Francine and Me

Desire, equipartition, and the proper role of computer algebra

Dan Styer, Professor of Physics, Oberlin College 25 March 2019

When I was an undergraduate student at Swarthmore College, back in the 1970s, there weren't a lot of women who majored in physics. But one of my physics classmates, I'll call her Francine, was a smart, curious, small, curvy, blond, and intensely attractive young woman, with a round face and a ready smile. One day she walked into the science library and announced "I've gone through the whole course catalog and ruled out those courses I think would be good to take, keeping only those courses I find essential — courses in physics and mathematics, of course, but also chemistry, sociology, linguistics, literature, history — and I find that I'd have to spend eight years in college just to take the bare essentials." What an intellectual adventurer! At that moment my feelings toward Francine morphed from generalized desire to intense craving. It got to be hard for me to concentrate on physics when she was around. I knew that Francine was surrounded by a lot of young men — all the other physics majors. Was there some way I could make myself stand out from this pack of admirers?

Perhaps there was. The previous semester, I had taken a course in physical chemistry, which none of my rivals had. In that course, I had been asked to prove the equipartition theorem: That the thermal average of the kinetic energy for one degree of freedom was equal to $\frac{1}{2}k_BT$. I had slaved over that problem, and come up with a solution — of which I was immensely proud — that stretched over twenty pages of algebra. I was then (and remain today) a nerd, so I did the sort of thing a nerd would do to attract the romantic interest of a highly-desirable colleague: I emphasized my solution of the equipartition theorem.

Here's the gist of my solution. The thermal average was equal to

$$\frac{\displaystyle\int_{-\infty}^{+\infty} \frac{p^2}{2m} e^{-p^2/2mk_BT}\, dp}{\displaystyle\int_{-\infty}^{+\infty} e^{-p^2/2mk_BT}\, dp}.$$

I worked on the denominator first. Using the substitution $z = p^2/2mk_BT$, so that

$$dp = \frac{\sqrt{2mk_BT}}{2z^{1/2}}\, dz,$$

I wrote

$$\begin{aligned}
\int_{-\infty}^{+\infty} e^{-p^2/2mk_BT}\, dp &= 2\int_0^{\infty} e^{-p^2/2mk_BT}\, dp \\
&= \sqrt{2mk_BT}\int_0^{\infty} e^{-z} z^{-1/2}\, dz \\
&= \sqrt{2mk_BT}\;\Gamma(\tfrac{1}{2}),
\end{aligned}$$

where the gamma function is defined through

$$\Gamma(t) = \int_0^{\infty} e^{-z} z^{t-1}\, dz.$$

So much for the denominator. If you like gamma functions, you should be happy. (I happen to like gamma functions. And who knows? Perhaps Francine did too.)

Now for the numerator. Using the same substitution gives

$$\begin{aligned}\int_{-\infty}^{+\infty} \frac{p^2}{2m} e^{-p^2/2mk_BT}\,dp &= 2\int_0^{\infty} \frac{p^2}{2m} e^{-p^2/2mk_BT}\,dp \\ &= \sqrt{2mk_BT}\,k_BT \int_0^{\infty} z e^{-z} z^{-1/2}\,dz \\ &= \sqrt{2m(k_BT)^3}\int_0^{\infty} e^{-z} z^{1/2}\,dz \\ &= \sqrt{2m(k_BT)^3}\;\Gamma(\tfrac{3}{2}).\end{aligned}$$

Another gamma function!

The thermal average was thus equal to

$$\frac{\sqrt{2m(k_BT)^3}\;\Gamma(\frac{3}{2})}{\sqrt{2mk_BT}\;\Gamma(\frac{1}{2})} = k_BT\frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{1}{2})}.$$

But I happened to know (as one can prove easily using integration by parts) that

$$\Gamma(z+1) = z\Gamma(z),$$

whence

$$\Gamma(\tfrac{3}{2}) = \tfrac{1}{2}\Gamma(\tfrac{1}{2}).$$

Thus the thermal average is

$$\frac{\displaystyle\int_{-\infty}^{+\infty} \frac{p^2}{2m} e^{-p^2/2mk_BT}\,dp}{\displaystyle\int_{-\infty}^{+\infty} e^{-p^2/2mk_BT}\,dp} = \frac{1}{2}k_BT$$

and the equipartition theorem is proved!

It's astounding: every intermediate expression involves the mass m, but in the final expression an m in the numerator cancels an m in the denominator. This is the origin of the term "equipartition": if you have a mixture of helium and argon, then the average thermal energy in a helium atom is the same as the average thermal energy in an argon atom: despite the difference in masses, the thermal energy is partitioned equally.

Now, as I said, my efforts as an undergraduate were somewhat less elegant than the treatment above — stretching out over some twenty pages — and I really didn't know whether Francine shared my love of gamma functions. But I thought it was worth a shot: With a fine hand, I wrote out my entire twenty-page proof on a single large sheet of cardboard, and posted this proof on my dorm room door.

The next semester I studied thermal physics. In that course, I encountered a different treatment of the equipartition theorem. The thermal average is (using the common shorthand $\beta = 1/k_BT$)

$$\frac{\displaystyle\int_{-\infty}^{+\infty} \frac{p^2}{2m} e^{-\beta p^2/2m}\,dp}{\displaystyle\int_{-\infty}^{+\infty} e^{-\beta p^2/2m}\,dp} = \frac{\displaystyle -\frac{\partial}{\partial\beta}\int_{-\infty}^{+\infty} e^{-\beta p^2/2m}\,dp}{\displaystyle\int_{-\infty}^{+\infty} e^{-\beta p^2/2m}\,dp} = -\frac{\partial}{\partial\beta}\log\int_{-\infty}^{+\infty} e^{-\beta p^2/2m}\,dp.$$

What a cute trick! (It's called "parametric differentiation".) This means I needed to perform only one integral, not two. I love it when my work cuts in half.

But it gets even better than that. Use the substitution $u^2 = \beta p^2/2m$ so that the thermal average is

$$-\frac{\partial}{\partial\beta}\log\left\{\frac{1}{\sqrt{\beta/2m}}\int_{-\infty}^{+\infty} e^{-u^2}\,du\right\} = -\frac{\partial}{\partial\beta}\log\left\{\frac{1}{\sqrt{\beta}}\sqrt{2m}\,(\text{number})\right\}.$$

Perhaps you know that the integral evaluates to $\sqrt{\pi}$. Perhaps you don't. In either case you know that the integral is some number, independent of β. Thus the thermal average is

$$-\frac{\partial}{\partial\beta}\left\{\log\frac{1}{\sqrt{\beta}} + \log\left[\sqrt{2m}\,(\text{number})\right]\right\} = -\frac{\partial}{\partial\beta}\left\{-\tfrac{1}{2}\log\beta\right\} = \tfrac{1}{2}\frac{1}{\beta} = \tfrac{1}{2}k_BT.$$

There it is! You don't have to evaluate two integrals, you don't even have to evaluate one integral. You don't need to know any properties of gamma functions. You simply need to know that a definite integral produces a number. This quick, three-line proof of equipartition is both easier and carries a lot more insight than my twenty-page proof laden with gamma functions.

That evening I walked back to my dorm room, pulled down the sheet of cardboard, and tore it to shreds. Francine had never remarked on it anyway.

It strikes me that this story illuminates the difference between computer algebra and clear thinking. My first way of doing the problem involved mechanically walking through the two integrals, the way a computer would approach the problem. The second way involved creativity and insight, and it not only produces the result, it also sheds light on how to generalize the result to other terms in the Hamiltonian, and on the physical origin of the mass independence. This is the sort of proof that a computer would not be able to create. Computers are great tools but poor masters.

I never did manage to attract the affections of Francine, but that's actually for the better. I wouldn't trade my wife Linda for anyone in the world.