Statistical Mechanics

September 2, 2009

Work 2 of the 3 problems. Please put each problem solution on a separate sheet of paper and put your name on each sheet.

Problem 1

Consider a simple mono-atomic solid consisting of N atoms. Assume that the Einstein approximation can be used to describe the vibrational motion of the atoms.

a. Assume that the vibrational level spacing has a value of $\epsilon = 0.037\,\text{eV}$. Consider the probability that an atom of this solid is in the ground state. At what temperature is this probability equal to 0.1?

b. For a given N and ϵ, how high does the temperature need to be to ensure that effectively no atoms are in the ground state? Is such temperature achievable in an ordinary solid?

c. How would hydrostatic pressure affect the above observations?

Problem 2

Evaluate the equilibrium constant

$$K_P = \frac{P_N{}^2}{P_{N_2}}$$

of the dissociative reaction

$$N_2 \rightleftharpoons 2N$$

at a temperature of $5000\,K$ under the following assumptions:

1. The characteristic temperatures of rotation and of vibration of the N_2 molecule are

$$\begin{aligned} \Theta_r &= 2.84\,K \\ \Theta_v &= 3.36 \times 10^3\,K\ , \end{aligned}$$

   respectively.

2. The dissociation energy is $D_0 = 169.3\,kcal/mole$. This includes the correction for the zero point energy of the vibrations.

3. The electronic ground state of the N_2 molecule has no degeneracy but the electronic ground state of the N atom has a degeneracy of 4 due to electron spin.

Problem 3

Consider an ideal gas composed of N absolutely rigid (i.e. no vibrations) diatomic molecules. Each molecule consists of two atoms of masses m and M, separated by distance d. The gas is held at constant volume V and temperature T. **(a)** Find the partition function of a single molecule, assuming that $T >> \hbar^2(M+m)/Mmd^2k_B$. **(b)** Starting from the total partition function, calculate the internal energy and specific heat of this gas at high temperature. Show that your result is consistent with the equipartition theorem.