Indian Institute of Science Education and Research, Trivandrum

PHY-321 Statistical mechanics end semester exam 20.4.2015

Instructions:

1. **Be clear. Be neat. Be specific.**
2. **Total is 50 points.** You are expected to answer
   (a) All 5 problems in Part A [5×4 points = 20 points]
   (b) All 4 problems in Part B [4×5 points = 20 points]
   (c) 1 out of the 2 problems in Part C [1×10 points = 10 points]
3. Useful formulae are given in Page 5.

Part A

1. **Van der Walls gases** **4 points**

   The partition function for an interacting gas is assumed to be:

$$Z = \left(\frac{V - Nb}{N}\right)^N \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3N/2} e^{N^2a^2/(Vk_B T)}$$

   where a and b are constants. Show that the pressure is of the same form as Van der Waals equation.

   Note: The Van der Walls equation of state is

$$\left(P + \frac{N^2}{V}a\right)(V - Nb) = Nk_B T$$

2. The average kinetic energy of the hydrogen atom in a certain stellar atmosphere (assumed to be in thermal equilibrium) is 1.0 eV.
   (a) What is the temperature of the stellar atmosphere in Kelvin? **(2 points)**
   (b) What is the ratio of the number of atoms in the second excited state ($n = 3$) to the number in the ground state? **(2 points)**

3. **Magnetic atoms** **4 points**

A solid contains N magnetic atoms having spin 1/2. At sufficiently high temperatures each spin is randomly oriented. At sufficiently low temperatures all the spins become oriented along the same direction (i. e. Ferromagnetic). Let us approximated the heat capacity as a function of temperature T by

$$C_V(T) = \begin{cases} c_1 \left(\frac{2T}{T_1} - 1\right) & \text{if } T_1/2 < T < T_1 \\ 0 & \text{otherwise} \end{cases}$$

where T_1 is a constant. Find the maximum value of c_1 of the specific heat.

4. **Classical Hard sphere gas** **4 points**

Calculate b_2 and b_3 (Virial coefficients) for a classical hard sphere with hard-sphere diameter a.

Express the equation of state of a classical hard-sphere gas in the form of a virial expansion. Include terms up to the third virial coefficient.

5. A system consists of N non-interacting, distinguishable two-level atoms. Each atom can exist in one of two energy states, $E_0 = 0$ or $E_1 = \epsilon$. The number of atoms in energy level, E_0 is n_0 and the number of atoms in energy E_1 is n_1. The internal (macroscopic) energy of this system is $U = n_0 E_0 + n_1 E_1$.

   (a) Compute the number of microstates for energy U. **(1 point)**

   (b) Compute the entropy of this system as a function of U. **(1 point)**

   (c) Compute the temperature of this system. Under what conditions can it be negative? **(1 point)**

   (d) Compute the heat capacity for a fixed number of atoms N. **(1 point)**

Part B

6. **The Massieu Function** $J(\beta, V, N)$

Whereas the entropy is an extremum function $S(U, V, N)$, it is sometimes useful to use a related extremum function, $J(\beta, V, N)$ where $\beta = 1/(k_B T)$ and T is temperature. For this function, β and U are conjugate variables (like pressure and volume).

   (a) Derive an expression for the differential quantity dJ in terms of variations $d\beta$, dV, and dN. **(1 point)**
   (Hint: as an initial guess for J, try either $J = S + \beta U$ or $J = S - \beta U$).

(b) Using additional reduced variables $\pi = p/T$ and $m = \mu/T$, write Maxwell relations for: **(3 points)**

$$\text{(i)} \quad \left(\frac{\partial \pi}{\partial N}\right)_{\beta,V} \qquad \text{(ii)} \quad \left(\frac{\partial U}{\partial V}\right)_{\beta,N} \qquad \text{(iii)} \quad \left(\frac{\partial U}{\partial N}\right)_{\beta,V} \tag{1}$$

(c) What is the relation between J and the Helmholtz free energy $F(T, V, N)$? **(1 point)**

7. **Proton NMR**

The nucleus of a hydrogen atom, a proton, has a magnetic moment. In a magnetic field, the proton has two states of different energy — spin up and spin down. This is the basis of proton NMR. The relative populations can be assumed to be given by the Boltzmann distribution, where the difference in energy between the two states is $\Delta E = g\,\mu\,B$, $g = 2.79$ for protons, and $\nu = 5.05 \times 10^{-24} J\ Tesla^{-1}$. For a 300 MHz NMR instrument, $B = 7\ Tesla$.

(a) Compute the relative population difference,

$$\frac{|N_+ - N_-|}{N_+ + N_-} \tag{2}$$

at room temperature for a 300 MHz machine. **(2 points)**

(b) Describe how the population difference changes with temperature. At what temperature population inversion occur? **(2 points)**

(c) What is the partition function? **(1 point)**

8. **Proteins and Quantum mechanics**

Let us assume for a moment that a protein of mass $50,000 g/mol$ can freely move in the cell. Approximate the cell as a cubic box 10m on a side.

(a) Compute the translational partition function for the protein in the whole cell. Are quantum effects important? **(2 points)**

[Hint: Use the density of states for a non-relativistic particle to compute the partition function.]

(b) The living cell, however, is very crowded with other molecules. Now assume that the protein can freely move only 5Angstrom along each, $x-, y-$ and $z-$direction before it bumps into some other molecule. Compute the partition function and conclude whether quantum mechanical effects are important in this case. **(2 points)**

(c) Now assume that we deuterate all the hydrogens in the protein (replace hydrogens with deuterium atoms). If the protein mass is increased by 10%, what happens to the free energy of the modified protein? By how much does it change? **(1 point)**

9. **Black-holes and canonical ensemble**

A black hole is a region of space time which has a sufficiently high matter density that the escape velocity exceeds the speed of light. A black hole of mass M has radius

$$R_s = \frac{2GM}{c^2},$$

where G is the gravitational constant and c is the speed of light. Hawking showed that black holes emit black body radiation with a temperature

$$T_{BH} = \frac{\hbar c^3}{8\pi\, G\, M\, k_B},$$

where $\hbar$ is the Planck constant, k_B is the Boltzmann constant. The energy of the black hole is $E = M\, c^2$.

(a) Calculate the specific heat of a black hole. Can we use canonical ensemble to derive thermodynamic quantities for this system? State your reasons. **(3 points)**

(b) Using the relation,

$$\frac{1}{T} = \frac{\partial S}{\partial E},$$

calculate the entropy of the black hole (assume that the entropy is zero for M = 0). Express your answer in terms of the surface area

$$A = 4\pi R_s^2$$

measured in units of the Planck length

$$\ell_P = \sqrt{\frac{\hbar G}{c^3}}$$

Is this entropy extensive? **(2 points)**

Part C

11. **Bose Einstein Condensation in 1 and 2-dimensions** **10 points**

Consider a gas of non-interacting, non-relativistic, identical Bosons. Explain whether and why the Bose-Einstein Condensation that applies to 3-dimensional gas also applies to a 2-dimensional or 1-dimensional gas.

Hint: Bose-Einstein Condensation occurs at $\mu = 0$.

OR

Suppose that for some sample the density of states of the electrons $D(\epsilon)$ is a constant D_0 for energy $\epsilon > 0$ ($D(\epsilon) = 0$ for $\epsilon < 0$) and that the total number of electrons is equal to N.

(a) Calculate the Fermi energy at 0 K **4 points**

(b) For non-zero temperatures, derive the condition that the system is non-degenerate. **3 points**

(c) Show that the electronic specif heat is proportional to the temperature, T, when the system is highy degenerate. **3 points**

Useful formulae

1. $k_B = 1.38 \times 10^{-23} m^2\, kg\, s^{-2} K^{-1}$; $\hbar = 1.06 \times 10^{-34} m^2 kg s^{-1}$
   $1eV = 1.60 \times 10^{-19}\, J$; $m_e = 9.10 \times 10^{-31}\, Kg$

2. Stirling's approximation $\ln n! \simeq n \ln n - n$

3. Multinomial distribution

$$(a_1 + a_2 + a_3 + \cdots)^M = \sum_{n_i=0}^{M} \frac{M!}{n_1!\, n_2!\, \cdots} a_1^{n_1} a_2^{n_2} \cdots$$

4. $dU = T\, dS - P\, dV \qquad dF = -S\, dT - P\, dV \qquad dG = -S\, dT + V\, dP$

5.

$$\frac{1}{T} = \frac{\partial S}{\partial U}; \qquad \frac{P}{T} = \frac{\partial S}{\partial V}; \qquad \frac{\mu}{T} = -\frac{\partial S}{\partial N}; \qquad C_V = \left.\frac{\partial U}{\partial T}\right|_{V,N}$$

6.

$$\langle E \rangle \equiv \bar{E} = -\frac{\partial \ln Z}{\partial \beta}; \qquad \langle P \rangle \equiv \bar{P} = k_B T \frac{\partial \ln Z}{\partial V}$$

7.

$$F = U - T\, S; \qquad G = E - T\, S + P\, V$$

$$S = -\left.\frac{\partial F}{\partial T}\right|_{V,N}; \qquad P = -\left.\frac{\partial F}{\partial V}\right|_{T,N}; \mu = \left.\frac{\partial F}{\partial N}\right|_{T,V}$$

8. Density of states in $k-$ space is given by $g(k)dk$.

Geometric series $\displaystyle\sum_{m=0}^{\infty} r^m = \frac{1}{1-r}$ $(r < 1)$ Gaussian integral $\displaystyle\int_0^{\infty} dx\, e^{-x^2/a^2} = a\sqrt{\pi}$
