

Topics for Today

- Case Studies in Thermal Physics
 - An Ideal Gas
 - Distribution of Molecular Velocities
 - The Ising Model of a Magnetic Film
 - Phase Transitions

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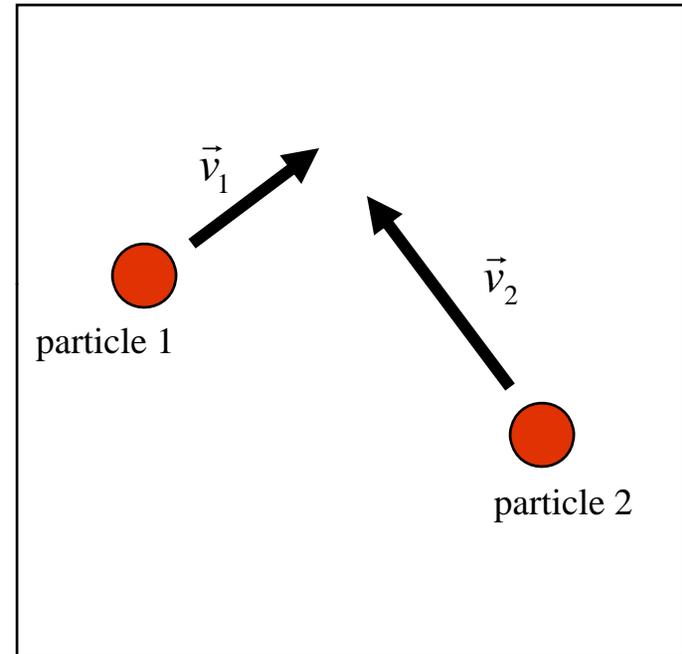
An Ideal Gas

- A system consisting of N molecules of mass m in a rigid box with energy E
- When the density of the gas is low, the particles move freely most of the time.

Particle collisions are rare.

The particles' kinetic energies account for essentially all of the system's energy.

- They account for all of the system's energy in the “ideal gas” approximation



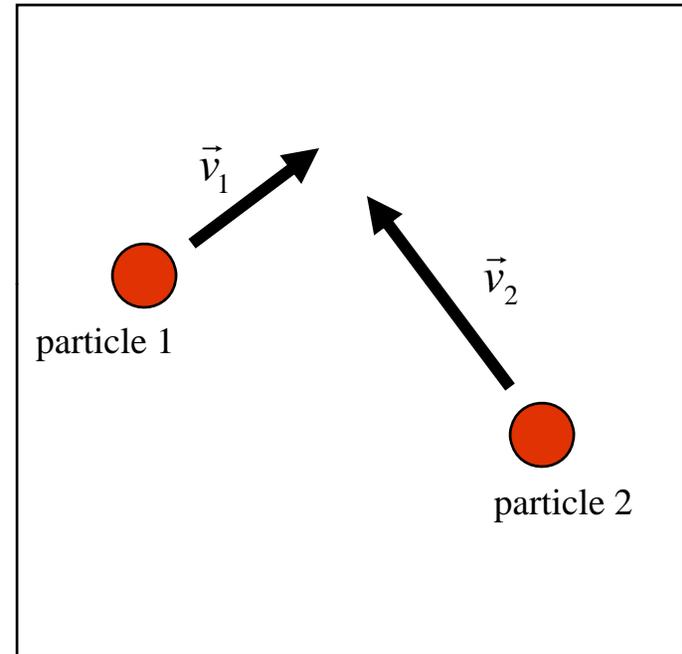
An Ideal Gas

- Since the energy of our ideal gas is

$$E = \frac{m}{2} \sum_{i=1}^N v_i^2,$$

each of its microstates can be represented by a list of the N particle velocities

- On average, the left-right, forward-back and up-down motions of particles in the gas are the same, so, we can deal separately with just one of them. We will, therefore, simulate an ideal gas in one-dimension.



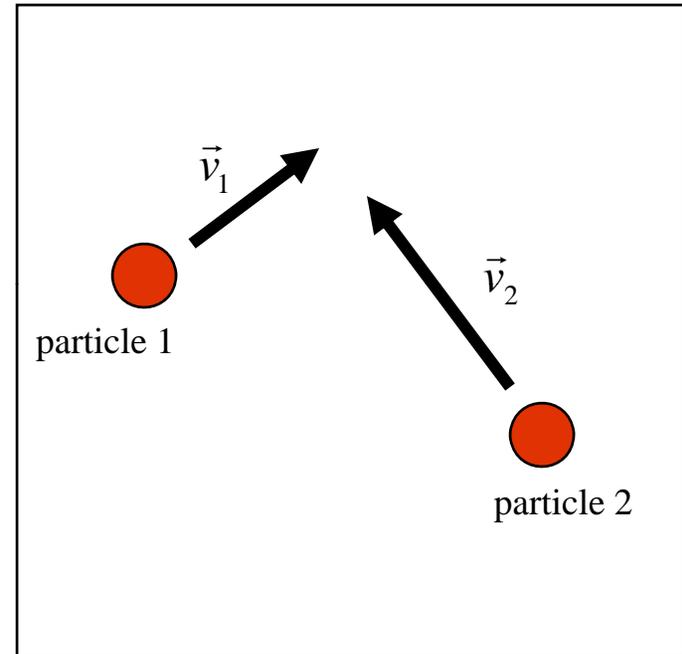
An Ideal Gas

- Each microstate of our 1d gas can be represented by list of numbers representing the velocities of the N molecules in that state

$$[v_1, v_2, \dots] = [535.4, -245, \dots] \text{ m/s}$$

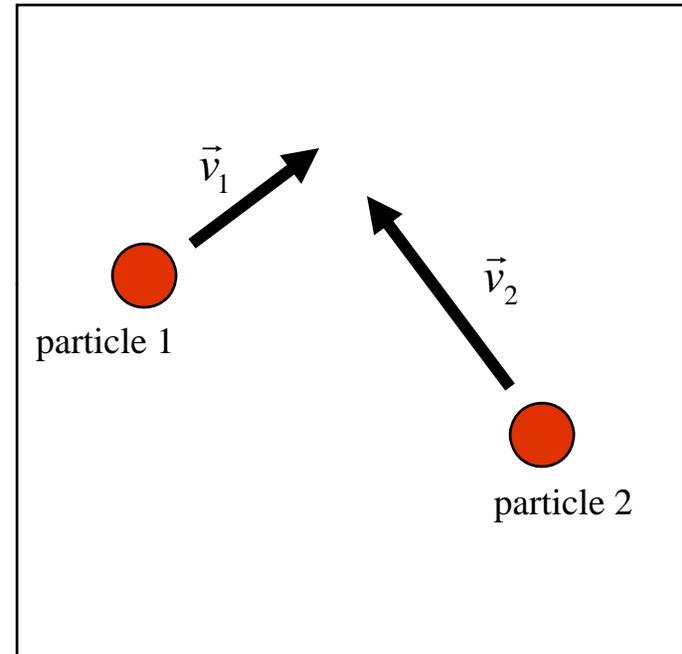
- The only constraint on these lists of N numbers is that the corresponding kinetic energies of the particles add up to the system energy

$$E = \frac{m}{2} \sum_{i=1}^N v_i^2$$



An Ideal Gas in Equilibrium

- Every possible microstate of our 1d gas with energy E is equally likely
- A random sampling yields mostly microstates with the energy spread as evenly as possible among the gas molecules because these states are most numerous.
- we can use such sampled states to estimate average properties of our gas because random measurements of the real gas system would yield a similar microstate sample.



Demon Algorithm Simulation: 1d Ideal Gas

- Start:

Specify an initial microstate of the combined gas-demon system that has the energy E of the gas we want to simulate.

No matter what state we start with the random changes the demon algorithm makes will quickly produce members of the most numerous class of microstates with energies spread as evenly as possible among the molecules.

We may as well assign each gas particle the same initial velocity so that each has one N^{th} of the energy E and assign the demon no initial energy.

Generate New Microstates Using the Demon Algorithm

Select a particle at random and consider making a random change in its velocity component, ΔV . The corresponding change in the energy of the particle is

$$\Delta E = \frac{m}{2}(V + \Delta V)^2 - \frac{m}{2}V^2$$

If this is negative, accept the change (the new microstate) and increase the demon's energy by a corresponding amount so that the energy of the combined gas-demon system does not change.

If it is positive and less than or equal to the demon energy, accept the change (the new microstate) and decrease the demon's energy by a corresponding amount so that the energy of the combined gas-demon system does not change.

If it is positive and greater than the demon energy, do not accept the change (the new microstate) and try again.

Monte Carlo Simulation Using the Demon Algorithm

A “step” in a Monte Carlo simulation of an N -particle gas consists of N of these trials.

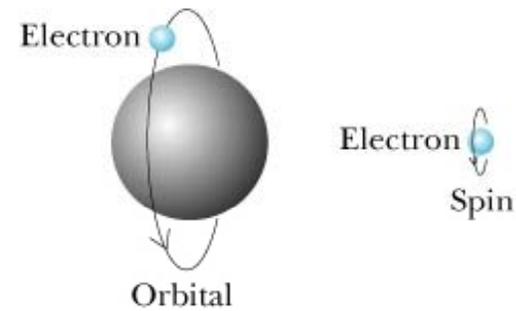
After each “step” you store or display information about the microstate of the gas needed to predict the gas properties you are interested in. For example, as we discussed last time, you can use the distribution of demon energy that accumulates during a simulation to estimate the temperature of the gas.

After a specified number of “steps” you stop the simulation and display results.

Magnetic Systems

Magnetic fields are generated by electric currents.

Atoms can generate such fields because of the currents circulating within them and within the particles they are made of.



The magnetic fields generated by single atoms are minute, but if many of them are aligned so that currents circulate in the same direction, then the magnetic fields can add up to become significant.



Remember how big Avogadro's number is!

Thermal Phase Transitions

Atoms in ferromagnetic materials like iron and nickel interact in ways that keep atoms aligned in this way at ordinary temperatures.

If you heat these materials, you discover that each has a critical temperature above which the atoms no longer remain aligned.

The materials are not magnetized above their Curie temperatures.

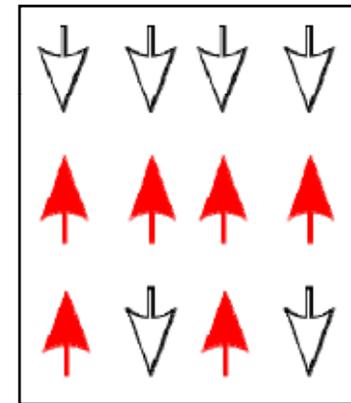
Let's look briefly at a simple model that predicts this interesting behavior.

Magnetic Systems and the 2d Ising Model

A tractable project simulates the behavior of a magnetic film with simple interactions between its atoms.

Arrange atoms in a regular rectangular lattice to represent the film.

Ising-model atoms have their magnetic orientations point up or down. The arrows in this figure represent one microstate of a 3 by 4 lattice of “spins”.



$$M = \mu \sum_{i=1}^N s_i$$

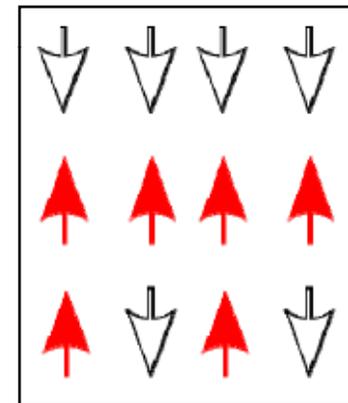
The magnetization of the system is the (vector) sum of the magnetization of its atoms.

The Energy of an Ising Film

To predict the equilibrium properties of the magnetic film we must know the energies of its possible microstates.

The energy of an Ising film is the sum of contributions representing the interactions between each spin and its nearest neighbors

$$E = -\frac{J}{2} \sum_{i=1}^N \sum_{j=nn(i)} S_i S_j$$

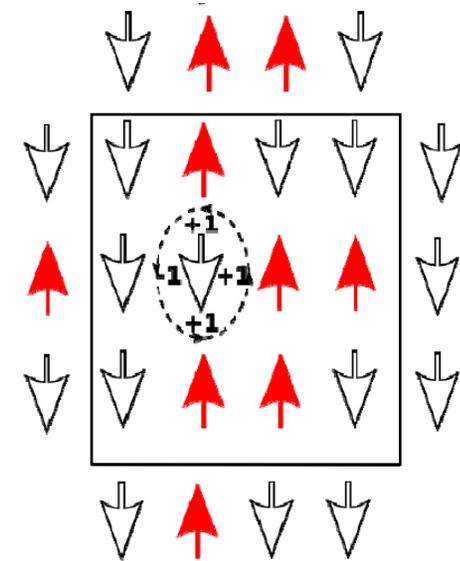


The “coupling constant” J is positive for a ferromagnetic film. The energy of a spin that is aligned with its neighbors is then lower than when it points in opposite direction.

What About Spins on the Edges?

Did you notice that spins at an edge of a finite Ising lattice have different environments?

To remove “edge effects” and, so, model a larger magnetic system, we “identify” the grid’s opposite edges so that every spin has 4 nearest neighbors.



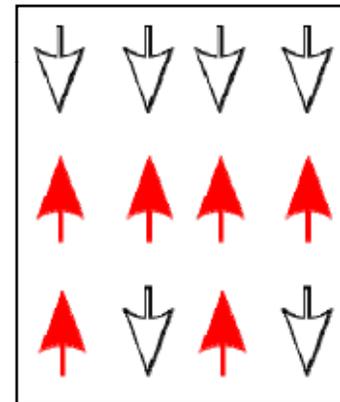
This actually represents a magnetic film on the surface of a torus [donut]!

Monte Carlo Simulation of an Ising Film

Represent a microstate of an n by n lattice of spins by an n by n array of the numbers +1 or -1, representing the “up” or “down” orientation of each spin.

$$\begin{bmatrix} -1 & -1 & -1 & -1 \\ +1 & +1 & +1 & +1 \\ +1 & -1 & +1 & -1 \end{bmatrix}$$

\Leftrightarrow



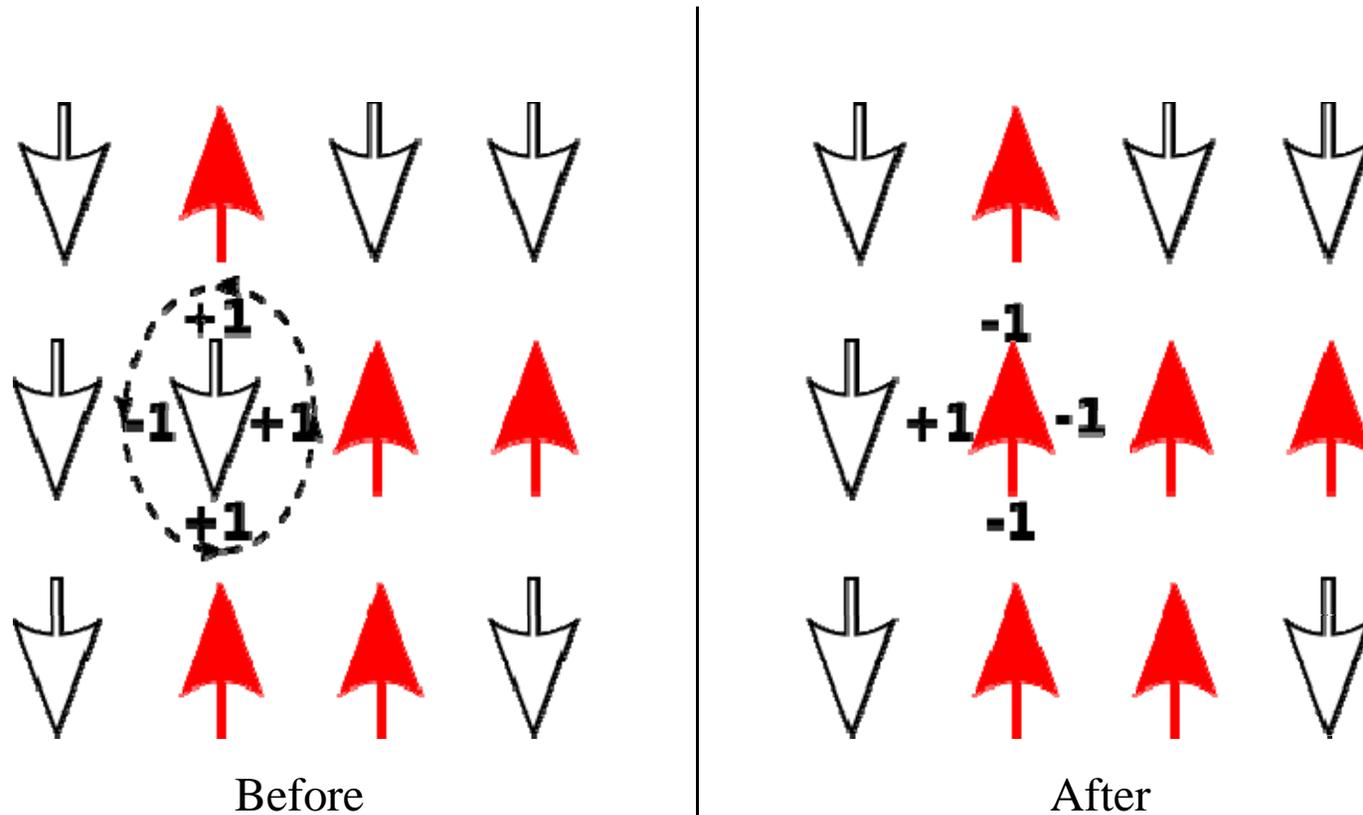
The efficiency of the demon algorithm for Ising systems stems from the fact that we avoid calculating the total system energy at each step.

We need deal with nearest neighbors when computing the energy effect of “flipping” a spin to change microstates.

Generating New Microstates Using the Demon Algorithm

Select an atom at random and consider making a random change in its orientation.

Compute the corresponding change in the energy of the atom. For example,



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$$\Delta E = -4J$$

- If this energy change is negative, accept the change (the new microstate) and increase the demon's energy by a corresponding amount so that the energy of the combined gas-demon system does not change.
 - If it is positive and less than or equal to the demon energy, accept the change (the new microstate) and decrease the demon's energy by a corresponding amount so that the energy of the combined gas-demon system does not change.
 - If it is positive and greater than the demon energy, do not accept the change (the new microstate) and try again.
-

A “step” in a Monte Carlo simulation of an n^2 atom system consists of n^2 of these trials.

After each step, we can compute and display the system's magnetization to see how it behaves when the system is in equilibrium.

We terminate simulation after a specified number of steps.

