Identifying Student Difficulties with Conflicting Ideas in Statistical Mechanics

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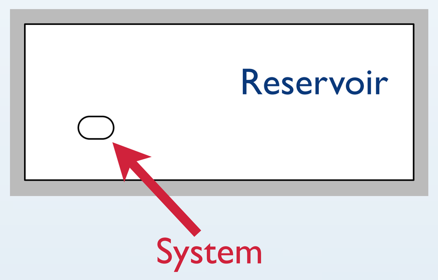
Supported in part by grant DUE-0817282

The Physics



Physical scenario under investigation is the *canonical ensemble*: a relatively small system in contact with a thermal reservoir.

- The temperature of the system is fixed by the reservoir, but its energy may fluctuate.
- The total energy of the system-reservoir combination is constant.

The Density of States Function

The Density of States function, $D(E)$, provides the number of states per unit energy that are accessible *to the system* for a given energy. The multiplicity of the system when it is in the "$\mathcal{E}$ energy state," (where $E \in \mathcal{E} \pm \Delta E$) is:

$$\omega_{sys} = \int_{\mathcal{E}-\Delta E}^{\mathcal{E}+\Delta E} D(E)\,\mathrm{d}E$$

The Boltzmann Factor

The Boltzmann factor is a decaying exponential function of the system's energy that is proportional to the multiplicity *of the reservoir* by the 2nd Law of Thermodynamics:

$$S_{res} = k\ln(\omega_{res})$$

$$S_{res} = S_{res}(E_{tot}) + \left(\frac{\partial S_{res}}{\partial E_{res}}\right)_{E_{tot}}(E_{res} - E_{tot}) + \ldots$$

$$\omega_{res} = \exp\frac{1}{k}\left(S_{res}(E_{tot}) - \frac{E_{sys}}{T}\right) = Ce^{-E_{sys}/kT}$$

Joint Probability

To determine the probability of the system having a particular energy, one must consider the total multiplicity of the system-reservoir combination: the product of the individual multiplicities. (See Ref. 3 for student difficulties with this concept.)

$$Prob(\mathcal{E}) = \frac{\omega_{sys}\omega_{res}}{\sum \omega_{sys}\omega_{res}} = \frac{1}{Z}\int_{\mathcal{E}-\Delta E}^{\mathcal{E}+\Delta E} D(E)e^{-E/kT}\,\mathrm{d}E \quad \text{where,} \quad Z = \int_{All\ E} D(E)e^{-E/kT}\,\mathrm{d}E$$

is the canonical partition function (i.e., probability normalizing factor)

The Course

- Data were collected near the end of an upper-division undergraduate statistical mechanics course.
- Interviews were conducted after all relevant instruction but before the final exam
- Instruction included lectures and tutorials on the Density of States[1] and the Boltzmann factor.[2]

References

1. B. R. Bucy, PhD Dissertation, University of Maine, 2007.
2. T. I. Smith, J. R. Thompson, and D. B. Mountcastle, in 2010 PERC Proceedings, 2010, pp. 305–308.
3. M. E. Loverude, in 2009 PERC Proceedings, 2009, pp. 189–192.
4. V. K. Otero, and D. B. Harlow, in Getting Started in PER, 2009, URL http://www.per-central.org/items/detail.cfm?ID=9122.
5. R. Baierlein, Thermal Physics, Cambridge University Press,1999.

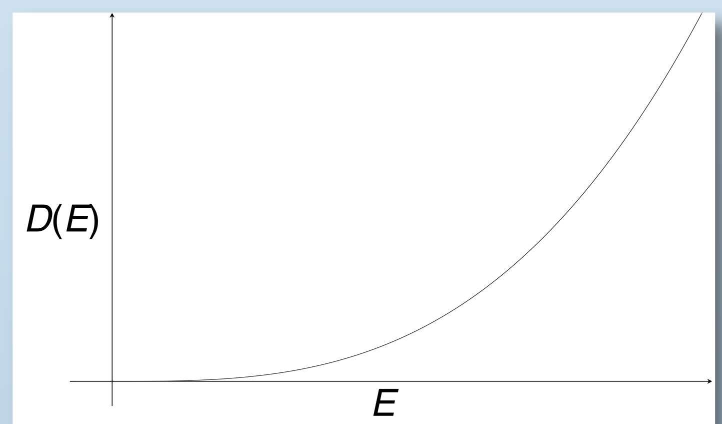
Interview ($N = 5$)

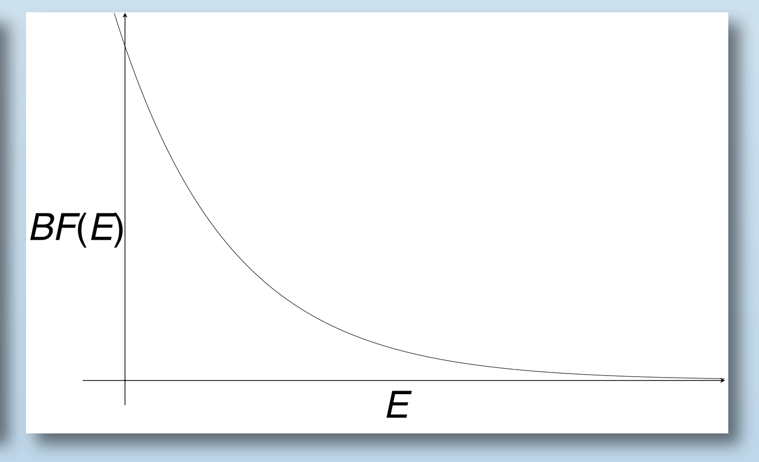
- Think-aloud, artifact-based interviews[4]
- 3 individual interviews
- 1 two-person interview
- Given graphs of $D(E)$ vs. E and $BF(E)$ vs. E individually

I) Students first given graph of Density of States ($D(E)$ vs. E) for a particular system (a multi-particle monatomic ideal gas)

- Asked if they could use it to make claims about which (if any) energies are more probable or less probable than others
- Asked explicitly how $D(E)$ relates to probability

II) Students then given graph of Boltzmann factor ($BF(E)$ vs. E) for the same system and asked the same questions





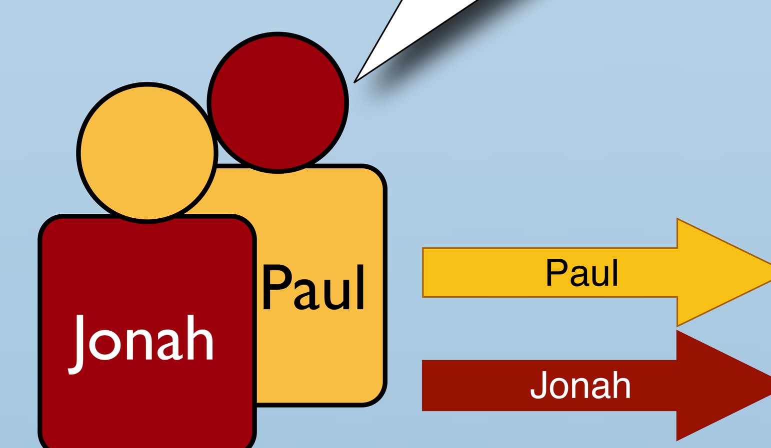
Connection to multiplicity and probability

Density of States		Boltzmann Factor	
Connected on their own	3	Connected on their own	3
Memorized connection (easily dismissed)	1	Connected only to probability	2
No connection	1	No connection	0

Paul and Jonah were interviewed together. They each had good ideas but frequently convinced each other to abandon those (both correct and incorrect) that did not seem to fit with their confident idea that the Boltzmann factor is related to probability. Paul was particularly explicit about his cognitive conflict.

III) Students asked to reconcile the fact that the graphs of $D(E)$ and $BF(E)$ indicate opposite results

"It's weird, when we look at each of these individually – Density of States and the Boltzmann Factor (or probability) – we look at this one [BF] and we say, 'Oh, well, ***this*** [low E] is the most probable,' and when we were thinking about this one conceptually [DoS], we're like, 'Oh, well, ***this*** [high E] is the most probable.' So maybe if we multiply them together it's somewhere in the middle."

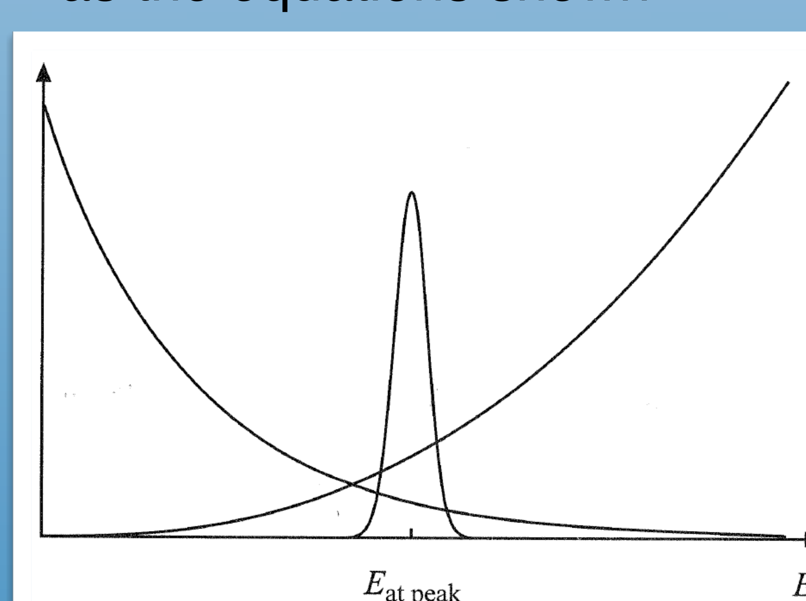


Reconciled trends in D(E) and BF(E)	
Multiplicity is multiplicative	3
Recalls multiplying	1
No recall	1

Ability to justify multiplication	
On own	0
With guidance	2
Not complete	3

Written Final Exam Question ($N = 12$)

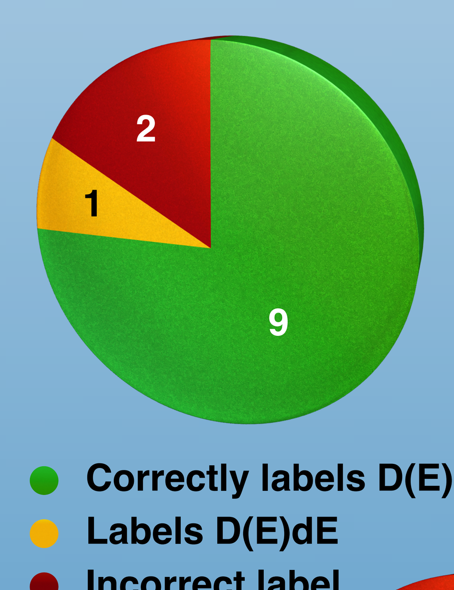
- Students given graph of $D(E)$, $BF(E)$ and their product (with only the energy axis labeled) as well as the equations shown

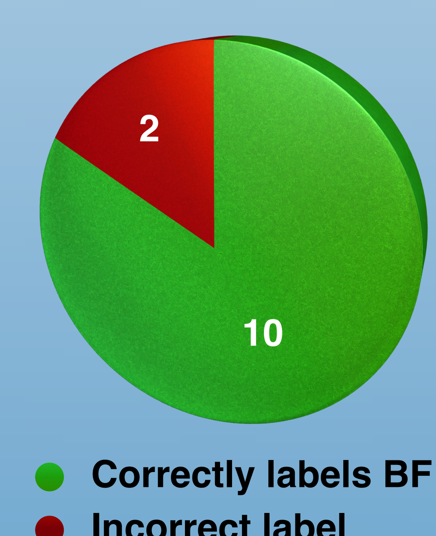


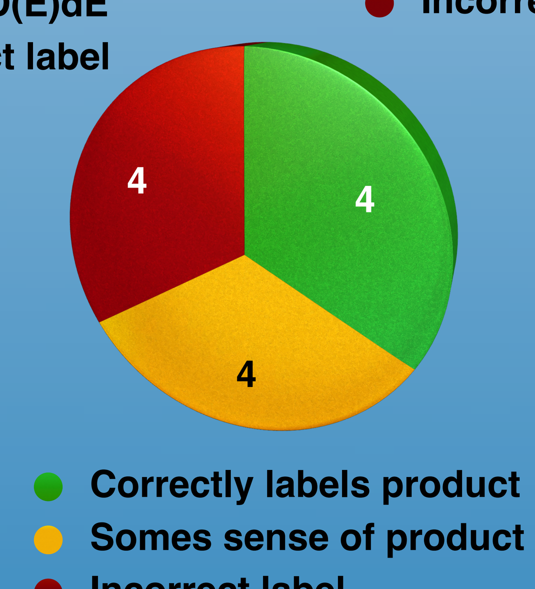
$$Z = \sum_j \exp(-E_j/kT)$$
$$= \int e^{-E/kT} D(E)\,\mathrm{d}E$$
$$= e^{-\langle E\rangle/kT} D(\langle E\rangle)\delta E$$

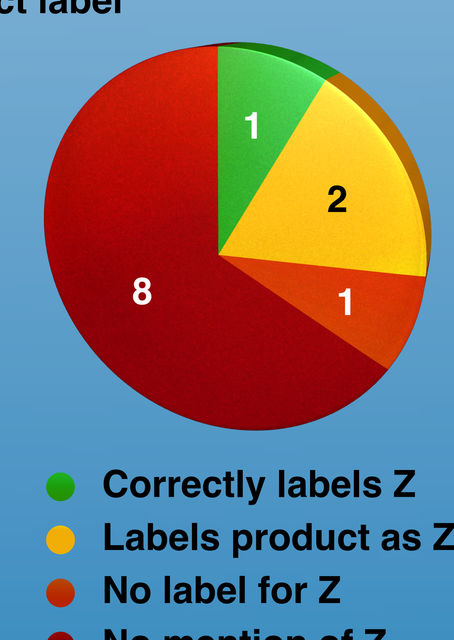
Recreated from Ref. 5.

- Asked to "identify everything that appears more than once" in the various representations and "describe what each of them refers to."









Exam Results

- 10 out of 12 students correctly identified both $D(E)$ and $BF(E)$
- 8 students indicated that the gaussian curve was *related to* the product of the other two functions (only 4 completely correctly)
- Only 1 student correctly identified Z as the integral of the product function

Conclusion

After lecture ***AND*** tutorial instruction, most students have the necessary pieces of knowledge but have ***NOT*** synthesized them to gain a robust understanding of ***WHY*** and ***HOW*** the product of $D(E)$ and $BF(E)$ is needed for a normalized probability distribution