UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:-

M.Sci.

Phys & Astro 4472: Order and Excitations in Condensed Matter

COURSE CODE : **PHAS4472**

UNIT VALUE : **0.50**

DATE : **27-APR-06**

TIME : **10.00**

TIME ALLOWED : **2 Hours 30 Minutes**

06-C1113-3-40

TURN OVER

Answer THREE questions

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

Boltzmann's constant, k_B=1.38 × 10^{-23} JK^{-1}
Bohr magneton, μ_B=9.27 × 10^{-24} JT^{-1}
Permeability of free space, μ_0=4π × 10^{-7} Hm^{-1}

1. (a) The unit cell structure factor F for the scattering of X-rays from a single crystal may be written in the form

$$F = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}.$$

Starting from the scattering amplitude for a distribution of electrons, outline the derivation of this expression, taking care to define all of the terms appearing on the right hand side of the equation. [4]

(b) Alkaline metals combine with the "Buckyball" molecule C_{60} to form a series of compounds with interesting structural and transport properties. For example, Rb_xC_{60} adopts the face centered cubic structure (*fcc*) for x=3, the body centered tetragonal (*bct*) structure for x=4, and the body centered cubic (*bcc*) structure for x=6. Using the conventional cubic cell draw cross-sections at z=0, 1/2 and 1 perpendicular to the [001] direction through the structure of Rb_xC_{60} for x=3 and 6. (You can ignore the Rb atoms and the internal structure of the C_{60} molecule, i.e. represent the molecule as a sphere of charge.) [4]

(c) Write down the structure factors for the *fcc* and *bcc* structures (again ignoring the Rb atoms and the internal structure of the C_{60} molecule) and identify the Miller indices and scattering angles (2θ) of the first three *allowed* Bragg peaks for each structure in a X-ray powder diffraction experiment performed at a wavelength of 1.54 Å. (The lattice parameter of Rb_3C_{60} is a=14.436 Å, and that of Rb_6C_{60} is a=11.548 Å) [6]

(d) The charge density $\rho(r)$ of a Buckyball molecule may be approximated as a surface of charge of radius R:

$$\rho(r) = \frac{360}{4\pi R^2}\delta(r - R).$$

Calculate the form factor within this approximation. X-ray diffraction experiments on Rb_3C_{60} show that instead of a steady decrease in the observed scattered intensity, the (311) Bragg peak is the most intense. Use this observation to estimate the radius of the C_{60} molecule. [6]

2.(a) Consider a material with n non-interacting localised magnetic ions per unit volume, each with a magnetic moment of $\mu = m_J g \mu_B$ with g=2 and where the quantum number m_J has allowed values of $m_J = \pm\frac{1}{2}$. Show that the magnetization M of the localised moments is given by [4]

$$M = n\mu_B \tanh\left(\frac{\mu_B \mathrm{B}}{k_B T}\right)$$

where **B** is the applied field. Hence show that in the small B limit the susceptibility is given by

$$\chi = \frac{n\mu_0\mu_B^2}{k_B T}$$

(b) Now assume that the moments interact, and that the interaction between them produces an effective mean field B_{mf}=$\mathrm{B} + \lambda M$, and λ is the molecular field constant. Show that the material becomes ferromagnetic in zero applied field below the Curie temperature

$$T_C = \frac{n\lambda\mu_B^2}{k_B}$$

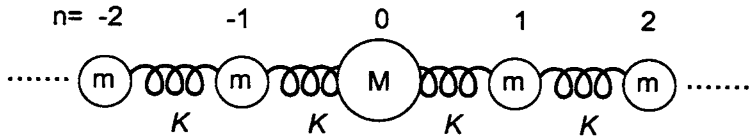
and make a sketch of the spontaneous magnetization versus temperature. [4]

(c) In the *inter-metallic* compound $GdAl_2$ the Gd^{3+} ions sit on a face centred cubic lattice (a = 7.9 Å) and have the electronic configuration $4f^7$. Apply Hund's rules to calculate J for Gd^{3+} and hence determine the effective magnetic moment μ_{eff} of the free ion. (The Landé g factor of the Gd^{3+} ion is 2.) [4]

(d) Experiments show that $GdAl_2$ orders ferromagnetically at T_C = 168 K and that at low temperatures the saturated value of the moment μ_{eff}=7.4 μ_B. Determine the value of the mean field B_{mf}, and estimate the magnitude of the dipolar field acting between two Gd ions. (Note that in general, $T_C = n\lambda\mu_{eff}^2/3k_B$.) [4]

(e) Using the results you have obtained above discuss the nature of the coupling between magnetic moments in $GdAl_2$. [4]

3.(a) Potassium metal adopts the body centered cubic structure. Neutron spectroscopy reveals that the transverse acoustic and longitudinal acoustic modes propagating along the [001] direction are degenerate. Explain this result by evaluating the inter-planar force constants J_x, J_y and J_z. (You may use the fact that the inter-planar force constants are related to the inter-atomic force constant K by $J_x = K\sum_j x_j^2/r^2$, etc., where r is the bond length.) [5]



(b) Consider the figure above, in which a mass defect has been inserted in a linear chain of atoms interacting through nearest-neighbour springs of constant K. In contrast to the travelling wave solutions found for the uniform chain, the mass defect can be expected to produce localised modes of vibration. One possible trial solution for the atomic displacements u_n is given by

$$u_n = Ae^{-q|n|-i\omega t}.$$

Assuming Hooke's law to be valid, write down the equations of motion for the atoms at $n = 1, 0$ and -1 and use the trial solution to show that this leads to two equations: [6]

$$M\omega^2 = 2K(1 - e^{-q})$$
$$m\omega^2 = K(2 - e^{q} - e^{-q}).$$

(c) Hence show that the angular frequency and wavevector are given by [4]

$$\omega^2 = \frac{4K}{M}\frac{m}{2m - M}$$
$$q = log_e\left(1 - \frac{2m}{M}\right).$$

(d) For the trial solution to be valid we require that the values of ω and q are such that the solution is oscillatory in time and does not diverge as a function of n. Investigate the restrictions that this places on the ratio of m/M. (Hint: Do not assume that $M > m$ as implied by the relative sizes of the atoms shown in the figure.) [5]

4. (a) Starting with the Heisenberg exchange interaction, describe the key assumptions of linear spin wave theory and discuss their limitations. Sketch a spin wave propagating in a classical ferromagnet. [4]

(b) The magnon dispersion for a three-dimensional Heisenberg ferromagnet on a body centered cubic lattice is

$$\hbar\omega = 16\mathcal{J}S[1 - \cos(q_x a/2)\cos(q_y a/2)\cos(q_z a/2)].$$

where $\mathcal{J}$ represents the nearest-neighbour exchange, S the spin quantum number and a the lattice parameter. Show that in the small $q = \sqrt{q_x^2 + q_y^2 + q_z^2}$ limit the dispersion is $\hbar\omega = 2\mathcal{J}Sq^2a^2$. [2]

(c) Hence by assuming periodic boundary conditions show that at low temperature the density of magnon states $g(\omega)$ is given by [3]

$$g(\omega) = \frac{V}{4\pi^2}\left(\frac{\hbar}{2\mathcal{J}Sa^2}\right)^{3/2}\omega^{1/2}.$$

(d) By evaluating the number of magnons excited as the magnet is warmed from low temperatures show that the decrease in magnetization is proportional to $T^{3/2}$ (Bloch's Law). [5]

(e) In the case of a one-dimensional ferromagnet the dispersion simplifies to

$$\hbar\omega = 4\mathcal{J}S[1 - \cos(qa)].$$

Use this result to argue that long-range magnetic order is impossible at finite temperature in one dimension. [6]

(You may make use of the result that

$$\int_0^\infty \frac{x^{1/2}}{e^x - 1}\,dx = \text{Constant}$$

)

5. (a) Compare and contrast the relative merits of neutrons and x-rays for studies of structure and dynamics of condensed matter. [5]

(b) Describe how scattering techniques can be used to tackle three of the following four problems. In each case provide sketches of the required equipment, explain principles of operation and identify the key physical quantities obtained.

i. The structure of dilute colloids in solution.

ii. The determination of the magnetic structure of an antiferromagnet using powder diffraction.

iii. The measurement of phonon dispersion using x-ray inelastic scattering.

iv. The exchange constants in a magnet using neutron scattering techniques. [15]