# Sándor Nagy: Tricky Dimensions – a Spin-off of a Sim
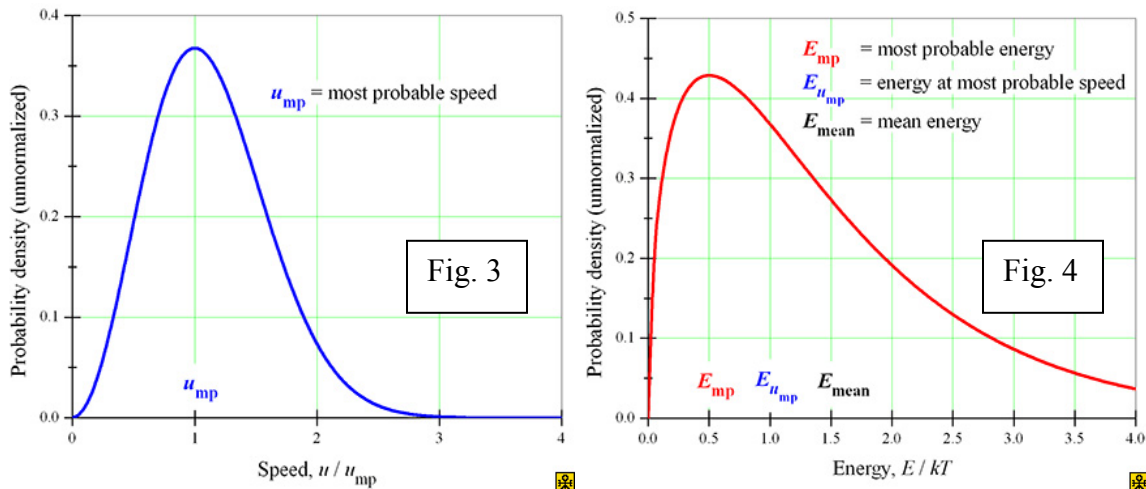
Abstract The Gas Properties sim – and probably all the other simulations on this topic I know of (see e.g. the one by Paul Falstad) – consider a 2D gas rather than a 3D one to make the simulation run faster (I believe). This approach still yields a qualitatively reasonable speed distribution (which looks very much similar to the Maxwell distribution), yet it "spoils" the energy distribution (from the point of view of 3D persons like you and me). However, this unavoidable flaw that goes with the simplification gives us an interesting insight into the world of dimensions.

It is a coincidence of two stimuli that caused me to write this "contribution" to the Gas Properties sim.

One stimulus has come from the simulation itself. If you are familiar with the Maxwell distribution of the monatomic ideal gas, then you will have no problem with accepting the speed histogram (Fig. 1) calculated by the program, however you will find the shape of the energy histogram (Fig. 2) rather puzzling.

Fig. 1
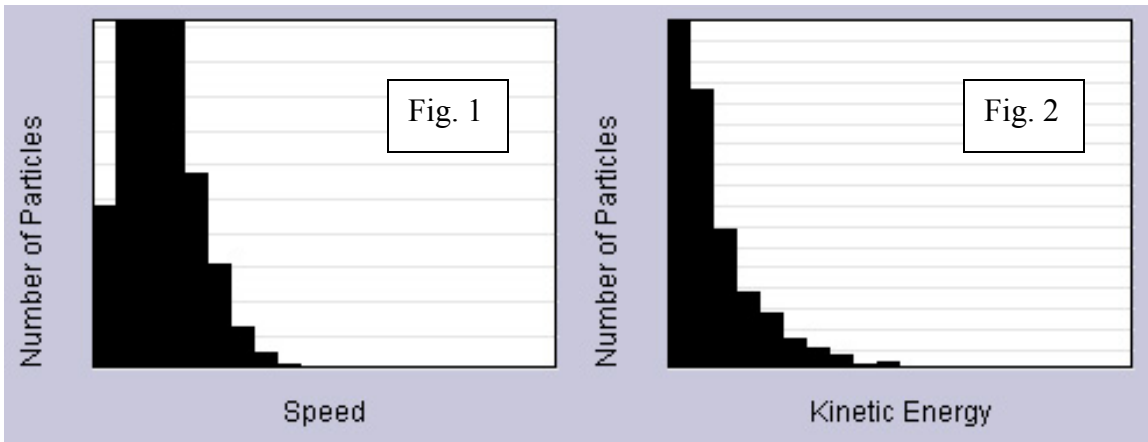
Fig. 2

If you can't remember how the probability densities should look like, have a glance at the respective distributions below obtained from the kinetic theory of the monatomic ideal gas. Whereas Figs. 1 and 3 are pretty similar, Fig. 2 seems to represent rather an exponential distribution than the red curve in Fig. 4.


Fig. 3

Fig. 4

E_{mp} = most probable energy
$E_{u_{mp}}$ = energy at most probable speed
E_{mean} = mean energy

(I have labeled some characteristics in Figs. 3 and 4 for my students to see that the most probable energy is not the energy of a molecule moving at the most probable speed.)

When I noticed the difference, my first thought was that the apparent exponential shape of the histogram was just an artifact caused by the poor resolution (large bin width) combined with the skewness of the red curve which it should represent. As it turns out further below, my assumption was wrong: the histogram *indeed* represents an exponential distribution rather than the red curve that I expected.

My second stimulus came from an effort to give my students some chemistry-related background to χ^2 distribution which makes it more appealing to them than the more abstract knowledge that χ^2 distribution is a useful tool for judging the goodness of fit of nuclear spectra (see the [Curve Fitting](#) sim). (You may want to know that I teach the basics of nuclear science to chemistry majors at a Hungarian university, but I also try to teach them a little statistics and probability theory on the side.)

If you are not too familiar with statistics, then you must take my word for the following. [Note that I have also prepared an electronic handout for my students in Hungarian with the details ([ValSum.pdf](#), Section 6.2), but it isn't very popular, so I have not translated it.]

Fig. 5
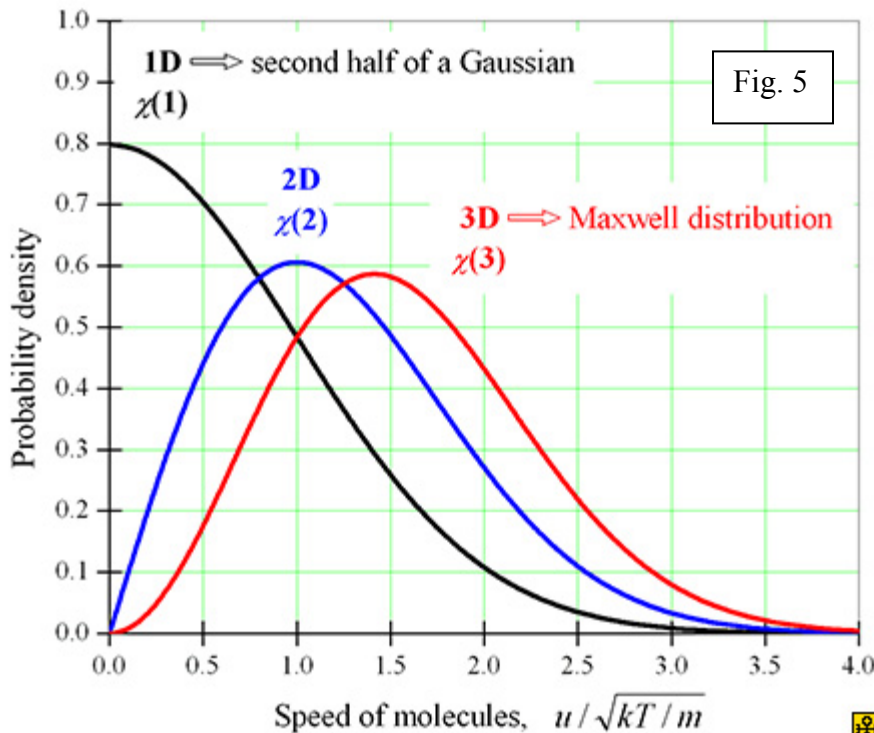
Let the speed u (i.e. the absolute value of the velocity vector) be given in the special unit of $\sqrt{kT/m}$. Now if you consider an ideal gas in 1D, 2D, and 3D, then it turns out that the speed has [chi distribution](#) with degree of freedom being equal to the dimension of the gas, i.e. $\chi(1)$, $\chi(2)$, and $\chi(3)$, respectively. The black curve in

Fig. 5 shows that $\chi(1)$ – which applies to 1D – happens to be a half Gaussian (normalized to 1). For 2D and 3D the curves are qualitatively similar to each other, but not quite the same. From a low-resolution histogram like the one in Fig. 1, one can only tell for sure that it cannot represent a 1D gas. However, it can represent a 2D gas just as well as a 3D gas. (If you have difficulty of picturing a 1D gas, think about it as an arbitrary direction in a 3D gas along which you measure the 1D distribution of a speed component.) The 3D curve gives you the Maxwell distribution known from books on physical chemistry:

$$f(u) == \sqrt{\frac{2}{\pi}} \left(\frac{m}{kT}\right)^{3/2} u^2 \exp\left(-\frac{mu^2}{2kT}\right)$$

Let us determine now the kinetic energy distributions of the same gases (i.e., 1D, 2D, and 3D). It turns out now that if we measure the kinetic energy ε in unit of $kT/2$ (which is the most probable energy in 3D according to the label in Fig. 4), then the energy distributions will be $\chi^2(1)$, $\chi^2(2)$, and $\chi^2(3)$, respectively, where the degree of freedom of the chi square distribution equals the number of dimensions of the gas.

As we can see in Fig. 6, the qualitative shape of the distribution curve sensitively depends on the dimension of the gas.

For a 1D gas, the probability density approaches infinity at $\varepsilon = 0$, then it decreases sharply.

Fig. 6
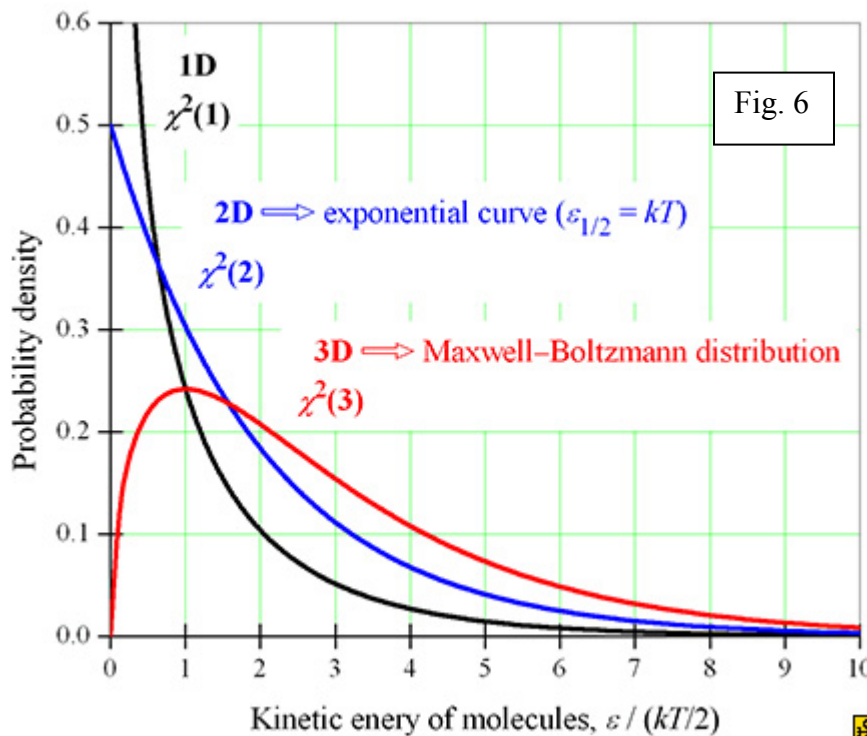
For a 2D gas, the maximum of the distribution curve is a finite value at $\varepsilon = 0$, then it decreases exponentially just like in the case of Fig. 2. This leads to the conclusion that the simulation must represent a 2D gas. (This conclusion has been confirmed by **Samuel Robert Reid** of **PhET**.) The median of the exponential is at $\varepsilon_{1/2} = kT$[♣]. This means that half of the molecules possess energy less than kT, while the other half more than kT.

For 3D, we get the Maxwell–Boltzmann distribution whose unnormalized curve is shown in Fig. 4:

$$f(\varepsilon) = \frac{2}{\sqrt{\pi}kT}\sqrt{\frac{\varepsilon}{kT}}\exp\left(-\frac{\varepsilon}{kT}\right)$$

[♣] Note that in 3D, according to Fig. 4, the value of the median in 2D (i.e. kT) happens to be equal to the kinetic energy of a molecule moving at the most probable speed. In 2D, however, the energy belonging to the most probable speed $\sqrt{kT/m}$ (see the maximum position of the blue curve in Fig. 5) is only $kT/2$.

Conclusion

So what is the point of this "contribution"? – you may ask.

The main point is that dimensions are tricky.

When you went to college, you must have met with the concept of *n*-dimensional Euclidean spaces during your math studies. You probably had the same feeling as I had.

Is that so simple? Wow! – you thought.

Maybe you were just as naive as I was as a student. I, for instance, would never have suspected that dimensions have any surprise in store for me. This was, of course, way before I first heard about fractal dimensions.

The first big shock came when I studied applied mathematics as a chemist and learned about a certain type of random walk in probability theory. The theorem I am referring to throws light on a big difference between $\leq$ 2D and $\geq$ 3D cases. The difference can be phrased in simple words like this. In 1D and 2D you cannot be lost hopelessly in an infinite maze if you choose your moving direction at random. In 3D or higher however, you will get lost for good sooner or later.

The final message (which may be appreciated by some of your students) is that the simulation works fine, but it is not about our 3D world, which can be most markedly seen from the energy distribution. However, if our world were "flatter" by one dimension, then gases would behave in that 2D universe just as the simulation predicts.