite understand what a macrostate is. I only learned microstate and I don't understand what it means from the explanation? Can you clarify?
- In the reading, it states that when we look at a system at a large scale "the only macrostate that we ever see is the most probable one." Does this mean that after a while we will only see that macrostate or does it mean that that macrostate will occur so often that we can't really tell what others occurred?
- I can see how it is possible to find the macrostate from the microstate, but can the reverse be done too...can you find the microstate from the macrostate? Or can you only guess what the possible microstates are?

2/1/13

Physics 132

17