

Identifying Student Difficulties with Conflicting Ideas in Statistical Mechanics

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Abstract. In statistical mechanics there are two quantities that directly relate to the probability that a system at a temperature fixed by a thermal reservoir has a particular energy. The density of states function is related to the multiplicity of the system and indicates that occupation probability increases with energy. The Boltzmann factor is related to the multiplicity of the reservoir and indicates that occupation probability decreases with energy. This seems contradictory until one remembers that a complete probability distribution is determined by the total multiplicity of the system and its surroundings, requiring the product of these two functions. We present evidence from individual and group interviews that students knew how each of these functions relates to multiplicity but did not recognize the need to combine the two to characterize the physical scenario.

Keywords: Physics Education Research, Statistical Mechanics, Partition Function, Boltzmann Factor, Density of States, Upper Division

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INTRODUCTION

As part of an ongoing collaborative project we have documented student difficulties with thermal physics and the associated mathematics. We have also made efforts to address these difficulties by developing and implementing guided-inquiry worksheet activities (a.k.a. tutorials). We have previously reported the development and implementation of a tutorial designed to help students in an upper-division statistical mechanics course develop a robust understanding of the Boltzmann factor.[1] Here we present the results of an investigation into student understanding of the connection between the Boltzmann factor and the density of states function.

When considering the canonical ensemble, one may imagine a small system of interest in contact with a large thermal reservoir. The temperature of the system is held fixed by the reservoir, but its energy will fluctuate. In systems where energy is a continuous quantity, the multiplicity of the system is given by the integral of the appropriate density of states function over a small range,

$$\omega_{\text{sys}} = \int_{\mathcal{E}-\Delta E}^{\mathcal{E}+\Delta E} D(E) dE, \quad (1)$$

where the limits of integration are chosen such that all values of energy within the range $\mathcal{E} \pm \Delta E$ are considered to be in what is commonly referred to as the “ \mathcal{E} macrostate.”

The Boltzmann factor is a mathematical expression for the probability that a thermodynamic system has a certain energy, based on that energy. The Boltzmann factor

may be used to determine many properties of the system and is, therefore, a cornerstone of statistical thermal physics. In the physical scenario above, the Boltzmann factor is proportional to the multiplicity of the *reservoir* as a function of the energy of the *system* ($\omega_{\text{res}} \propto e^{-E/kT}$).¹ To discuss the probability of the system having a particular energy, one must consider the total multiplicity given by the product of ω_{sys} and ω_{res} :

$$\text{Prob}(\mathcal{E}) = \frac{\omega_{\text{sys}}\omega_{\text{res}}}{Z} = \frac{1}{Z} \int_{\mathcal{E}-\Delta E}^{\mathcal{E}+\Delta E} D(E)e^{-E/kT} dE, \quad (2)$$

where Z (the normalizing factor) is the canonical partition function, the sum (integral) of the total multiplicity over all system states (i.e. values of E):

$$Z = \int_{\text{All } E} D(E)e^{-E/kT} dE. \quad (3)$$

As can be seen from Eqs. 2 and 3, an increase in either $D(E)$ or the Boltzmann factor individually results in an increased probability, provided the other is (relatively) constant over the range in question. For simplicity, conclusions are often made by considering only one of these quantities. A complete analysis, however, requires considering both simultaneously (by taking their product).

In the following sections we describe the methods and results of our research on student understanding of how

¹ The constant of proportionality becomes irrelevant in the context of probability, which is normalized.

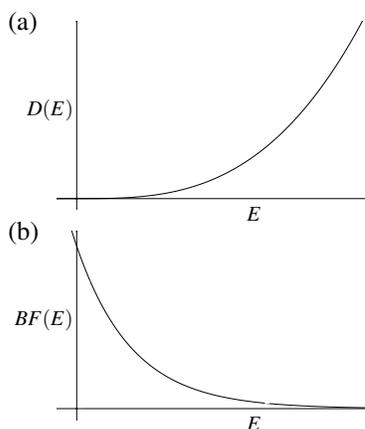


FIGURE 1. Graphs of (a) the density of states and (b) the Boltzmann factor as functions of energy of the system. Graphs were given to students one at a time during the interviews.

the density of states and the Boltzmann factor contribute to the probability distribution of a thermodynamic system. We present evidence from clinical interviews and written surveys suggesting that students at the end of an undergraduate statistical mechanics course display a reasonable familiarity with each of these quantities individually but often lack a robust understanding of how they are related and why they must be used in conjunction with one another.

RESEARCH SETTING AND METHODS

We conducted our study within an upper-division undergraduate statistical mechanics course at a public research university in the northeastern United States. During the investigation, 13 students were enrolled in the course (nine undergraduate physics majors, one chemistry major, and three graduate students in physics). As part of regular class meetings, students participated in lectures and tutorials designed to help them understand how the density of states function ($D(E)$) relates to the multiplicity of the system and how the Boltzmann factor relates to the multiplicity of the reservoir. Students also spent a significant amount of class time investigating how multiplicity relates to probability.

After all instruction on related topics, we interviewed students either as individuals or in pairs (based on student preference) to investigate their ideas about the relationship between the density of states and the Boltzmann factor. We interviewed five students (two undergraduate physics majors, and three physics graduate students) using a think-aloud, artifact-based protocol[2] in order to examine their ideas more deeply than we could using either written surveys or classroom observations.

During the interviews, students were given generic

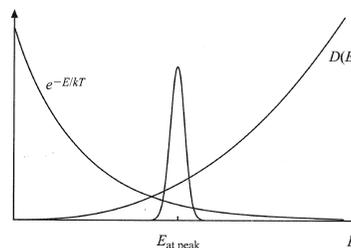


FIGURE 2. Graph of the Boltzmann factor, the density of states, and their product as functions of energy (all on different vertical scales). Taken from Figure 5.4 in Ref. 5, p. 100. Figure used without “ $e^{-E/kT}$ ” and “ $D(E)$ ” labels on the final exam.

graphs of $D(E)$ and the Boltzmann factor as functions of system energy (Figure 1). The graphs were presented one at a time (with $D(E)$ given first), and students were asked to determine which values of energy, if any, were more probable and which were less probable. They were also asked to articulate *how* these graphs relate to the probability of the system having a particular value of energy (E). We were looking for evidence of student understanding of (i.e., the ability to clearly articulate and apply) three pieces of information that could be synthesized to gain a picture of total probability in this context: 1) $D(E)$ is related to the multiplicity of the *system*; 2) the Boltzmann factor is proportional to the multiplicity of the *reservoir*; and 3) the total multiplicity needed to determine probabilities is the product of the multiplicities of the system and the reservoir, i.e., the product of $D(E)$ and the Boltzmann factor (the peak in Figure 2 and the integrand in Eq. 2).²

As a follow-up and broadening of the interview task, a question on the final exam (given after the interviews had been conducted) presented students with the graph from Figure 2 (without either function label) as well as several expressions for the canonical partition function (Z):

$$Z = \sum_j \exp(-E_j/kT) = \int e^{-E/kT} D(E) dE. \quad (4)$$

Students were asked to indicate which features of the graph corresponded to which items in the equations. Our goal for question was to determine if students could connect the algebraic and graphical representations of those physical quantities. The desired result is that students would recognize the graphs of $D(E)$ and the Boltzmann factor and determine that the canonical partition function is represented by the area under the gaussian peak (Figure 2), corresponding with the integral of the product of $D(E)$ and the Boltzmann factor (Eqs. 3 & 4).

² Loverude has reported student difficulties related to combining multiplicities of various systems.[3]

Data from interviews and final exams were analyzed using a grounded theory approach in order to find interesting and common trends. These trends were examined using the framework of identifying specific student difficulties[4] associated with the Boltzmann factor. However, with our small data set, trends were not always apparent, and several data are treated as case studies with an emphasis on description before interpretation.

INTERVIEW RESULTS

Four of the students were able to articulate how $D(E)$ determines the multiplicities and, therefore, relative probabilities of various energy levels, but two of these students, Paul and Jonah (senior physics majors, interviewed together) were not confident in this relationship. Three students also indicated in some way that the Boltzmann factor is related to the multiplicity of the reservoir, but only one, Kyle (a graduate student), seemed to have a robust understanding of this relationship.

All students had an understanding that combining multiplicities requires multiplication. Two students articulated this fact by stating that “multiplicity is multiplicative.” Moreover, all students recalled the figure from the text (Figure 2) that overlays the Boltzmann factor, $D(E)$, and the product of the two.[5] Three students referred to this figure even before the graph of the Boltzmann factor was introduced, often discussing the “bell-curve” shape. Paul mentioned the figure almost as soon as the graph of $D(E)$ was first presented, and continued to refer to it throughout the interview, but could not remember the details of what the various curves represent or the paragraph explaining why it was important.

Kyle and Malcolm (another graduate student) also used conservation of energy arguments: (Malcolm commenting on $D(E)$) “Energy conservation stops energy from increasing too far”; (Kyle trying to combine the two) “We don’t see liquid nitrogen or shining air in this room, so neither high energies nor low energies are very likely.” However, none of the students correctly stated that the product of the two functions was necessary to determine the relative probabilities of energy values without assistance from the interviewer.

Kyle had the strongest understanding of the material based on the time it took him to answer questions and the accuracy of his responses. He was confident in both how $D(E)$ can be used to determine the multiplicity of the system and that the Boltzmann factor is proportional to the multiplicity of the reservoir. He was articulate about the multiplicative nature of multiplicities; he had good intuitions regarding practical limits on energy values; and he spontaneously reflected on topics with which he was and was not comfortable. With all of these desirable cognitive and metacognitive traits, however, Kyle still

had not synthesized all available information to articulate that the bell-curve in Figure 2 results from considerations of the multiplicity of the system-reservoir combination and thus requires the product of the two functions.

The weakest interviewees by far were Paul and Jonah. (Jonah did not participate in the *Boltzmann Factor* tutorial.) Between the two of them they expressed many good ideas about thermodynamics and statistical mechanics that were relevant to the interview scenario. Their confidence in any of those ideas, however, was quite low. Every time a new piece of information seemed to contradict what they had previously said, they would dismiss one or the other as incorrect or try to reconcile them without concern for previously expressed factors (e.g., appropriate units). In fact, the only idea they were completely sure about was that probability is proportional to the Boltzmann factor. After much prodding Paul expressed the need to maximize the entropy of the system-reservoir combination as a whole (i.e., maximize total multiplicity) to determine the most probable state, indicating that all of the information needed to succeed was available to them, but their lack of confidence in the physical meaning of the various terms seemed to impede their understanding of the combined probability distribution.

These results indicate that, for our interview sample, students understand that a) $D(E)$ is related to the multiplicity of the system, b) the Boltzmann factor is related to the multiplicity of the reservoir, c) “multiplicities are multiplicative,” and the total multiplicity is determined by the product of individual multiplicities, and d) multiplicity is directly related to probability. These students had *not*, however, synthesized this information to gain a robust understanding of the physical reasoning behind taking the product of $D(E)$ and the Boltzmann factor to determine the probability distribution.

EXAM RESULTS

As mentioned previously, a question on the final exam asked students to relate algebraic expressions of Z in terms of $D(E)$ and the Boltzmann factor to an unlabeled graph of $D(E)$, the Boltzmann factor and their product. Ten out of 12 students correctly labeled the graphical representation of both the Boltzmann factor and $D(E)$, and eight of these students related the gaussian-shaped curve to the product of the two. Only one student (Kyle) correctly interpreted Z as the area under the curve of the graph of the product. Two students indicated that the gaussian-shaped graph itself would be Z (Figure 3), while eight students made no mention of Z in their response. These exam results strengthen the claim that students recognize graphs of the Boltzmann factor, $D(E)$, and their product (the integrand of Eq. 4), but may not have a robust understanding of the physical implications

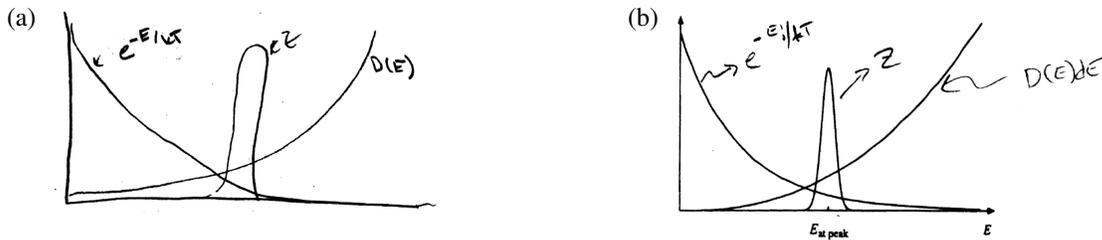


FIGURE 3. Samples of student work from the final exam: incorrect interpretations of Z . (a) Bill: “The partition function, Z , ... is the peak gaussian shaped curve.” (b) Jayne: “... the ‘hump’ is the product of the two, otherwise known as Z , the partition function.”

(as evidenced by their failure to properly interpret the integral of the product as Z). This failure to recognize an integral as represented by the area under a graph of a function has been documented by several researchers in thermal physics education [6, 7, 8, 9] and is known in the mathematics education research literature (e.g., [10]). It is particularly interesting here since Z is first introduced as a *constant* normalizing factor that is equivalent to the *sum* of Boltzmann factors (see Eqs. 2 & 4).

SUMMARY AND IMPLICATIONS

In virtually all physically interesting systems modeled with the canonical ensemble, one must consider the interactions between a system and its surroundings and how the entropy and multiplicity of each affects thermodynamic equilibrium. Though a necessary first step toward understanding more complex systems, the Boltzmann factor on its own is only applicable in a handful of cases; otherwise one needs knowledge of the multiplicity of the system obtained from the density of states function. It is unclear at this point how well students understand the physical connection between these two mathematical expressions. It is also unclear how well they understand the underlying physics sufficiently to see why the product of the two (rather than the sum or any other combination) yields an expression for the probability of a system having a particular energy. The bell-shaped curve that is the graph of this product, however, is virtually the definition of thermodynamic equilibrium, with the vast majority of states in a system having energies within a narrow range of values around an expected energy, $\langle E \rangle$. A robust understanding of the product of the Boltzmann factor and the density of states and why they are physically relevant is, therefore, vital to a comprehensive understanding of statistical mechanics.

Our research has focused on identifying specific student difficulties; data analysis used a grounded theory approach. Both of these frameworks emphasize description before interpretation. Future studies will seek to determine the prevalence of the difficulties identified here and reasons for why students display these difficulties.

We will also investigate instructional strategies that may help students gain a more complete understanding of the physical and mathematical issues involved in relating the Boltzmann factor and the density of states.

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