Phy 632: Problem Set 5
(Due: March 31, 2011)

25). In this problem we derive the distribution law in three different ensembles.

a) Consider an ensemble of $\mathcal{A}$ members in which the energy and particle number of each member is *fixed*. This is the microcanonical ensemble. Let E_j denote the energy of a single-particle state j. Use the method of the most probable distribution to recover the Gibbs distribution law, namely

$$P_j = \frac{\exp(-\beta E_j)}{\sum_j \exp(-\beta E_j)} , \tag{1}$$

where β is constant. (Appealing to thermodynamics we find $\beta = 1/k_B T$.)

b) Consider an ensemble of $\mathcal{A}$ members in which the particle number of each member is *fixed*, but the energy is allowed to vary, subject to the constraint that the total energy of the ensemble is fixed. This is the canonical ensemble. Use the method of the most probable distribution to recover the Gibbs distribution law.

c) Consider an ensemble of $\mathcal{A}$ members in which the energy and particle number of each member is allowed to vary, subject to the constraints that the total energy and the total number of particles in the ensemble are fixed. This is the grand canonical ensemble. Let E_{Nj} be the energy of an ensemble member with N particles in the j^{th} quantum state, and let a_{Nj} denote the number of ensemble members in the state j which contain exactly N particles. Use the method of the most probable distribution to determine, ultimately, the distribution law of the grand canonical ensemble, namely,

$$P_\alpha = \frac{\exp(-\beta(E_\alpha - \mu N_\alpha))}{\sum_\alpha \exp(-\beta(E_\alpha - \mu N_\alpha))} , \tag{2}$$

where α is a compact notation for N and j.

26). In the Einstein model of a crystalline solid, each atom sits in a three-dimensional harmonic oscillator potential. The lattice sites on which the atoms sit are all distinguishable. Moreover, all $3N$ oscillators possess the same natural frequency ω_0. Each oscillator has a spectrum given by

$$\varepsilon_n = \hbar\omega_0(n + \frac{1}{2}) , \tag{3}$$

where $n = 0, 1, 2, \cdots$.

a) Show that the free energy of the solid is given by

$$F = 3Nk_{\rm B}T \log\left[1 - \exp(-\hbar\omega_0/k_{\rm B}T)\right] + \frac{3}{2}N\hbar\omega_0 \tag{4}$$

b) Find the average value of n as a function of temperature, $\overline{n}(T)$.

c) Compute the amount of energy required to add one more atom to the solid, without changing the entropy at fixed volume.

d) Determine the heat capacity C (at fixed volume) as a function of temperature. Compute C in the low and high temperature limits.

27). A weight of mass W hangs on a chain of N links, each of length l and of negligible weight. Each link can rotate freely in a vertical plane, so that if θ_n denotes the deflection of link n from the direction a plumb bob hangs, then θ_n ranges from $-\pi$ to π. Note that the energy of the system is given by the configuration of its links, $E = -Wgl\sum_{n=1}^{N}\cos\theta_n$. Determine the average energy of the system. Should your result agree with the prediction of the equipartition theorem in the $k_BT \ll gWl$ limit? Does it?

(*Hint:* Note that $\int_{-\pi}^{\pi} d\theta \exp(z\cos\theta) = 2\pi I_0(z)$, where $I_0(z)$ is a modified Bessel function of the first kind. Note $I_0(z) \sim e^z/\sqrt{2\pi z}[1 + \frac{1}{8z} + \mathcal{O}(z^{-2})]$ as $z \to \infty$.)

28). Consider a two-dimensional classical harmonic oscillator with the Hamiltonian

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{k}{2}(x^2 + y^2)\ . \tag{5}$$

According to the principle of the equipartition of energy, the average energy will be $2k_\mathrm{B}T$. Show that upon transformation to polar coordinates the Hamiltonian becomes

$$H = \frac{1}{2m}(p_r^2 + \frac{p_\theta^2}{r^2}) + \frac{k}{2}r^2\ . \tag{6}$$

What would you predict for the average energy now? Show by direct integration in polar coordinates that $\langle\varepsilon\rangle = 2k_\mathrm{B}T$. Is there anything wrong here? Why not?

29). Polarized proton targets are useful for a variety of investigations in high energy and nuclear physics. Consider a "frozen-spin target," in which the protons in especially prepared ammonia or butanol targets are polarized by applying a magnetic field at low temperatures. It is appropriate to model the target as if it were a system of N distinguishable protons. The proton's magnetic moment μ can be either aligned (+) or anti-aligned (−) with the magnetic field H in the positive z direction, so that the energy of the moments is given by $E = \pm\mu H$. Note that the "+" is associated with the anti-aligned magnetic moment.

a) If the applied magnetic field is 3.5 T and the target is kept at a temperature of 200 mK (1mK = 10^{-3}K), then what is the polarization of the protons in the target? Note that the proton's magnetic moment is 2.793 μ_N, where the nuclear magneton $\mu_N = 3.152 \cdot 10^{-14}$MeV T^{-1}. (The above parameters were taken from H. Dutz *et al.*, "The Bonn Frozen Spin Target for Experiments with Real Photons," in *High Energy Spin Physics, Volume 2: Workshops* (W. Meyer, E. Steffens, and W. Thiel, eds.), Springer-Verlag, Berlin, 1991, p.241.))

b) What are the energy, entropy, and heat capacity (at fixed volume) as a function of temperature? Sketch them. Can the temperature of this system ever be negative? What is the physical origin of this behavior?

(*Hint:* Note N.F. Ramsey, Phys. Rev. **103**, 20 (1956).)

30). Consider a system of fixed particle number N at constant T and V. Use the canonical ensemble to prove that the mean square fluctuations in the energy $\langle(\Delta E)^2\rangle$, where $\langle(\Delta E)^2\rangle \equiv \langle(E - \langle E\rangle)^2\rangle$, are given by $\langle(\Delta E)^2\rangle = k_B T^2 C_V$, where C_V is the specific heat at constant volume. If we assume that $\langle E\rangle$ is given by $3Nk_BT/2$, that is, that the system is an ideal gas, then what is the behavior of $\sqrt{\langle(\Delta E)^2\rangle}/E$ for large N?