

The Question 1.1 of Homework 1

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October 2020

While scoring this homework, I observed that there are students having some serious misunderstanding of the properties of our dear temperature, hence, I would like to review some of these ideas and explain why they go wrong in this letter.

1 Temperature and Energy

Some of you stated that the energy shall go to infinity as the temperature approaches the infinity, but you shall notice that we only have to states with either energy zero or ϵ . With the total particle number fixed, the system cannot have energy more than $N\epsilon$, so, it's impossible for the energy of this system to approach infinity.

In fact, any system with bounded energy spectrum and finite particles have an upper bound for its internal energy. Conversely, for system with unbounded energy spectrum such as idea gas, the energy is not bounded and might go to infinity as the temperature does.

2 Equipartition Theorem

Some of you claimed that the system shall have equally probable states as a result of the equipartition theorem, this is an serious misconception of this theorem and have nothing to do with this question. Now I will introduce this theorem and its limitation first and explain why it doesn't work on our question.

The equipartition theorem indicates that if the energy of the system is a positive definite quadratic form in some variables $\{u_1, u_2, \dots, u_N\}$, that is, energy $E(u) = u^T A u$ for some positive matrix A , and $u = (u_1, u_2, \dots, u_N)^T$, then the part of energy from the re-defined variables based on the eigenvectors of A are all equal, in fact, each of them are $\frac{1}{2}k_B T$.

The proof is kind of trivial, diagonalize $A = S^T E S$, where E is diagonal, and let $v = S u$. Thus, the calculation of partition function reduces to Gaussian integrals, and one can easily find that the energy in the direction of v_i is given by

$$\frac{1}{Z} \int_v E_i v_i^2 \exp\left\{-\frac{v^T E v}{k_B T}\right\} = -\sqrt{\alpha} \frac{\partial}{\partial \alpha} \frac{1}{\sqrt{\alpha}} \Big|_{\alpha=\frac{1}{k_B T}} = \frac{1}{2} k_B T$$

Hence, to make the Equipartition theorem works, the energy spectrum of the system must obey the Boltzmann distribution and have a Gaussian or, in general, a positive quadratic form of energy spectrum.

For a two state system with bounded energy spectrum (a quadratic form of energy spectrum is clearly not bounded since we can take the eigenvector to the limit of infinite norm), the equipartition theorem just doesn't work, and we cannot say the energy of a system is proportional to the temperature in general, in fact, it's not true for many kinds of systems.

3 Maximization of Entropy and the Second Law

Another great misunderstanding in the Homework 1 is the maximization of entropy and the second law. Some said the entropy shall be maximized when the temperature goes to infinity. Most of these student didn't explain why this is true. Some of these even claimed that this is true because of the second law or the requirement of entropy maximization in a system that reaches equilibrium. I will explain later why the two claims do not work.

Originally, I gave no credits to those replying that the entropy shall be maximized without any further explanation. However, after some struggling discussion with Prof Hsu, we decided to give full credits to those answering that the entropy shall be maximized without any further explanation (out of mercy).

What is the second law? It's a complicated stuff to explain, and the law itself has many different statements or understanding in different level. However, in any form or aspect of it, one thing is certainly true : the increase of entropy is an dynamical property. For example, engines are of dynamics, classical and (open) quantum relaxations are dynamical process, Boltzmann's H theorem was proved under the assumption of a dynamical system, and even the quantum version of H theorem of completely positive trace preserving maps proved by Lindblad talks about a dynamical process. However, in this question, we are asking the probability of a single state in the limit of infinity temperature. It's more about the property of a function rather than a dynamical process. Some of you may say we can view the process of making the temperature higher as such a dynamical process. But you shall notice that lowering the temperature can also be taken as a dynamical process but with a opposite behaviour of entropy. If you want to explain it in this way, then the difference between these two opposite processes shall be explained in a logical, detailed, and physical manner.

The more detailed you reply, the more possible it is for you to get credits. And I cannot guarantee that one can still get full or even any credit if he or she claims an answer without further explanation in a question like this.

Another misconception is the maximization of entropy. But, in fact, we are talking about a system that has been in equilibrium and has fixed energy and particle numbers. There's no need of further relaxation for the system to increase its entropy and reach equilibrium. It's already one. Also, we don't even expect any system in equilibrium to have infinite temperature based on our common sense.

4 Summary

Correct understanding of facts, laws, principles, and results in physics, in my own point of view, is one of the most important part in this field. Wrong application of physics laws and abuse of scientific facts may cause dangerous consequences.

This class requires you to reply your answer as clear as possible. A precise understanding of questions also matters. Some of you answered this problem in a mathematical manner, and I, sadly, cannot give you any credit. In the coming midterm or final, there're still chances to answer a question like this (with the line "explain in physics"), and those who replies in a mathematical manner will still get no points.