- **<u>Theme Music:</u> Duke Ellington**
  Take the A Train
- **<u>Cartoon:</u> Lynn Johnson**
  For Better or for Worse

Foothold principles: Newton's Laws

- Newton 0:
  - An object responds **only** to the forces it feels and only at the instant it feels them.
- Newton 1:
  - An object that feels a net force of 0 keeps moving with the same velocity (which may = 0).
- Newton 2:
  - An object that is acted upon by other objects changes its velocity according to the rule

$$\vec{a}_A = \vec{F}_A^{net} / m_A$$

- Newton 3:
  - When two objects interact the forces they exert on each other are equal and opposite.

$$\vec{F}_{A\to B}^{type} = -\vec{F}_{B\to A}^{type}$$

Foothold ideas: Kinetic Energy and Work

- Newton's laws tell us how velocity changes. The Work-Energy theorem tells us how speed (independent of direction) changes.
- Kinetic energy = $\frac{1}{2}mv^2$
- Work done by a force = $F_x \Delta x$ or $F_{||}\Delta r$ (part of force || to displacement)
- Work-energy theorem: $\Delta(\frac{1}{2}mv^2) = F_{||}^{net}\ \Delta r$ (small step)

$$\Delta(\tfrac{1}{2}mv^2) = \int_i^f F_{||}^{net}\ dr \quad \text{(any size step)}$$

Foothold ideas: Potential Energy

- The work done by some forces only depends on the change in position. Then it can be written

$$\vec{F} \cdot \Delta\vec{r} = -\Delta U$$

U is called a *potential energy*.

- For gravity, $U_{gravity} = mgh$

For a spring, $U_{spring} = \frac{1}{2} kx^2$

For electric force, $U_{electric} = k_C Q_1 Q_2 / r_{12}$

- Potential to force:

$$\vec{F} = -\frac{\Delta U}{\Delta\vec{r}} = -\left(\frac{\partial U}{\partial x}\hat{i} + \frac{\partial U}{\partial y}\hat{j} + \frac{\partial U}{\partial z}\hat{k} \right) = -\vec{\nabla} U$$

The force associated with a PE at a given place points "downhill" – in the direction where the PE falls the fastest.

Foothold ideas: Energy

- Kinds of energy (macro)
  - Kinetic
  - Potential
  - Thermal
  - Chemical
- Kinds of energy (micro)?
- First law of thermodynamics
  - Conservation of total energy

Internal energy

Thermal energy entering

Work done on the rest of the world

$$\Delta U = Q - W$$

Energy needed to add internal energy at constant pressure (Enthalpy)

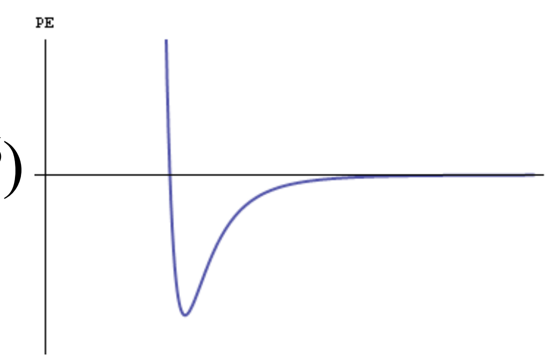
$$\Delta H = \Delta U + p\Delta V$$

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.

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)



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.

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.

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.

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.
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Foothold ideas: Entropy

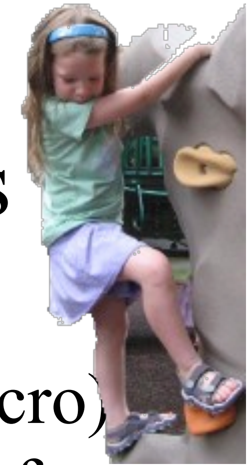
- ***Entropy*** – an extensive measure of how well energy is spread in an object.
- ***Entropy measures*** –
  - The number of microstates in a given macrostate

$$S = k_B \ln(W)$$

  - The amount that the energy of a system is spread among the various degrees of freedom
- ***Change in entropy*** upon heat flow

$$\Delta S = \frac{Q}{T}$$

Foothold ideas:
The Second Law of Thermodynamics



- Systems composed of a large number of particles spontaneously move toward the thermodynamic (macro) state that correspond to the largest possible number of particle arrangements (microstates).
  - The 2nd law is probabilistic. Systems show fluctuations – violations that get proportionately smaller as N gets large.
- Systems that are not in thermodynamic equilibrium will spontaneously transform so as to increase the entropy.
  - The entropy of any particular system can decrease as long as the entropy of the rest of the universe increases more.
- The universe tends towards states of increasing chaos and uniformity. (Is this contradictory?)

Foothold ideas: Transforming energy

- Internal energy: thermal plus chemical ΔU
- Enthalpy: internal plus amount needed to make space at constant p $\Delta H = \Delta U + p\Delta V$
- Gibbs free energy: enthalpy minus amount associated with raising entropy of the rest of the universe due to energy dumped $\Delta G = \Delta H - T\Delta S$
- A process will go spontaneously if $\Delta G < 0$.

Spontaneity…

$$\Delta G = \Delta H - T\Delta S$$

$-T\Delta S_{total}$ → ΔG

$-T\Delta S_{surroundings}$ → ΔH

$T\Delta S_{system}$ → $T\Delta S$

The sign of the Gibbs Free Energy change indicates spontaneity!

$\Delta G < 0$ → $\Delta S_{total} > 0$ → spontaneous

$\Delta G > 0$ → $\Delta S_{total} < 0$ → not spontaneous

Foothold ideas: Energy distribution

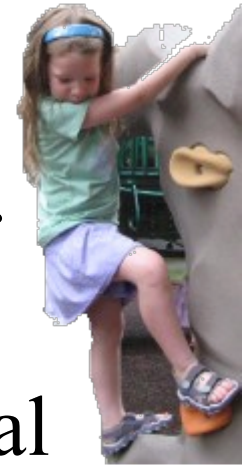
- Due to the randomness of thermal collisions, even in (local) thermal equilibrium a range of energy is found in each degree of freedom.
- The probability of finding an energy E is proportional to the Boltzmann factor

$$P(E) \propto e^{-E/k_B T} \quad \text{(for one DoF)}$$

$$P(E) \propto e^{-E/RT} \quad \text{(for one mole)}$$

- At 300 K, $k_B T \sim 1/40$ eV
  $N_A k_B T = RT \sim 2.4$ kJ/mol

Foothold ideas: Charge – A hidden property of matter



- Matter is made up of two kinds of electrical matter (positive and negative) that usually cancel very precisely.
- Like charges repel, unlike charges attract.
- Bringing an unbalanced charge up to neutral matter polarizes it, so both kinds of charge attract neutral matter
- The total amount of charge (pos – neg) is constant.

Foothold ideas: Conductors and Insulators

- Insulators
  - In some matter, the charges they contain are bound and cannot move around freely.
  - Excess charge put onto this kind of matter tends to just sit there (like spreading peanut butter).
- Conductors
  - In some matter, charges in it can move around throughout the object.
  - Excess charge put onto this kind of matter redistributes itself or flows off (if there is a conducting path to ground).

Foothold idea: Coulomb's Law

- All objects attract each other with a force whose magnitude is given by

$$\vec{F}_{q\to Q} = -\vec{F}_{Q\to q} = \frac{k_C qQ}{r_{qQ}^2}\hat{r}_{q\to Q}$$

- k_C is put in to make the units come out right.

$$k_C = 9\times 10^9 \text{ N-m}^2/\text{C}^2$$

Foothold ideas: Energies between charge clusters

- Atoms and molecules are made up of charges.
- The potential energy between two charges is

$$U_{12}^{elec} = \frac{k_C Q_1 Q_2}{r_{12}}$$

No vectors!

- The potential energy between many charges is

$$U_{12...N}^{elec} = \sum_{i<j=1}^{N} \frac{k_C Q_i Q_j}{r_{ij}}$$

Just add up all pairs!

Foothold idea:
Fields

- *Test particle*
  - We pay attention to what force it feels.
    We assume it does not have any affect on the source particles.
- *Source particles*
  - We pay attention to the forces they exert and assume they do not move.
- *Physical field*
  - We consider what force a test particle would feel if it were at a particular point in space and divide by its coupling strength to the force. This gives a vector at each point in space.

$$\vec{g} = \frac{1}{m}\vec{W}_{E\to m} \qquad \vec{E} = \frac{1}{q}\vec{F}_{\text{all charges}\to q} \qquad V = \frac{1}{q}U^{elec}_{\text{all charges}\to \text{q}}$$

Foothold ideas:
Electric potential energy and potential

- The potential energy between two charges is

$$U_{12}^{elec} = \frac{k_C Q_1 Q_2}{r_{12}}$$

- The potential energy of many charges is

$$U_{12...N}^{elec} = \sum_{i<j=1}^{N} \frac{k_C Q_i Q_j}{r_{ij}}$$

- The potential energy added by adding a test charge q is

$$\Delta U_q^{elec} = \sum_{i=1}^{N} \frac{k_C q Q_i}{r_{iq}} = qV$$

= the voltage at the position of the test charge

Units

- Gravitational field
  units of g = Newtons/kg
- Electric field
  units of E = Newtons/C
- Electric potential
  units of V = Joules/C = Volts
- Energy = qV so $e\Delta V$ = the energy gained by an electron (charge $e = 1.6 \times 10^{-19}$ C) in moving through a change of ΔV volts.
  1 eV = 1.6×10^{-19} J

Foothold ideas: Electric charges in materials

- The electric field inside the body of a static conductor (no moving charges) is zero.
- The entire body of a static conductor (no charges moving through it) is at the same potential.
- The average electric field in an insulator is reduced (due to the polarization of the material by the field) by a factor that is a property of the material: the dielectric constant, κ. (Sometimes written in biology as ε) Since κ is the ratio of two fields, it is dimensionless.

Foothold ideas: Capacitors

$$\Delta V = E\Delta x = Ed$$

$$E = 4\pi k_C \sigma = 4\pi k_C \frac{Q}{A} \quad \Rightarrow \quad Q = \left(\frac{A}{4\pi k_C}\right) E$$

$$Q = \left(\frac{A}{4\pi k_C d}\right) \Delta V$$

$$Q = C\Delta V$$

What does this "Q" stand for?

$$C = \frac{\kappa \varepsilon_0 A}{d}$$

If plates are separated by a material

Energy stored $= \frac{1}{2} Q\Delta V$