PHY 5524: Statistical Mechanics

January 25^{th}, 2012
Assignment # 4
(Due Wednesday February 1^{st}, 2012)

Problem 1

Consider the problem of N spin-1/2 particles (*e.g.* electrons) occupying the N sites of a one-dimensional lattice in the presence of a constant magnetic field $\mathbf{B} = B_0\hat{\mathbf{z}}$.

1.a) First consider the problem using the *microcanonical* ensemble and calculate the entropy of the system as a function of N and E.

1.b) Then consider the problem using the *canonical* ensemble and

1.b.i) Show that the partition function for the system, $Z(N, T)$, may be written as,

$$Z(N, T) = [Z_1(T)]^N \ ,$$

where $Z_1(T)$ is the *single-particle* partition function. Provide explicit expressions for $Z_1(T)$ and for the Helmoltz free energy.

1.b.ii) Obtain the average energy of the system E(N,T).

1.b.iii) Obtain the entropy of the system $S(N, T)$.

1.b.iv) By manipulating the above two expressions, obtain the entropy of the system in terms of N and E. Compare the expression for $S(N, E)$ to the one obtained in **(1.a)** using the *microcanonical* ensemble.

Problem 2

Consider a network of $N = 1006$ non-interacting spin-1/2 particles fixed to the sites of a one-dimensional lattice. The network is placed in an external uniform magnetic field so that its total (fixed) energy is given by $E = -(N_\uparrow - N_\downarrow)\epsilon_0 = -100\epsilon_0$, where ϵ_0 is a positive constant describing how the magnetic moment of each particle couples to the external magnetic field. Now divide the network into a very large component ("*the reservoir*") and a very small one ("*the system*"), with the system containing only 6 spins and the reservoir containing the remaining 1000.

2.a) Compute the probability of finding the system in each of its allowed $2^6 = 64$ microstates.

2.b) Compute the average energy of the system.

2.c) Use the fact that the probability of finding the system in each of its allowed microstates is given by $P_\alpha = \exp(-\beta E_\alpha)/Z$ (where Z is a normalization constant) to compute the temperature of the reservoir in units of ϵ_0. This is the simplest to obtain by taking the ratio of the probabilities of two microstates (*e.g.*, the one having all spins up and the one having all spins down).

2.d) How sensitive is the temperature of the reservoir to the choice of microstates selected in part **(2.c)**? That is, what value do you obtain if you select a different ratio? What do you think will happen to any possible discrepancy in the temperature for $N \to \infty$, i.e. in the thermodynamic limit?

2.e) Without doing any calculation, what do you expect will happen to the temperature if you reverse the spin population? That is, when the energy is $E = +100\epsilon_0$.

Problem 3

Consider N non-interacting distinguishable molecules. The internal Hilbert space of each molecule can be described by two states $|1\rangle$ and $|2\rangle$. When the Hamiltonian is applied to these states one obtains:

$$\begin{aligned} H|1\rangle &= \epsilon|1\rangle - t|2\rangle \ , \\ H|2\rangle &= \epsilon|2\rangle - t|1\rangle \ , \end{aligned}$$

where both ϵ and t are positive constants. Neglect all other degrees of freedom, such as translational or rotational motion of the molecules.

3.a) Find the partition function of the system.

3.b) Find the average energy of the system.

3.c) Find the leading temperature-dependent term of the average energy of the system at low temperatures.

3.d) Find the constant-volume specific heat at low temperatures.