Name____________________________

ME 501

Exam #2
2 December 2009
Prof. Lucht

1. POINT DISTRIBUTION

Choose two (2) of problems 1, 2, and 3:

Problem #1	**50 points**	__________________
Problem #2	**50 points**	__________________
Problem #3	**50 points**	__________________

You are required to do two of the problems. Please indicate the problems you have chosen.

2. EXAM INSTRUCTIONS

- Write your name on each sheet.
- This exam is closed book and closed notes.
- Seven 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.

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1. **(50 points)** The system shown below has available energy levels of 0, $\alpha\, k_B$, $2\alpha\, k_B$, and $3\alpha\, k_B$ units, where α = 100 K. The degeneracy of each of the four levels is given by g_j = 10,000 + 10,000 j. The thermodynamic assembly has 1000 particles (N = 1000) and the temperature of the assembly is 200 K. For this dilute assembly, the population distribution for the most probable macrostate is given by the Boltzmann distribution law,

$$N_j = N_{jmp} = N \frac{g_j \exp\left(-\varepsilon_j / k_B T\right)}{\sum_j g_j \exp\left(-\varepsilon_j / k_B T\right)} = N \frac{g_j \exp\left(-\varepsilon_j / k_B T\right)}{Z}$$

(a) Using the Boltzmann distribution law, calculate the most probable macrostate $\{N_{0mp}, N_{1mp}, N_{2mp}, N_{3mp}\}$. Round the populations to the nearest integer.

(b) For corrected Maxwell-Boltzmann statistics, the number of microstates in a particular macrostate $\{N_j\}$ is given by

$$W_{CMB}\left(\left\{N_j\right\}\right) = \prod_j \frac{g_j^{N_j}}{N_j!}$$

Use the Stirling approximation ($\ln N! \approx N \ln N - N$) to show

$$\ln\left[W_{CMB}\left(\left\{N_j\right\}\right)\right] = N + \sum_j N_j \ln\frac{g_j}{N_j}$$

(c) What is the entropy (J/K) of the assembly?

(d) What is the energy (J) of the assembly?

(e) Calculate the number of microstates associated with two macrostates that are very similar to the most probable macrostate. Macrostate A is given by $\{N_{0mp}, N_{1mp}+5, N_{2mp}-10, N_{3m}+5\}$. Macrostate B is given by $\{N_{0mp}, N_{1mp}-5, N_{2mp}+10, N_{3m}-5\}$. Comment on the results.

j	ε_j	g_j
3	300 k_B	40,000
2	200 k_B	30,000
1	100 k_B	20,000
0	0	10,000

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2. Diatomic hydrogen gas is contained in a rigid pressure vessel with $\forall = 1.0 \; m^3$. The initial pressure is 1 kPa and the temperature is 50 K.

(a) Calculate the amount of heat transfer required to raise the temperature of the gas from 50 K to 100 K. Assume that the H_2 is an ideal gas (translational mode fully excited), a rigid rotator, and a harmonic oscillator (see equation sheets). For H_2, odd-J rotational levels have a nuclear spin statistical weighting factor (NSSW) of 3, and even-J rotational levels have an NSSW of 1. **Do not assume that** $Z_{rot} = T / \sigma \theta_{rot}$. Instead use the combined rotational-nuclear partition function:

$$Z_{rot,nuc} = \sum_J \left(NSSW\right)_J \, g_{rot,J} \exp\left(-\frac{\varepsilon_J}{k_B T}\right)$$

Consider rotational levels with $0 \le J \le 4$. Recall that $P\forall = N k_B T$. You may the tables on the next page to be useful in organizing your work.

Answer: 2975 J

(b) Calculate the change in entropy $S_2 - S_1$ as the hydrogen gas is heated from 50 K to 100 K at constant volume.

For H_2: $\theta_{vib} = 6339 \, K$, $\theta_{rot} = 87.5 \, K$, $B_e = 60.848 \; cm^{-1}$, $\omega_e = 4405.3 \; cm^{-1}$.

The ground electronic level has a degeneracy of 1: **Level 0:** $g_0 = 1$, $\left(\varepsilon_0 / hc\right) = 0 \; cm^{-1}$

Answer: 42.24 J/K

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T= 50 K

J					
0					
1					
2					
3					
4					

T = 100 K

J					
0					
1					
2					
3					
4					

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3. A rigid pressure vessel with a volume of 1 m^3 contains 0.1 kmols of diatomic oxygen (O_2) at 300K. The gas is heated to 3500 K. How many O-atoms (monatomic oxygen) does the pressure vessel contain at 3500 K, and what is the assembly pressure in Pascals?

Hint: Consider the reaction $O_2 \leftrightarrow 2O$. Also, remember that $P\forall = N k_B T$. The general solution for quadratic equations is in the equation sheets. Alternatively, you could iteratively solve the equation that you get by assuming for the initial step that N_{O2} at 3500 K is the same as the initial value at 300K.

Assume that diatomic oxygen is a rigid rotator and harmonic oscillator, neglect any ionization, and use the following characteristic temperature and dissociation energy data:

	Θ_{rot}(K)	**Θ_{vib}(K)**	**(D_0/hc) (cm^{-1})**
O_2	2.08	2280	41,300

Consider the following electronic levels:

O_2: **Level 0:** $g_0 = 3$, $(\varepsilon_0 / hc) = 0 \ cm^{-1}$

Level 1: $g_1 = 2$, $(\varepsilon_1 / hc) = 7{,}920 \ cm^{-1}$

O: **Level 0:** $g_0 = 5$, $(\varepsilon_0 / hc) = 0 \ cm^{-1}$

Level 1: $g_0 = 3$, $(\varepsilon_0 / hc) = 158 \ cm^{-1}$

Level 2: $g_0 = 1$, $(\varepsilon_0 / hc) = 226 \ cm^{-1}$

Answers: 5.484×10^{24}, 3.043 MPa