Physics 415
Spring 2025
Homework 6
Due Friday, March 14, 2025

This assignment covers material in Chapter 6 of Reif. I recommend reading through the text and also Lectures Notes 18-21.

Problem 1: (Canonical ensemble: harmonic oscillator, adapted from Reif 6.1) A simple harmonic one-dimensional oscillator has energy levels given by $E_n = (n+1/2)\hbar\omega$, where ω is the characteristic (angular) frequency of the oscillator and where the quantum number n can assume the possible integral values $n = 0, 1, 2, \ldots$. Suppose that such an oscillator is in thermal contact with a heat reservoir at temperature T low enough so that $T/\hbar\omega \ll 1$.

(a) Find the ratio of the probability of the oscillator being in the first excited state to the probability of it being in the ground state.

(b) Assuming that only the ground state and first excited state are appreciably occupied, find the mean energy of the oscillator as a function of the temperature T.

Problem 2: (Canonical ensemble: decoupled spins, adapted from Reif 6.2) Consider a system of N decoupled spin-$\frac{1}{2}$ particles with magnetic moments μ, in an external field H. Suppose the system is in thermal contact with a heat reservoir at absolute temperature T. Calculate the mean energy $\bar{E}$ as a function of T and H.

Problem 3: (Canonical ensemble: spin-$\frac{1}{2}$, adapted from Reif 6.4) A sample of mineral oil is placed in an external magnetic field H. Each proton has spin-$\frac{1}{2}$ and a magnetic moment μ; it can, therefore, have two possible energies $\epsilon = \mp\mu H$, corresponding to the two possible orientations of its spin. An applied radio-frequency field can induce transitions between these two energy levels if its frequency ν satisfies the Bohr condition $h\nu = 2\mu H$. The power absorbed from this radiation field is then proportional to the *difference* in the numbner of nulcei in these two energy levels. Assume that the protons in the mineral oil are in thermal equilibrium at a temperature T which is so high that $\mu H \ll T$. How does the absorbed power depend on the temperature T of the sample?

Problem 4: (Canonical ensemble: two-level system, adapted from Reif 6.6) A system consists of N non-interacting particles, each of which can be in either of the two states with respective ϵ_1 and ϵ_2, where $\epsilon_1 < \epsilon_2$.

(a) Without explicit calculation, make a qualitative plot of the mean energy $\bar{E}$ of the system as a function of its temperature T. What is $\bar{E}$ in the limit of very low and very high temperatures? Roughly near what temperature does $\bar{E}$ change from its low to its high temperature limiting value?

(b) Using the result of (a), make a qualitative plot of the heat capacity C_V (at constant volume) as a function of the temperature T.

(c) Calculate explicitly the mean energy $\bar{E}(T)$ and heat capacity $C_V(T)$ of this system. Verify that your expressions exhibit the qualitative features discussed in (a) and (b).

Problem 5: (Canonical ensemble: spin-1, adapted from Reif 6.7) The nuclei of atoms in a certain crystalline solid have spin one. According to quantum theory, each nucleus can therefore be in any one of three quantum states labeled by the quantum number m, where $m =$ -1, 0, or 1. This quantum number measures the projection of the nuclear spin along a crystal axis of the solid. Since the electric charge distribution in the nucleus is not spherically symmetrical, but ellipsoidal, the energy of a nucleus depends on its spin orientation with respect to the internal electric field existing at its location. Thus a nucleus has the same energy $E = \epsilon$ in the state $m = 1$ and the state $m = -1$, compared with energy $E = 0$ in the state $m = 0$.

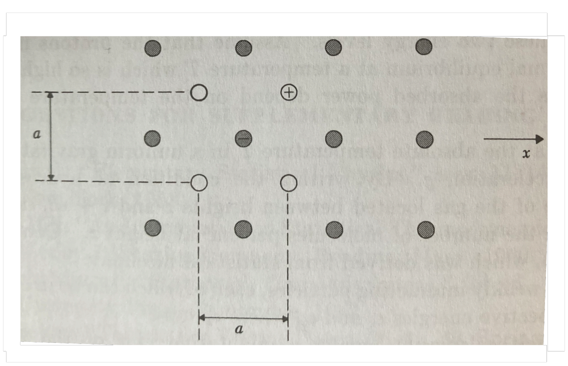
(a) Find an expression, as a function of absolute temperature T, of the nuclear contribution to the molar internal energy of the solid.

(b) Find an expression, as a function of T, of the nuclear contribution to the molar entropy of the solid.

(c) By directly counting the total number of accessible states, calculate the nuclear contribution to the molar entropy of the solid at very low temperatures. Calculate it also at very high temperatures. Show that the expression in part (b) reduces properly to these values as $T \to 0$ and $T \to \infty$.

(d) Make a qualitative graph showing the temperature dependence of the nuclear contribution to the molar heat capacity of the solid. Calculate its temperature dependence explicitly. What is its temperature dependence for large values of T?

Problem 6: (Canonical ensemble: electrical polarization, adapted from Reif 6.8) The following describes a simple two-dimensional model of a situation of actual physical interest. A solid at absolute temperature T contains N negatively charge impurity ions per cm^3, these ions replacing some of the ordinary atoms of the solid. The solid as a whole is, of course, electrically neutral. This is so because each negative ion with charge $-e$ has in its vicinity one positive ion with charge $+e$. The positive ion is small and thus free to move between lattice sites. In the absence of an external electric field it will, therefore, be found with equal probability in any one of the four equidistant sites surrounding the stationary negative ion (see diagram; the lattice spacing is a).



If a small electric field $\mathcal{E}$ is applied along the x direction, calculate the electric polarization, i.e., the mean electric dipole moment per unit volume along the x direction.

Problem 7: (Canonical ensemble: thermal expansion, adapted from Reif 6.11) Two atoms of mass m interact with each other by a force derivable from a mutual potential energy of the form

$$U = U_0 \left[\left(\frac{a}{x} \right)^{12} - 2 \left(\frac{a}{x} \right)^{6} \right], \tag{1}$$

where x is the separation between the two particles. The particles are in contact with a heat reservoir at temperature T low enough so that $T \ll U_0$, but high enough so that classical statistical mechanics is applicable. Calculate the mean separation $\bar{x}(T)$ of the particles and use it to compute the quantity

$$\alpha \equiv \frac{1}{\bar{x}} \frac{\partial \bar{x}}{\partial T}. \tag{2}$$

(This illustrates the fundamental procedure for calculating the coefficient of linear expansion of a solid.) Your calculation should make approximations based on the fact that the temperature is fairly low; thus retain only the lowest order terms which yield a value of $\alpha \neq 0$. *Hint:* Expand the potential function about its minimum in a power series in x.

Problem 8: (Grand canonical ensemble: two-level system) This problem is similar to Problem 4, but now you consider a system in the grand canonical ensemble, that is, a system in contact with a heat and particle reservoir, so that the temperature T and chemical potential μ are fixed (while the energy and particle number will fluctuate).

(a) Consider a system that may be unoccupied with energy zero or occupied by one particle in either of two states, one of energy ϵ_1 and one of energy ϵ_2. Show that the grand partition function for this system is

$$\mathcal{Z} = 1 + z e^{-\epsilon_1/T} + z e^{-\epsilon_2/T}, \tag{3}$$

where $z = \exp(\mu/T)$ is the "fugacity."

(b) Show that the average occupancy of the system is

$$\overline{N} = \frac{z e^{-\epsilon_1/T} + z e^{-\epsilon_2/T}}{\mathcal{Z}}. \tag{4}$$

(c) Show that the average occupancy of the state at energy ϵ_1 is

$$\overline{N(\epsilon_1)} = \frac{z e^{-\epsilon_1/T}}{\mathcal{Z}}. \tag{5}$$

(d) Find an expression for the average energy of the system.

(e) Allow the possibility that the energy level ϵ_1 and ϵ_2 may be occupied each by one particle at the same time; show that

$$\mathcal{Z} = 1 + z e^{-\epsilon_1/T} + z e^{-\epsilon_2/T} + z^2 e^{-(\epsilon_1+\epsilon_2)/T} = (1 + z e^{-\epsilon_1/T})(1 + z e^{-\epsilon_2/T}). \tag{6}$$

Because $\mathcal{Z}$ can be factorized as shown, we have in effect two independent systems corresponding to the energy levels ϵ_1 and ϵ_2.