Answer EVERY question from section A and TWO questions from section B.

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

Mass of the electron	m_e	$=$	9.11×10^{-31} kg
Charge on the electron	e	$=$	-1.602×10^{-19} C
Permittivity of free space	ϵ_0	$=$	8.854×10^{-12} F m^{-1}
Bohr magneton	μ_B	$=$	9.273×10^{-24} J T^{-1}
Boltzmann's constant	k_B	$=$	1.38×10^{-23} J K^{-1}
Planck's constant/2π	$\hbar$	$=$	1.05×10^{-34} J s

SECTION A

[Part marks]

1. For an ionic solid, give an equation describing the interaction between any two ions at long range. Define any symbols you use. **[3]**

   If the crystal structure is held fixed, but the lattice constant is increased by 1%, does the strength of the interaction increase or decrease? By how much? **[4]**

2. With the aid of a sketch, show that packing of spheres with the minimum of empty space between them can form a crystal lattice which obeys the definition of the hexagonal crystal system. **[4]**

   For this "hexagonal close-packed" lattice, determine the ratio of the a and c lattice constants. **[3]**

3. In a free electron metal, why is it not possible for all the electrons to have the same energy? **[4]**

   Imagine shining light on a piece of this metal. Suppose the wavelength of the light is varied, starting from a large value and gradually becoming smaller. At a certain value electrons begin to be emitted from the metal. Sketch the variation of the maximum kinetic energy of emitted electrons against the wavelength of the incident light. **[3]**

4. The "tight-binding" method considers the effect on the energy of electrons in a crystal of overlap between neighbouring atomic orbitals.

Sketch how the typical atomic wavefunctions on two adjacent sites in a crystal overlap to form *bonding* and *antibonding* configurations. Label the axes of your sketch. For this purpose, you should consider the atoms to be isolated from the rest of the crystal. **[3]**

Give two reasons why the energy of the antibonding wavefunction should be higher than that of the free atom. **[3]**

5. The densities of electrons and holes in a certain semiconductor are given respectively by:

$$n = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(\mu - E_C)/k_B T}$$

$$p = 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(E_V - \mu)/k_B T}$$

Explain the meaning of the symbols m_e and m_h and why they do not necessarily have the same value. **[3]**

For the case of an intrinstic (undoped) semiconductor with $m_e = m_h$, derive an expression for the Fermi level μ in terms of the symbols used above. **[4]**

6. Since electrons are particles that can move they can carry a thermal current; as they are charged they can carry an electric current as well. How does the ratio of the thermal conductivity to electrical conductivity in a metal vary with temperature? **[2]**

To obtain this temperature dependence the same relaxation time has been used for the electric and thermal currents. Explain why this is not always a correct thing to do. **[4]**

7. A p-n junction is formed when a block of p-type semiconductor (containing n_A acceptor atoms per unit volume) is brought into electrical contact with a block of n-type material (donor concentration n_D).

(a) Sketch how the concentration of free carriers varies across the junction and explain how this leads to the formation of an empty "depletion zone" . **[6]**

(b) Show that the width of the depletion zone on the n-side of the junction, w_n, varies with the potential difference across the junction, ΔV, according to the expression below. **[10]**

$$w_n = \left(\frac{2\epsilon\epsilon_0 n_A \Delta V}{e n_D (n_A + n_D)} \right)^{\frac{1}{2}}$$

(c) Deduce an analogous expression for the width on the p-side of the junction, w_p, and hence the total width of the depletion zone, w_{tot}. **[7]**

(d) Explain how w_{tot} changes when an additional voltage V is applied across the junction and hence how current rectification takes place. **[7]**

8. The internal energy of a harmonic crystal can be written as

$$U = \underbrace{U_0}_{1} + \int_0^\infty \underbrace{\sum_p D_p(\omega)}_{2} \underbrace{\hbar\omega}_{3} \underbrace{\frac{1}{\mathrm{e}^{\hbar\omega/k_BT} - 1}}_{4} \, \mathrm{d}\omega$$

Explain the meanings of the numbered terms in this expression. **[8]**

Consider a single two-dimensional sheet of graphite (usually called graphene). In its unit cell there are two carbon atoms. How many branches in the phonon spectrum are there? What kind of phonons do they correspond to? **[4]**

Part of the phonon spectrum of graphene can be described by the Debye model, and part by the Einstein model. The total spectrum can then be described by the sum of the two parts. What type of phonons does the Debye model describe? What type of phonons does the Einstein model describe? **[2]**

For the Debye model, the relation between the phonon frequency ω and wavevector k is $\omega = ck$. What is c? **[1]**

For one branch, the k-space density of states is

$$\tilde{D}_p(k) \, \mathrm{d}k = \frac{Na}{2\pi} k \, \mathrm{d}k$$

where a is the area of the graphene unit cell. Determine the corresponding $D_p(\omega)$ for the Debye model. **[3]**

For the Einstein model the phonon frequency ω is independent of k and $D_p(\omega) = N\delta(\omega - \omega_{Einstein})$ for N unit cells. Using this result, and the results obtained earlier for the Debye model, construct $D(\omega) = \sum_p D_p(\omega)$ for graphene. **[2]**

Show that

$$U = U_0 + 3N \left\{ \frac{\hbar\omega_{Einstein}}{\mathrm{e}^{\hbar\omega_{Einstein}/k_BT} - 1} + k_BT \left(\frac{T}{\theta}\right)^2 \int_0^{x_D} \frac{x^2}{\mathrm{e}^x - 1} \, \mathrm{d}x \right\}$$

where $k_B\theta = \hbar c\sqrt{2\pi/a}$ and $x_D = \hbar\omega_D/k_BT$. What is ω_D? **[5]**

At low temperature $U \approx U_0 + 6\zeta N k_B T(T/\theta)^2$ where $\zeta = \int_0^\infty x^2/(\mathrm{e}^x - 1) \, \mathrm{d}x$. Which phonons are contributing to the thermal energy at low temperature? **[1]**

Determine the heat capacity at low temperature, and explain how the dimensionality of the system reveals itself in your expression. **[4]**

9. If a paramagnetic solid is placed in a magnetic field, is the magnetisation parallel or anti-parallel to the magnetic field? Briefly explain why. **[2]**

In a ferromagnet the magnetic dipoles spontaneously align parallel to one another. What interaction causes this, and what is its origin? **[3]**

Sketch the variation with temperature of the magnetisation of a ferromagnet in the absence of an applied magnetic field. **[4]**

Consider a non-magnetic crystal in which a fraction α of the atoms have been replaced with magnetic atoms with spin $S = \frac{1}{2}\hbar$, and gyromagnetic ratio $g = 2$. If the z-component of the spin is $S_z = m\hbar$, what is the energy of interaction between the atom and a magnetic field aligned along the z direction with strength B? **[1]**

Show that the magnetisation of the crystal when a magnetic field B is applied is

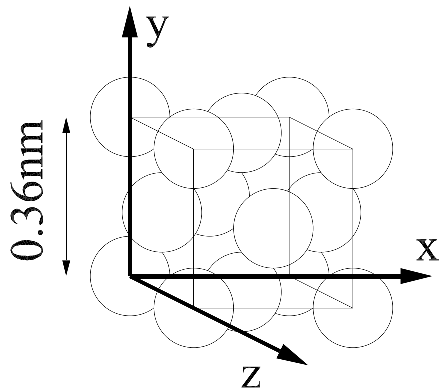
$$M = \alpha n \mu_B \tanh\left(\frac{B\mu_B}{k_B T}\right)$$

where n is the number of atoms per unit volume. **[10]**

Show that the high temperature susceptibility is $\chi = \partial M/\partial H = C/T$ and find C. **[5]**

If the fraction of magnetic particles is very low, would you expect the system to be ferromagnetic? Explain your answer. **[5]**

10. The following picture shows a face-centred cubic (FCC) lattice representing the arrangement of atoms inside a crystal of copper.



(a) Using the Cartesian coordinate system indicated in the picture, write down a set of *primitive* lattice vectors to describe the lattice. **[3]**

(b) What is the volume of the primitive unit cell described by these vectors? How many atoms are contained within the volume? **[7]**

(c) What are the corresponding reciprocal lattice vectors? Draw a sketch of the reciprocal lattice with clearly labelled axes. **[8]**

(d) In an X-ray diffraction experiment, $\mathbf{k}$ describes the wavevector of a beam incident on the crystal and $\mathbf{k}'$ describes the direction of the detector. What is the general condition under which diffraction will occur from this crystal? **[7]**

(e) How can your picture of the reciprocal lattice be used to explain the statement that "(hkl) = (111), (200), (220), (311) ... are the allowed Bragg reflections of the FCC lattice" ? **[5]**

END OF PAPER