Phys 362
Spring 2018

Statistical and Thermal Physics: Homework 11

Due: 3 May 2018

1 Two level system

Consider a system consisting of a single particle that could be in one of two possible states. The energies of the states are $-\epsilon$ and ϵ. Where possible, reduce to hyperbolic functions. MEDIUM

a) Determine an expression for the partition function of the system.

b) Determine an expression for the mean energy of the system.

c) Determine an expression for the heat capacity of the system.

d) Suppose that the energies of each state are each changed by adding the same constant energy, E_0. Show that this will change the partition function and the mean energy of the system but that it will not change the probabilities with which the system will be in either state. You can do this one the hard way or the smart way.

2 Energy for large systems of multiple distinguishable particles.

For a system of N identical distinguishable particles, the partition function is

$$Z_{N \text{ particles}} = Z^N_{\text{single particle}}$$

a) Use this to show that

$$\overline{E}_{N \text{ particles}} = N\,\overline{E}_{\text{single particle}}.$$

b) Use this result and

$$\sigma_E^2 = -\frac{\partial \overline{E}}{\partial \beta}$$

to show that

$$\sigma_{E \text{ for } N \text{ particles}} = \sqrt{N}\,\sigma_{\text{single particle}}.$$

c) Explain how you can use this result to justify the fact that the mean energy is a good representative for the system energy when the system contains a large number of particles.

3 Gould and Tobochnik, *Statistical and Thermal Physics*, 4.50, page 237. LONG

4 Absorption on a surface

A model for absorption involves a surfaces with absorption sites, each of which can accommodate at most one particle. If there is only one type of particle that can be absorbed, then the energy is 0 if the site is vacant and if it is occupied the energy is $-\epsilon$, where $\epsilon > 0$. Assume that the surface is in equilibrium with a bath (e.g. a surrounding gas) at temperature T and at chemical potential μ. MEDIUM

a) Suppose that $\epsilon > -\mu$. Determine the probability that the site is occupied for $T \to 0$ and for $T \to \infty$.

b) Suppose that $\epsilon < -\mu$. Determine the probability that the site is occupied for $T \to 0$ and for $T \to \infty$.

c) Determine the probability that the site is occupied for $\epsilon = -\mu$.

d) The hemoglobin molecule can absorb diatomic oxygen molecules. Data indicates that $\mu = -0.6\,\text{eV}$ and $\epsilon = 0.7\,\text{eV}$ at $T = 300\,\text{K}$. Determine the probability with which the hemoglobin molecule will absorb an oxygen molecule.

e) Suppose that, in addition to the first type of molecule, a second type of molecule can be absorbed at the site. Any site can be occupied by at most one molecule. For the second type of molecule, the energy when the molecule is absorbed is $-\epsilon'$, where where $\epsilon' > 0$. Assume that the chemical potential for this second type is the same as for the oxygen molecule. Derive an expression for the grand partition function for this situation and use the result to determine the probability with which the site is occupied by an oxygen molecule if $\epsilon' = 0.75\,\text{eV}$ and $T = 300\,\text{K}$.

5 Magnetic resonance

In magnetic resonance, a collection of spin-1/2 nuclei is placed in an external magnetic field. Suppose that the nuclei are protons, for which approximately $\mu = 5 \times 10^{-8}\,\text{eV/T}$. These are placed in an external field of 15 T (typical for state-of-the-art NMR spectrometers).EASY

a) Show that for a single spin-1/2 particle, the probability with which it is in the spin up state is

$$p_+ = \frac{1}{1 + e^{-2\mu B/kT}}.$$

b) Suppose that the temperature is 300 K. Find the fraction of particles in the spin up state. Determine the deviation from 1/2 for this fraction.

c) Determine the temperature at which the fraction of particles in the spin up state is greater than 90%. Practical NMR is simplified by having the sample be in a solution state. Is this likely in this case?

6 Gould and Tobochnik, *Statistical and Thermal Physics*, 5.4 a) b), page 246. Don't reinvent the wheel, you just found the probability in the up state in the last problem. Also, don't derive the form for the energy of the system, it is given in the book a page or two before this problem. EASY

7 Mean values of position and momentum for a particle in one dimension

Consider a particle that can move in one dimension. Let x and p denote the position and momentum of the particle respectively. Suppose that the energy of the particle is

$$E = \frac{p^2}{2m} + U(x)$$

where $U(x)$ is any potential energy. EASY

a) Show that the partition function takes the form

$$Z = Z_x Z_p$$

where

$$Z_x := \alpha_x \int e^{-U(x)\beta} \mathrm{d}x$$

and

$$Z_p := \alpha_p \int e^{-p^2\beta/2m} \mathrm{d}p$$

where α_x and α_p are constants that are independent of temperature.

The constants α_x and α_p are irrelevant for the thermodynamics that follows and can both be set equal to 1.

b) The probability density for the position of the particle, regardless of its momentum is

$$p(x) = \frac{1}{Z} \int e^{-E\beta} \mathrm{d}p.$$

Show that

$$p(x) = \frac{1}{Z_x} e^{-U(x)\beta}.$$

c) The mean value of the position, regardless of momentum, is

$$\overline{x} := \int x \, p(x) \mathrm{d}x.$$

Show that

$$\overline{x} = \frac{1}{Z_x} \int x \, e^{-U(x)\beta} \mathrm{d}x.$$

d) *Optional: extra credit up to 5% of the total assignment grade.* Evaluate $\overline{x}$ for a one dimensional classical harmonic oscillator. Really evaluate it, no cheats or integrators, start to finish it.

e) *Optional: extra credit up to* 5% *of the total assignment grade.* Consider a particle that is trapped in a vertical region $0 < y \leqslant \infty$ and which is subject to potential $u(y) = mgy$ where $m > 0$. Sketch the potential and indicate its minimum. If a particle were released from rest at any $y > 0$, where would you expect to eventually find it? Now suppose that the particle is in contact with a heat bath at temperature T. Determine an expression for $\overline{y}$. How does this compare to your previous expectation? Comment on this as $T \rightarrow 0$ and $T \rightarrow \infty$.

8 Thermal expansion coefficient for noble gases

This problem is long but worth it. It starts with very general statistical physics, works all the way through thermodynamics to the point where a readily measurable quantity of a real system can be predicted. HARD(est) so far?

Consider a classical particle restricted to one dimension and subject to potential $u(x)$. In general it is not possible to evaluate the mean value of position

$$\overline{x} = \frac{1}{Z_x} \int x \, e^{-u(x)\beta} \mathrm{d}x.$$

A scheme for approximating this is to expand $u(x)$ about the equilibrium point x_0.

$$u(x) = u(x_0) + (x - x_0) \left.\frac{du}{dx}\right|_{x_0} + \frac{1}{2}(x - x_0)^2 \left.\frac{d^2u}{dx^2}\right|_{x_0} + \frac{1}{3!}(x - x_0)^3 \left.\frac{d^3u}{dx^3}\right|_{x_0} + \cdots$$

where equilibrium means that the potential energy reaches a minimum.

a) If the expansion for $u(x)$ is terminated at the second order term, show that $\overline{x} = x_0$.

b) Suppose that the expansion is terminated at the third order term and rewrite this for convenience as

$$u(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + a_3(x - x_0)^3$$

for suitable $a_0, a_1, \ldots$. One cannot evaluate this exactly but it is possible if one approximates

$$e^{-a_3(x-x_0)^3} \approx 1 - a_3(x - x_0)^3.$$

Use this approximation to show that

$$\overline{x} = x_0 - \frac{3}{4} \, kT \, \frac{a_3}{a_2^2}.$$

You can look up Gaussian integrals that are needed.

c) Interacting noble gas atoms can be modeled using the Lennard-Jones potential

$$u(x) = u_0 \left[\left(\frac{x_0}{x}\right)^{12} - 2\left(\frac{x_0}{x}\right)^{6} \right].$$

Show that the linear thermal expansion coefficient defined as

$$\alpha := \frac{1}{x_0} \frac{d\overline{x}}{dT}$$

yields

$$\alpha = \frac{7}{48} \frac{k}{u_0}.$$

d) For argon, $x_0 = 3.9 \times 10^{-10}$ m and $u_0 = 0.010$ eV. Evaluate the linear expansion coefficient and compare the result to the measured value $\alpha = 0.0007\,\mathrm{K}^{-1}$.