Name_____

ME 501

Exam #2
November 15, 2007
Prof. Lucht
ME 255

1. POINT DISTRIBUTION

Problem #1　　　**30　points**　　　_____

Problem #2　　　**30　points**　　　_____

Problem #3　　　**30　points**　　　_____

Problem #4　　　**30　points**　　　_____

Problem #5　　　**30　points**　　　_____

2. EXAM INSTRUCTIONS

- **You must do four (4) out of the five (5) problems and indicate clearly which problem you decided not to have graded.** Please write "**DO NOT GRADE"** in the space next to the problem that you decide not to do.
- This exam is closed book and closed notes.
- Several equation sheets are attached.
- When working the problems, list all assumptions, and begin with the basic equations.
- If you do not have time to complete evaluation of integrals or of terms numerically, remember that the significant credit on each problem will be given for setting up the problem correctly and/or obtaining the correct analytical solution.

1. (30 points) The time-independent Schrödinger wave equation for the harmonic oscillator is

$$- \left(\hbar^2/2\mu\right) \frac{d^2\psi}{dx^2} + V(x)\psi(x) = \varepsilon \psi(x)$$

where $V(x) = k\, x^2/2$ and $x = r - r_e$.   The internuclear spacing is r, and the equilibrium internuclear spacing is r_e. The normalized eigenfunction and energy eigenvalue for the ground state (v = 0) are given by

$$\psi_0(x) = \beta \exp\left(-a\, x^2\right), \quad a = \frac{\pi \mu \nu}{\hbar}, \quad \beta = \left(\frac{2a}{\pi}\right)^{1/4}$$

$$\varepsilon_0 = \left(v + \frac{1}{2}\right) h\nu = \frac{1}{2} h\nu, \qquad k = \left(2\pi \nu\right)^2 \mu$$

Calculate the expectation values in Joules for the potential energy $\langle V(x) \rangle$ and for the kinetic energy $\langle p_x^2/2\mu \rangle$, for N_2 in its ground vibrational state. For nitrogen, the mass of each nucleus is 14 amu and the vibrational frequency $(\nu/c) = 2330$ cm^{-1}. Hint: you may find it useful to express the spring constant k in terms of the parameter a. Also note:

$$\int_0^\infty \exp\left(-b\, x^2\right) dx = \frac{1}{2}\sqrt{\frac{\pi}{b}} \qquad \text{for } b > 0$$

$$\int_0^\infty x^{2n} \exp\left(-b\, x^2\right) dx = \frac{1 \times 3 \times 5 \times \ldots \ldots \times (2n-1)}{2^{n+1}\, b^n} \sqrt{\frac{\pi}{b}} \qquad \text{for } \left(n = 1,\, 2, \ldots \ldots,\ b > 0\right)$$

$$\int_0^\infty x^{2n+1} \exp\left(-b\, x^2\right) dx = \frac{n!}{2\, b^{n+1}} \qquad \text{for } \left(n = 0,\, 1,\, 2, \ldots \ldots,\ b > 0\right)$$

ME 501   Final Exam   12/11/2007   Name_____

Problem #1 Extra Page

2. (30 points) The system shown below has energy levels of $\left(\varepsilon_j/k_B\right)$ = 0 K, 5 K, 10 K, 150K, and 200K. The degeneracy of each of three lower levels is 10^8 and the two upper levels is 10^{10}. The system has only these energy levels; there are no translational, rotational, or vibrational modes. The number of particles in the assembly is 10^5.

(a) Calculate the energy of the assembly at temperatures of 5, 25, and 50 K, assuming corrected Maxwell-Boltzmann statistics. Why is CMB statistics a good assumption?

(b) Estimate the heat capacity of the system at 15 K and at 37.5 K by considering the results of part (a). Comment on the results.

(c) Calculate the assembly entropy S (in J/K) at temperatures of 5, 25, and 50 K. Assume corrected-Maxwell-Boltzmann statistics. Comment on the results.

j	ε_j/k_B (K)	g_j
4	200	10^{10}
3	150	10^{10}
2	10	10^8
1	5	10^8
0	0	10^8

ME 501   **Final Exam**   **12/11/2007**   **Name**_____

Problem #2 Extra Page

ME 501   Final Exam   12/11/2007   Name_____

Problem #2 Extra Page

ME 501   Final Exam   12/11/2007   Name_____

3. (30 points)

(a)   Given the translational energy distribution for a Maxwell-Boltzmann gas

$$f\left(\varepsilon_{tr}\right)d\varepsilon_{tr} \;=\; \frac{2\left(\varepsilon_{tr}\right)^{1/2}}{\pi^{1/2}\left(k_{B}T\right)^{3/2}}\exp\left(-\varepsilon_{tr}/k_{B}T\right)d\varepsilon_{tr}$$

show that the speed distribution is given by

$$f\left(V\right)dV \;=\; \sqrt{\frac{2}{\pi}}\left(\frac{m}{k_{B}T}\right)^{3/2}V^{2}\exp\left(-mV^{2}/2k_{B}T\right)dV$$

(b)   Calculate the value of the mean reciprocal speed $\left\langle\dfrac{1}{V}\right\rangle$ for an assembly of nitrogen (N_2)

molecules at a temperature of 1000 K and a pressure of 2 bars. For N_2, the mass of each nucleus is 14 amu. You will need to use the definite integral formulae from Problem #1.

ME 501   **Final Exam**   **12/11/2007**   **Name**_____

Problem #3 Extra Page

4. (30 points) A rigid pressure vessel with a volume of 1 m^3 contains 0.1 kmols of diatomic oxygen (O_2) and 0.1 kmols of diatomic nitrogen (N_2) at 300K. The gas is then heated to 3000 K. At 3000 K, find the equilibrium ratio $\dfrac{N_N \, N_{NO}}{N_O \, N_{N_2}}$ for the reaction. Consider the reaction

$$O + N_2 \Leftrightarrow NO + N$$

Assume that the molecules are rigid rotators and harmonic oscillators, and use the following data:

Species	θ_{rot}(K)	θ_{vib}(K)	(D_0/hc) (cm^{-1})
N_2	1.998	2358	78,700
NO	1.704	1904	52,300

For the calculation of the electronic partition functions, consider the following electronic levels:

O: **Level 0** [g_0 =5, $\varepsilon_0/hc = 0$ cm^{-1}], **Level 1** [g_1 =3, $(\varepsilon_1/hc) = 158$ cm^{-1}],
    Level 2 [g_2 =1, $(\varepsilon_2/hc) = 226$ cm^{-1}]

N_2: **Level 0** [g_0 =1, $(\varepsilon_0/hc) = 0$ cm^{-1}]

NO: **Level 0** [g_0 =2, $(\varepsilon_0/hc) = 0$ cm^{-1}], **Level 1** [g_1 =2, $(\varepsilon_1/hc) = 121$ cm^{-1}]

N: **Level 0** [g_0 =2, $(\varepsilon_0/hc) = 0$ cm^{-1}]

ME 501   Final Exam   12/11/2007   Name_____
Problem #4 Extra Page

ME 501   Final Exam   12/11/2007   Name_____

5.   (30 points) The temperature of a 1.0 cm^3 copper metal crystal is raised from $T_1 = 400$ K to $T_2 = 500$ K. Calculate the internal energy change of the crystal $(U_2 - U_1)$ due to lattice vibrations $(U_2 - U_1)_{vib}$ and due to the free electron gas $(U_2 - U_1)_{elec}$. Assume that the temperature is high enough that the Einstein model is accurate for determining the internal energy due to lattice vibrations. The Einstein temperature of the copper crystal is $\theta_E = 265\ K$.

The density of the copper is 9000 kg/m^3, the atomic weight of the metal is copper is 63.5 kg/kmol, and there is one free electron per lattice site.

ME 501   **Final Exam**   **12/11/2007**   **Name**_____
Problem #5 Extra Page