Statistical Mechanics

September 12, 2003

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

a) Consider a single walled nanotube which metallic in nature (ie: full conjugated C sp2 hybridized orbitals) so that it is 1-Dimensional in nature. If that nanotube has 1 free electron per atom and an atomic spacing of 3.34 $\mathring{A}$ at $T = 0$, calculate the Fermi energy for the 1-D metal.

b) Consider a non-interacting non-relativistic gas of N spin $\frac{1}{2}$ fermions at $T = 0$ in a box of area A.

i) Find the Fermi Energy

ii) Show that the total energy is given by:

$$E = \tfrac{1}{2} n e_F$$

Problem 2

Consider a gas with a very short-range attractive interactions that can be approximated by

$$\exp\left(-\frac{V_{ij}}{kT}\right) = 1 + \alpha\delta(\mathbf{r}_i - \mathbf{r}_j),$$

where α is a temperature-dependent parameter with the dimension of volume. Assume for simplicity that the density of the gas is sufficiently low, so that one can neglect the probability of three or more particles being at exactly the same point in space. Find the second virial coefficient and the equation of state of this gas.

Problem 3

Carbon Dioxide, CO_2, is a linear triatomic molecule with an electronic ground state of $^1\Sigma_g^+$. It has four normal modes of vibration; two bending modes and one in phase and one out of phase stretching modes ($\tilde{\nu}_1 = \tilde{\nu}_2 = 667.3$ cm^{-1}, $\tilde{\nu}_3 = 1383.3$ cm^{-1}, $\tilde{\nu}_4 = 2439.3$ cm^{-1}), and a rotational constant of 0.390 cm^{-1}. Assuming ideal behavior, calculate the entropy and constant volume heat capacity at 298 K and 1 bar. (Note: the molar mass of CO_2=44 g/mole and the gas constant, R, is 8.314 J/mol K) Boltzman constant, $k = 1.381 \times 10^{-23}$ J/K; $c = 3 \times 10^8$ m/sec= 3×10^{10} cm/sec.