Exercise Problems - Week 5

Statistical Mechanics and Thermodynamics

SoSe 2018

May 14, 2018

JGU Mainz - Institut für Physik

Choose 4 of the 6problems below. Each problem is worth 12 points.

Problem 1

A hydrogen atom in equilibrium with a radiation field at temperature T can be in its ground state orbital level (the "$1-s$" level, which is two-fold spin degenerate with energy ϵ_0), or it can be in its first excited state energy level (the "$2-p$" level, which is six-fold degenerate with energy ϵ_1). For the purpose of this problem we shall assume that this atom does not have any other excited states (i.e., no $2s$ level and no levels with the principal quantum number $n > 2$).

1. (a) What is the probability that the atom will be in an "orbital s-state"?
   (b) What is the probability that the atom will be in an "orbital p-state"?
   (c) What is the probability that the atom will be in an "orbital s-level"?
   (d) What is the probability that the atom will be in an "orbital p-level"?
2. If the temperature is such that $k_BT = \epsilon_1 - \epsilon_0$, then show and state which of the two orbital levels is occupied more.
3. Derive an expression for the mean energy of the atom at temperature T and obtain the limiting value of this mean energy as $T \to \infty$.
4. Derive an expression for the entropy of the atom at temperature T and also, from the definition of entropy, state what should be the values of the entropy for this atom in the limits of $T \to 0$ and $T \to \infty$. (If you do not know the answer for the last question, you may obtain the limits from your general expression of entropy.)

Problem 2

An ensemble of non-interacting pairs of Ising spins is in a magnetic field h and at temperature T. Each spin variable s_i^z can only take on values $s_i^z \pm 1$. The two spins within each pair interact according to the Hamiltonian

$$H = -Js_1^z s_2^z - \mu_B h \left(s_1^z + s_2^z\right), \qquad \text{with } J > 0$$

1. Enumerate the possible states of a single pair and compute their corresponding energies.
2. Derive an expression for the average value of a spin, $\langle s_i^z \rangle, (i = 1, 2)$ as a function of J, T and h.
3. Given the above model, determine whether there exists a temperature T_c for which $\langle s_i^z \rangle$ can be non-zero at $h = 0$. Evaluate T.

Problem 3

Consider a system of N independent harmonic oscillators with the same frequency ω. The system is at, temperature T.

1. Show that the partition function of the system is

$$Q_N = \left[2\sinh\left(\frac{\hbar\omega}{2k_BT}\right)\right]^{-N}$$

2. Using this result, obtain the internal energy U of the system as a function of T and N.

3. Show that the heat capacity is

$$C = Nk_B \frac{e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2} \left(\frac{\hbar\omega}{k_B T}\right)^2$$

   and it approaches to 0 as $T \to 0$.

4. Determine its Helmholtz free energy F.

5. Determine its entropy S.

Problem 4

A 3D harmonic oscillator has mass m and the same spring constant k for all three directions. Thus, its quantum-mechanical energy levels are given by

$$E = \hbar\omega\,(n_1 + n_2 + n_3 + 3/2)$$

Neglect the zero point energy in what follows.

1. What are the energy E_0 and degeneracy g_0 of the ground sate? Of the first excited state? Of the second excited state?

2. What is the partition function for this system if only the lowest two (ground and the first exited) energy levels are important? When this approximation valid?

3. What is the free energy in this case?

4. What is the entropy in this case?

5. What is the rms fluctuation $\delta E \equiv \left(\overline{E^2} - (\overline{E})^2\right)^{1/2}$ in the energy in this case?

Problem 5

A quantum particle of charge q is in the potential $V(x) = m\frac{\omega^2 x^2}{2}$ in 1D at temperature T.

1. Find the heat capacity of this system.

2. Find the electric dipole susceptibility of the system. ($d = -(\partial F/\partial \mathcal{E})_{V,N,T}$, $\chi = (\partial d/\partial \mathcal{E})_{V,N,T}$ where $\mathcal{E}$ is the electric field.)

3. For the oscillator state ψ_n in the presence of electric field $\mathcal{E}$ calculate $x_n = \langle \psi_n | \hat{x} | \psi_n \rangle$, and then average displacement $\bar{x} = \sum_n x_n \omega_n$.

Problem 6

Consider N identical and independent particles of spin $1/2$ in a magnetic field so that the energy of each particle is either ϵ or $-\epsilon$ depending upon the orientation of the spin: down or up respectively. The probability of the energy $-\epsilon$ is p and of $+\epsilon$ is $q = 1 - p$.

1. Find the probability that N_1 spins are up and N_2 are down, with $N_1 + N_2 = N$.

2. From this probability find the average or expected value of the energy in terms of p, ϵ, and N.

3. By considering that N_1 and N_2 are continuous rather than discrete variables, find the most likely (i.e., maximal probability) for the values N_1 and N_2 using the approximation that $\log(x!) \approx x \log(x) - x$.
4. Write down a partition function for this system at a temperature T.
5. Find the free energy, the entropy, and the total energy from this partition function. For what value of p will your result in the second part agree with your result for the total energy in this part?