6304NSC HONOURS STATISTICAL AND CONDENSED MATTER PHYSICS

PROBLEM SHEET 2

1.
(a) Use the method of Lagrange Multipliers to find the maximum volume $f(\underline{x}) = x_1 x_2 x_3$ of a cuboid with orthogonal sides of length x_1, x_2, x_3 subject to the constraint

$$g(\underline{x}) \equiv 2x_1 + x_2 + x_3 = 12.$$

(b) As a check on your working, re-solve the same problem without Lagrange Multipliers, by using the constraint condition to eliminate one of the three x variables.

2. Use the method of Lagrange Multipliers to obtain the Grand Distribution $f(i,N)$ by maximising the Shannon Entropy S subject to three constraints:

 (i) Normalisation of the probability distribution
 (ii), (iii) Specified average values of energy E and particle number $\langle N \rangle$,

$$\sum_{i,N} f_{i,N} E_i = U, \quad \sum_{i,N} f_{i,N} N = \langle N \rangle$$

Note: do not be confused by notation: we are maximising S here, not f as in problem 1 and the Notes page discussing Lagrange multipliers in general. The $\{f(i,N)\}$ are now the independent variables – i.e. they are the "x" variables.

3. Consider two systems in weak thermal and diffusive contact with one another. Show that the Grand partition function for the combined system is the product of the separate Grand partition functions. Assume both are in contact with a larger thermal and particle bath which determines the temperature and chemical potential.

4. Just as temperature can be defined even for the micro-canonical ensemble (no thermal coupling) of a large system via $1/T = \partial S(U)/\partial U$, so too can chemical potential be defined for a system not in chemical equilibrium with a bath. Specifically, it can be shown (see Chap. 7) that

$$\mu = \left.\frac{\partial F}{\partial N}\right|_{V,T}$$

where F is the Helmholtz free energy, $F = U - TS = -k_B T \ln(Z)$.

(a) Consider a classical ideal gas consists of atoms of mass m. Calculate its chemical potential as a function of temperature and volume.

(b) Consider a certain surface which is able to adsorb these gas atoms. The atoms can be adsorbed at certain sites. At type-A sites only one atom can be adsorbed, and when present it has energy $-\varepsilon_A$ where ε_A is a positive number. Type-B sites are roomier and can adsorb either one atom with energy $-\varepsilon_B$, or two gas atoms with total energy $-2\varepsilon_C$. (Here the ε's are positive quantities.) Find the mean number of atoms on

 (i) an A site (ii) a B site

as a function of temperature and chemical potential.

(c) Hence calculate the mean number of atoms on an A site as a function of temperature and volume, when the surface of part (b) is exposed to the gas of part (a).

5. Compare the expression in 6g.2 to the uncertainty relation argument in section 6b.

6. Investigate the existence of Bose condensation of a *box-confined* gases of free Bosons
(a) in <u>two</u> dimensions
(b) in <u>one</u> dimension

7. Within continuum grand ensemble theory, investigate the existence of Bose condensation with *harmonic* confinement in *one dimension*.

8. Working with the grand ensemble description of a gas of noninteracting Bosons, find the fractional RMS fluctuation in occupation number of a single-particle orbital j.
i.e. find

$$\Delta n_j = \left[\frac{\left\langle (n_j - \overline{n}_j)^2 \right\rangle}{\overline{n}_j^2} \right]^{1/2}.$$

In particular, consider Δn_0 in the case where $T<T_c$, where Bose-condensation occurs. What does this last case imply about the uncertainty in the *total* number of atoms in the gas? What does this suggest about the appropriateness of the grand canonical ensemble description of BEC of a fixed number of atoms. (There has been some controversy about this: see e.g. H. D. Politzer, Phys. Rev. A **54**, 5048 (1996).).