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1.1: Background Material

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- kinetic theory of gases
- particle speed in a gas

Understanding the Simulator

To fully grasp what is going on with this lab, a deeper understanding of this simulator is needed. Its intent is to mimic the behavior of a three-dimensional gas, but the medium in which this is done (a flat screen) is two dimensions. This is certainly a visual shortcoming, but is that all, or is something more fundamental involved here? The answer is that it depends upon how you wish to use the program.

The simulator includes both numbers that are displayed and actual particle motions that obey physical laws (elastic collisions). Things get tricky because the numbers displayed can come from either plugging numbers directly into physics equations, or extracted from the results of the simulated motions. In the case of this particular simulator, the gases are modeled accurately, which is to say that the particles of each gas are imbued with their correct masses. These masses, along with a selected user setting (temperature), are used in a physics calculation that assumes three dimensions, and provides another number that is displayed (particle speed). The fact that the simulator is confined to two dimensions never comes into play here, because none of the numbers depends upon the physical nature of two-dimensional motion.

But the simulator allows us to do more, and this additional exploration depends intimately upon the statistical physics of the particle motions, and this includes the fact that they have two degrees of freedom, rather than the previously-assumed three. So although we are inclined to treat this as a three-dimensional simulator based on the purely calculated quantities (and the fact that the masses nicely match those of real gases), we find that this assumption breaks down when we let the simulator behave physically.

One might ask why one would bother to build a laboratory around such a flawed simulator. As you will see, exploring these very flaws turns out to be extremely instructive!

Average Speed vs. RMS Speed

There are many ways to compute a "characteristic" measurement of a quantities from a sample that contains many randomly-distributed such measurements. In this lab, we will be looking at the speeds of particles in a gas. We can define a "typical" speed of such a particle several ways. One way is to take a simple average of the speeds of all the particles. The simulator we are using keeps track of the speeds of all the particles at every moment in time, so computing this average is easy to do, and indeed it displays this average in real time.

Another way to define the speed of a typical particle is in terms of the *root-mean-square*, or *rms* value. This consists of averaging not the speeds of the particles, but rather the *squares* of those speeds. Of course, the average of squares is hardly characteristic of a speed, as this average doesn't even have the proper units. So to complete the calculation, we take the square root of this average. Summarizing the difference between these two measurements of a typical particle's speed:

$$\begin{aligned} v_{ave} &= \frac{1}{N}(v_1+v_2+\dots+v_N) \\ v_{rms} &= \sqrt{\frac{1}{N}\left(v_1^2+v_2^2+\dots+v_N^2\right)} \end{aligned} \tag{1.1.1}$$

There are a couple of important things to point out about these values when it comes to this lab:

1. Notice that if every particle has the same speed ($v_1=v_2=\dots=v$), then these quantities come out exactly equal. At the beginning of a simulation, it is possible to ensure that all the particles start at the same speed, which means that even though the display shows the average speed per particle, we know that this is also the starting rms speed.
2. Suppose instead of measuring the speeds of the particles, we measured their *kinetic energies*. An average of these measurements would look like this (note: all the particles are the same type, and therefore have equal masses):

$$\begin{aligned} KE_{ave} &= \frac{1}{N}(KE_1 + KE_2 + \cdots + KE_N) \\ &= \frac{1}{N}\left(\frac{1}{2}mv_1^2 + \frac{1}{2}mv_2^2 + \cdots + \frac{1}{2}mv_N^2\right) \\ &= \frac{1}{2}m\left[\frac{1}{N}\left(v_1^2 + v_2^2 + \cdots + v_N^2\right)\right] \\ &= \frac{1}{2}mv_{rms}^2 \end{aligned} \tag{1.1.2}$$

The simulator is designed so that all of the collisions between particles are elastic, which means that no matter what happens, the total kinetic energy of all the confined particles remains fixed, which in turn assures that the rms speed of the collection remains fixed, no matter what collisions occur. It is for this reason that when we define a typical speed for a particle in a gas (at given temperature), the definition of "typical" that we use is the rms speed.

These two properties will be useful to know, because we can see what happens when we start with a gas with non-random motion (all the particles at the same speed, not affecting each other), and then "randomize" their motions by allowing them to collide with each other, separating their average and rms speeds.

1.2: Activities

Things You Will Need

All you will need for this lab is the PhET simulator, which you can run now in a separate window.

Configuring the Simulator

Begin with the "Energy" panel of the simulator. Configure it as follows:

- **Open the "Particles" and "Injection Temperature" dropdowns (the "Average Speed" and "Speed" dropdowns should already be open, but if they are not, then open them as well).**
- **Select the units for the Pressure gauge to be kilopascals (kPa).**
- **Uncheck the "Collisions" box in the "Particles" dropdown.**

A few useful features of the simulator to know about:

- All the particles injected into the chamber come in with the same kinetic energy (which is proportional to their "temperature"). The injection temperature can be selected, or by default, the injection temperature is the same as the current temperature of the gas in the chamber.
- You can inject 50 particles at a time of a single variety with the button (fully extending the pump does the same, if you are into the animation). Using the button injects one particle at a time. The similar buttons whose arrows point to the left remove particles in the same number. [These removal buttons are of little use, as they choose particles at random to remove, and may select more "hot" particles than "cold" ones, meaning that while we can add particles without changing the gas temperature, we cannot remove them without changing the gas temperature.]
- You can remove all of the particles from the chamber at once with the button.

Deducing the Simulated Gases

We will start by assuming that this simulator is designed to demonstrate the three-dimensional kinetic theory of gases. Two gases are selected (one that is "heavy," and the other that is "light"), and in an effort to be as accurate as possible, the quantitative read-outs of the simulator are based on the correct masses of these gases.

1. Your task is to determine which of the five gases listed below is represented by the light particles, and which one is represented by the heavy particles. You are of course free to look up properties of these atoms and molecules to help you make this determination.

$$H_2\;,\quad He\;,\quad N_2\;,\quad O_2\;,\quad Ne$$

Timeout for Some Math

We now turn toward the question raised in the Background Material about whether this simulator actually does represent a gas in three dimensions. The Maxwell-Boltzmann distribution function gives us a measure of the probability of finding a random particle that has a speed in a given infinitesimal range:

$$P\left(v \leftrightarrow v+dv\right) = \mathcal{D}\left(v\right)dv \tag{1.2.1}$$

This Maxwell-Boltzmann distribution $\mathcal{D}\left(v\right)$ is derived using the assumption that the particles can "randomly" change their individual velocities, *subject to the constraint* that the sum of their kinetic energies remains fixed. In other words, all collisions (with the walls of the container, and with each other) must be elastic. Our simulator is programmed to exactly follow this constraint. Something else that is hidden within the distribution function is the dimension of the space within which the particles are constrained. What this means is that if you select a random particle from a gas, the probability that it will have a speed between v and $v+dv$ is different if that gas is constrained to two dimensions than if it occupies three dimensions. This is evidenced by the two distribution functions:

$$\begin{aligned} \mathcal{D}_{2d}\left(v\right) &= \alpha\;v\,e^{-\frac{1}{2}\alpha v^2} \\ \mathcal{D}_{3d}\left(v\right) &= \sqrt{\tfrac{2}{\pi}}\;\alpha^{\frac{3}{2}}\;v^2\;e^{-\frac{1}{2}\alpha v^2} \end{aligned} \tag{1.2.2}$$

In both cases, the constant α is defined in terms of the temperature of the gas and the mass of the particles (and the Boltzmann constant k_B):

$$\alpha \equiv \frac{m}{k_B T} \tag{1.2.3}$$

Multiplying each of these by dv gives the probability of selecting a random particle with a speed that falls in the range $v \leftrightarrow v+dv$ for its particular dimension. For what follows below, the following *definite gaussian integrals* will be useful:

$$\begin{aligned} \int_0^\infty x\, e^{-\beta x^2}\, dx &= \tfrac{1}{2}\beta^{-\frac{2}{2}} \\ \int_0^\infty x^2\, e^{-\beta x^2}\, dx &= \tfrac{1}{4}\sqrt{\pi}\,\beta^{-\frac{3}{2}} \\ \int_0^\infty x^3\, e^{-\beta x^2}\, dx &= \tfrac{1}{2}\beta^{-\frac{4}{2}} \\ \int_0^\infty x^4\, e^{-\beta x^2}\, dx &= \tfrac{3}{8}\sqrt{\pi}\,\beta^{-\frac{5}{2}} \end{aligned} \tag{1.2.4}$$

2. The probability of finding a random particle with *any* speed whatsoever (from $v=0$ to $v=\infty$) must obviously equal 1, and this is the sum of the probabilities of all the tiny ranges (which is of course an integral). Show that each of the two distributions given satisfies this important requirement.

The value of having a probability distribution is that it can be used to compute averages. An average of several possible values that can arise randomly is the product of each value and it corresponding probability, summed over all of the possible values:

$$\text{average of } x = \langle x \rangle = x_1 \cdot P(x_1) + x_2 \cdot P(x_2) + \dots \tag{1.2.5}$$

When the values lie on a continuum (like particle speeds), this sum becomes an integral. So multiplying every possible speed v by its corresponding probability $\mathcal{D}(v)\, dv$, and adding all of these products together gives a means for computing the average speed:

$$\langle v \rangle = \int_0^\infty v\, \mathcal{D}(v)\, dv \tag{1.2.6}$$

We can similarly take averages of other quantities, most notably the square of the velocity:

$$\langle v^2 \rangle = \int_0^\infty v^2\, \mathcal{D}(v)\, dv \tag{1.2.7}$$

3. Determine the relationship (i.e. the ratio) between the average and rms particle speeds for both a two and three-dimensional gas.

Simulated Evaluation

We are at last ready to examine the simulator. The average speed comes as a direct read-out in the simulator. The rms speed we can determine using the trick indicated in the Background Material – if we start with the "no collisions" configuration given above, the particle speeds remain constant and uniform. Then, without changing anything else about the gas, we can turn on collisions to introduce randomness.

4. Determine whether the simulator replicates a two or three-dimensional gas. This consists of several parts:
   a. Run the simulator "without randomness" to get the particle rms speed.
   b. Introduce randomness and get the average speed. Does the rms value change when you do this? Why or why not?
   c. The average speed fluctuates with time, so you will need to "sample" these numbers at random times, say by closing your eyes, waiting a second, and clicking the pause button, then writing down the number. Then un-pause the simulator and repeat several times. An average of these samples should be a good measure of the "true" average speed.
   d. The data obtained from the sampling method just described also allows you to calculate an uncertainty interval for the measurement. For a refresher on how to compute standard deviation, review this from your very first 9HA lab.
   e. Determine whether the relationship between the average and rms speeds is (to within uncertainty) characteristic of a two or three-dimensional gas.