PHYS 427 - Discussion 03

Feb 11, 2025

Over the last few weeks, we dealt with thermodynamics in the microcanonical ensemble. Unfortunately calculations in this formalism are particularly difficult, because computing the multiplicity function for most realistic systems is a hopeless task.

Thankfully most systems that we would like to probe aren't actually closed. We learned in class that if a system is in **thermal contact** with a reservoir at temperature T (i.e. the system and reservoir can exchange energy), then in thermal equilibrium the probability the system is in microstate "i" is given by

$$p_i = \frac{e^{-\beta\varepsilon_i}}{Z} \tag{1}$$

where ε_i is the energy of the system in state "i", $\beta \equiv 1/k_B T$, and Z is the **partition function**:

$$Z \equiv \sum_i e^{-\beta\varepsilon_i} \tag{2}$$

[**Note**: the sum is over all microstates of the system and not energy values (the distinction is important when there are degenerate energy levels).] When we work with equilibrated systems that are in thermal contact with a reservoir, we say we're working in the **canonical ensemble**. In this case, all of thermodynamics follows from the partition function!

Algorithm: Thermodynamics in the canonical ensemble
1. Compute the partition function of the system: Z.
2. Compute the thermodynamics of the system using the partition function (generally, this means taking an appropriate derivative of Z).

For instance, the average energy of a system is given by $U = \sum_i p_i \varepsilon_i$. However, in the canonical ensemble one can compute this sum by taking the following derivative of the partition function:

$$U = -\frac{\partial \ln Z}{\partial \beta} \tag{3}$$

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1. **Geometric series**: Repeatedly in statistical mechanics one encounters the sum:

$$S = \sum_{n=0}^{N} x^n. \tag{4}$$

[For instance, you'll encounter this sum on the upcoming homework!]

(a) Show that for $x \neq 1$:

$$\sum_{n=0}^{N} x^n = \frac{1 - x^{N+1}}{1 - x} \tag{5}$$

[Hint: explicitly write out the following sum: $(1-x)S$. You should notice that many terms cancel.]

(b) By taking a derivative of this result, show that for $x \neq 1$:

$$\sum_{n=0}^{N} n x^n = \frac{x}{(1-x)^2}\left[1 - (N+1)x^N + N x^{N+1}\right] \tag{6}$$

As an aside, it is very common to encounter this sum with $N \to \infty$ and $|x| < 1$. In this case $\lim_{N\to\infty} x^N = 0$ and the results above simplify considerably:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad , \quad \text{if } |x| < 1 \tag{7}$$

$$\sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2} \quad , \quad \text{if } |x| < 1 \tag{8}$$

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2. **2D non-interacting ultra-relativistic gas**: Consider a gas of N highly-relativistic particles confined to a square of area $A = L^2$. The particles have energy $\varepsilon_{\vec{p}} = |\vec{p}|c$ where the momentum is $\vec{p} = \hbar\vec{k}$ and the wavevectors are quantized as $\vec{k} = \pi\vec{n}/L$ with $n_x, n_y = 1, 2, \ldots, \infty$.

(a) Show that as $L \to \infty$ we can approximate a momentum sum by an integral:

$$\sum_{\vec{p}} F(\varepsilon_{\vec{p}}) \sim \frac{L^2}{(\pi\hbar)^2} \int_0^\infty dp_x \int_0^\infty dp_y F(\varepsilon_{\vec{p}}) \tag{9}$$

where $F(\varepsilon_{\vec{p}})$ is an arbitrary function of the dispersion $\varepsilon_{\vec{p}}$. *Hint: you can start by arguing that $\Delta p_x L/\hbar\pi = 1$ (or you can solve it another way).*

(b) Write the integral in polar coordinates (p, θ); then make a change of variables to show that:

$$\sum_{\vec{p}} F(\varepsilon_{\vec{p}}) \sim \frac{L^2}{2\pi(\hbar c)^2} \int_0^\infty d\varepsilon\, \varepsilon\, F(\varepsilon) \tag{10}$$

hence, we can approximate momentum sums by energy integrals!

(c) Compute the partition function of a single particle, Z_1.

(d) Compute the partition function of N indistinguishable particles, Z_N.

(e) Assuming the N particle system is in thermal equilibrium with a reservoir, compute its energy. You should find that

$$U = 2Nk_BT \tag{11}$$

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3. **(Optional) Metropolis algorithm:** If the energy of your system depends non-trivially on the configuration of your degrees of freedom (say the orientation of each spin on a chain), how do you compute the partition function? It would be a complicated multidimensional sum, almost impossible to solve analytically except in very special cases. So what do you do if you need to calculate an expectation value? You use computers!

   The Monte Carlo method is a trick to do huge multidimensional integrals (or sums) on a computer. This method generates configurations of your system following the Boltzmann distribution. That is, each configuration of spins will occur at a rate proportional to its Boltzmann weight. For each configuration that the computer generates, you compute the value of the quantity of interest (say the total magnetization, or the product of a number of spins). Since the configurations are already weighted by the Boltzmann factor, the arithmetic average of those numbers is the *weighted thermal average* that we seek. You could measure, for example, the average magnetization of a spin chain in this way.

   The Metropolis method is a specific form of Monte Carlo calculation. It gives a way to generate configurations that obey the Boltzmann distribution. For concreteness, consider your system to be a 1D spin chain. You can imagine that the energy of each configuration depends on the presence of an external magnetic field, and each spin gets an energy depending on whether it is aligned or anti-aligned with the field. The method goes as follows:

   (a) Start with some configuration of spins i with energy E_i.

   (b) Change some degrees of freedom (flip some spins) to obtain another configuration j from the first one.

   (c) If $E_j < E_i$, jump to configuration j with probability 1 (always), and if $E_j > E_i$, jump with probability $e^{-\beta(E_j - E_i)}$.

   After a very long time, you should find that the configuration appears with probabilities obeying

$$\frac{p(i)}{p(j)} = e^{-\beta(E_i - E_j)}, \tag{12}$$

   like in the Boltzmann distribution!

   Here is one way to understand this. Consider the rate of change of the probability $p(i)$:

$$\frac{dp(i)}{dt} = -p(i)\sum_j R(i \to j) + \sum_j p(j)R(j \to i), \tag{13}$$

   where $R(i \to j)$ is the rate of jumping from i to j and vice versa. In equilibrium, or steady state, we have $\frac{dp(i)}{dt} = 0$. One sufficient condition for equilibrium is to ensure that the contribution from every value of j is separately zero, not just the sum. That is,

$$-p(i)R(i \to j) + p(j)R(j \to i) = 0, \qquad \forall j. \tag{14}$$

   This is called *detailed balance*. When this happens,

$$\frac{p(i)}{p(j)} = \frac{R(j \to i)}{R(i \to j)}. \tag{15}$$

   Show that if you use the rates specified by the Metropolis algorithm in the equation above, you recover Eq. (12). *(Hint: first assume $E_j > E_i$, then the reverse.)* Given

a computer that can generate a random number between 0 and 1, how will you accept a jump with probability $e^{-\beta(E_j-E_i)}$?

(Adapted from Shankar's *Quantum Field Theory and Condensed Matter - An Introuction*)