University of Durham

EXAMINATION PAPER

May/June 2011 Examination code: 043531/01 or 044111/01

LEVEL 3 PHYSICS: CONDENSED MATTER PHYSICS
LEVEL 4 PHYSICS: CONDENSED MATTER PHYSICS 4

SECTION A. SEMICONDUCTORS
SECTION B. MAGNETIC PROPERTIES
SECTION C. ORGANIC ELECTRONICS and DIELECTRICS

Time allowed : 3 hours

Examination material provided : None

Answer the compulsory question that heads each of sections A, B and C. These **three** questions have a total of 15 parts and carry 50% of the total marks for the paper. Answer **one** other question from **each** section. If you attempt more than the required number of questions only those with the lowest question number compatible with the rubric will be marked: **clearly delete** those that are not to be marked. The marks shown in brackets for the main parts of each question are given as a guide to the weighting the markers expect to apply.

ANSWER EACH SECTION IN A SEPARATE ANSWER BOOK

Do **not** attach your answer booklets together with a treasury tag, unless you have used more than one booklet for a single section.

APPROVED TYPES OF CALCULATOR MAY BE USED.

Information

Elementary charge:	$e = 1.60 \times 10^{-19}$ C
Speed of light:	$c = 3.00 \times 10^{8}\,\mathrm{m\,s^{-1}}$
Boltzmann constant:	$k_\mathrm{B} = 1.38 \times 10^{-23}\ \mathrm{J\,K^{-1}}$
Electron mass:	$m_\mathrm{e} = 9.11 \times 10^{-31}$ kg
Gravitational constant:	$G = 6.67 \times 10^{-11}\ \mathrm{N\,m^2\,kg^{-2}}$
Proton mass:	$m_\mathrm{p} = 1.67 \times 10^{-27}$ kg
Planck constant:	$h = 6.63 \times 10^{-34}$ J s
Permittivity of free space:	$\epsilon_0 = 8.85 \times 10^{-12}\ \mathrm{F\,m^{-1}}$
Bohr magneton:	$\mu_\mathrm{B} = 9.27 \times 10^{-24}\ \mathrm{J\,T^{-1}}$
Magnetic constant:	$\mu_0 = 4\pi \times 10^{-7}\ \mathrm{H\,m^{-1}}$
Nuclear magneton:	$\mu_\mathrm{N} = 5.05 \times 10^{-27}\ \mathrm{J\,T^{-1}}$
Molar Gas constant:	$R = 8.31 \times 10^{3}\ \mathrm{J\,K^{-1}\,kmol^{-1}}$
Avogadro's constant:	$N_\mathrm{A} = 6.02 \times 10^{26}\ \mathrm{kmol^{-1}}$
Gravitational acceleration at Earth's surface:	$g = 9.81\ \mathrm{m\,s^{-2}}$
Stefan-Boltzmann constant:	$\sigma = 5.67 \times 10^{-8}\ \mathrm{W\ m^{-2}\ K^{-4}}$

SECTION A. SEMICONDUCTORS

Answer Question 1 and **either** Question 2 **or** Question 3.

1. (a) A particular sp^2 hybrid orbital is given by

$$|A\rangle = \frac{1}{\sqrt{3}}|s\rangle + \frac{1}{\sqrt{6}}|p_x\rangle + \frac{1}{\sqrt{2}}|p_y\rangle$$

where $|s\rangle$, $|p_x\rangle$ and $|p_y\rangle$ are orthonormal atomic orbitals with associated s and p orbital energies $\epsilon_s = -17.52$ eV and $\epsilon_p = -8.97$ eV respectively. What is the energy of the sp^2 hybrid orbital? [4 marks]

(b) Sketch and identify the structure of the top of the valence energy bands near the centre of the Brillouin zone of a typical semiconductor, when spin-orbit interaction terms are included. [4 marks]

(c) Explain briefly why gallium nitride and its alloys have become important in a number of practical applications and why this has only occurred relatively recently. [4 marks]

(d) The electron mobility in a semiconductor at $T = 50$ K has the value $\mu = 15000$ cm^2 V^{-1} s^{-1} and may be assumed to be limited by charged impurity scattering. What value of mobility would you expect at 25 K? [4 marks]

(e) Write down an expression of Fick's Law for electrons and explain its significance. [4 marks]

2. (a) The energy of an electron in the conduction band of a fictitious simple cubic structure semiconductor with lattice constant a is given by

$$E(\underline{k}) = 3B - B[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$$

where $\underline{k}$ is the wavevector and B is a positive constant. Sketch the form of $E(\underline{k})$ along the [100] direction, indicating values at key points. [6 marks]

(b) Show that in the limit $k \to 0$, near the centre of the Brillouin zone, the effective mass may be represented by the expression

$$m^* \approx \frac{\hbar^2}{Ba^2}$$

along the [111] direction. [8 marks]

(c) Given that the energy band has a total width of 3.6 eV and that $a = 2 \times 10^{-10}$ m, what is the value of the relative effective mass along the [111] direction near the centre of the Brillouin zone? Comment on this result compared to that of a typical realistic, direct gap semiconductor with a face-centred cubic structure. [6 marks]

3. (a) Write down expressions for the electron concentration in the conduction band and the hole concentration in the valence band of a semiconductor in terms of N_c and N_v, the effective densities of states in the conduction and valence bands respectively. [4 marks]

   (b) An intrinsic semiconductor has $N_\mathrm{c} = 1.0 \times 10^{25}\ \mathrm{m}^{-3}$, $N_\mathrm{v} = 6.0 \times 10^{24}\ \mathrm{m}^{-3}$ and a band gap of 0.67 eV at $T = 300$ K. How far below the conduction band edge is the Fermi level under these conditions? [6 marks]

   (c) What is the value of the intrinsic carrier concentration at this temperature? [2 marks]

   (d) If the semiconductor has an introduced donor concentration $N_\mathrm{d} = 1 \times 10^{22}\ \mathrm{m}^{-3}$ what is the value of the resultant hole concentration, and what then is the position of the Fermi level relative to the conduction band edge? State any assumptions made. [6 marks]

   (e) For most semiconductors we have that $N_\mathrm{v} > N_\mathrm{c}$ but this is clearly not the case in the above example. What is the most likely explanation for this? [2 marks]

SECTION B. MAGNETIC PROPERTIES

Answer Question 4 and **either** Question 5 **or** Question 6.

4. (a) Calculate the energy difference between the spin states of an isolated, spin-only electron in the presence of a magnetic field of $B = 4$ T. [4 marks]

   (b) State or derive an expression relating the magnetic moment and orbital angular momentum of an electron orbiting the nucleus in the simple Bohr model of a hydrogen atom. What would be the orbital magnetic moment of an electron in the ground state of a hydrogen atom? [4 marks]

   (c) Sketch the typical hysteresis curve for a magnetically hard material and give one possible technological application for such a material. [4 marks]

   (d) Give a brief description of the RKKY indirect exchange mechanism and explain why it can lead to both ferromagnetic and antiferromagnetic order in rare earth metals. [4 marks]

   (e) State Bloch's law for the decrease in spontaneous magnetization in a three dimensional ferromagnet when temperature is increased from a value of $T = 0$ K. Briefly explain the origin of Bloch's law. [4 marks]

5. (a) Describe, with the aid of a sketch, a Bloch domain wall. [4 marks]

(b) A Bloch wall exists in a cubic material, between two neighbouring ferromagnetic domains in which the atomic spins (of magnitude S) point in the positive z and negative z directions. The Heisenberg exchange energy associated with two neighbouring spins $\underline{S}_i$ and $\underline{S}_j$ is given by

$$E_{ex} = -2J_{ex}S_iS_j\cos\phi\ ,$$

where ϕ is the angle between the direction of the spins and J_{ex} is the exchange integral. Also, the anisotropy energy per unit area of Bloch wall is of the form

$$\sigma_{anis} \approx KNa\ ,$$

where K is the anisotropy constant and a is the lattice spacing. $N+1$ is the number of atoms in a single atomic row, running from one side of the Bloch wall to the other. Use this information to derive an expression for the total energy per unit area of the Bloch wall in terms involving N. [4 marks]

(c) A rectangular slab of the ferromagnet magnetic material is spontaneously magnetized along its longest axis when $T < T_C$. Calculate the magnetostatic energy associated with the ferromagnet, of dimensions length $L = 2$ cm, width $W = 0.5$ cm and thickness $t = 0.01$ mm, given that the demagnetization factor is $D \approx 1.7 \times Wt/L^2$. The saturation magnetization of the ferromagnet is 8.7×10^5 A m^{-1}. [4 marks]

(d) This ferromagnet consists of atoms with $S = 2$ arranged in a simple cubic lattice with $a = 0.35$ nm. The Curie temperature of the material is 650 K and $K = 2.6 \times 10^4$ J m^{-3}. At very low temperatures Bloch walls are found to exist within the material. The width of each wall is typically 40 nm. Calculate the energy of such a Bloch wall. [6 marks]

(e) Estimate the maximum number of Bloch walls that can be created in the ferromagnet stating any assumptions that you make. [2 marks]

6. (a) Sketch the magnetic field dependence of the magnetization of a paramagnet at a low temperature. Indicate the part of your sketch where Curie's law is applicable. [3 marks]

(b) Calculate the magnetic moment of an isolated Cr^{2+} ion which has 4 electrons in the $3d$ shell and state any assumptions that you make. Comment on the nature of the magnetic susceptibility of a solid made from such ions. [4 marks]

(c) A solid consists of Cr^{2+} ions in a face centred cubic arrangement with a unit cell length of $a = 0.42$ nm. Halfway between neighbouring Cr^{2+} ions, separated along the edge of the unit cell by the distance a, there is a non-magnetic anion, O^{2-}. The paramagnetic susceptibility of the solid is of a Curie-Weiss form with the Curie-Weiss temperature $\theta = -10$ K and Curie's constant $C = 3.38$ K. Also, the magnetization is found to saturate at a value of 2×10^6 A m^{-1} at very high magnetic fields. Calculate the number of Cr^{2+} ions per unit volume and hence determine the values for the total angular momentum quantum number J and the Landé g factor. [6 marks]

(d) Calculate the magnetic moment per Cr^{2+} using the values of J and g obtained in part (c). Compare this value with that calculated in part (b) and explain any differences in the two values. [3 marks]

(e) The Curie-Weiss temperature, θ, is attributed to be a consequence of a superexchange interaction. Give a brief description of this exchange mechanism and explain the nature of the magnetic state expected to exist at very low temperatures. What would be the value of the low field magnetic susceptibility of the solid at $T = 0$ K? [4 marks]

SECTION C. ORGANIC ELECTRONICS and DIELECTRICS
Answer Question 7 and **either** Question 8 **or** Question 9.

7. (a) The fluorescence lifetime of a blue molecular material used to fabricate light emitting devices, shows a pronounced temperature dependence, varying from 500 ps at room temperature to 3 ns at 50 K. Assuming the device shows an ideal charge balance (100%), an optical output coupling (light extraction yield) of 25%, and a singlet recombination yield of 25%, estimate the device maximum external quantum efficiency. [4 marks]

   [Hint: Assume that the radiative decay rate constant is independent of temperature, and that at low temperatures the non radiative decay rate constant (k_{NR}) is $\approx 0 \ s^{-1}$.]

   (b) Consider a polymer light emitting device, emitting in the blue spectral region, when submitted to a voltage bias. Discuss the role of triplet-triplet annihilation on the possibility of achieving internal quantum efficiencies larger than 25%. Explain why thermal delayed fluorescence is not normally active in conjugated polymers, and establish the relationship between the polymer singlet and triplet energies, that will allow triplet-triplet annihilation to contribute to the device emission. [4 marks]

   (c) A thin dielectric slab of area $A = 2.5\times10^{-4}$ m^2 and thickness $d = 0.001$ m has a relative permittivity $\epsilon(\omega) = 7.6 - 0.3i$ at angular frequency $\omega = 2000$ s^{-1}. Estimate the magnitude of the peak current through the dielectric at this frequency. You may neglect edge effects. [4 marks]

   (d) Describe, briefly, the significance of the individual terms in the expression for the local electric field in a dielectric material,

$$E_{local} = E_a + E_{LOR} + E_{SPH},$$

   and explain why this can mean that the electric field experienced by an individual dipole within a dielectric can be significantly greater than the average macroscopic field. [4 marks]

   (e) Sketch the hysteresis diagram for a ferroelectric material below the Curie temperature ensuring that all key features are labelled and defined. [4 marks]

8. Consider an organic photovoltaic solar cell (OPV) made of a mixture of polymer and charge acceptor materials in a bulk heterojunction architecture.

   (a) Identify the basic constituents of such an OPV device, and explain their roles in device operation. [4 marks]

   (b) Using a HOMO-LUMO energy diagram for P3HT (HOMO: –5.2 eV; LUMO: –3.2 eV) and PCBM (HOMO: –6.0 eV; LUMO: –4.2 eV) materials, show that both excitation of P3HT and PCBM will lead to the same charge separated intermediate. Give a justified estimation of the maximum open circuit voltage of such a solar cell based on P3HT and PCBM.[4 marks]

   (c) Discuss the potential strategies for optimizing the efficiency of an organic solar cell device. Highlight the important roles of light absorption, exciton diffusion, charge separation, recombination, and charge transport to the electrodes. [6 marks]

   (d) A major problem in organic solar cells is the poor spectral match between the absorption of the cell's constituent materials and the Sun's photon flux. For example, P3HT absorption is only active above 650 nm and the Sun's photon flux peaks at 780 nm, this is a major source of loss for OPVs. One possible approach to solve this problem is to make use of dyes which absorb light in the red and near infrared (NIR) regions of the spectrum, and use them as dopants to extend the light absorption of the cell to the NIR region.

   Discuss the conditions that such dyes have to fulfill in order to promote light absorption and contribute to charge generation without acting as charge traps. In particular discuss the role of such dyes in the photoinduced charge generation mechanism for two different situations: First, when the dye is located at the polymer:acceptor interface, and then secondly when the dye is located in a polymer rich phase. [6 marks]

9. Describe, briefly, the electronic and ionic polarisation mechanisms in a dielectric material and explain in simple terms why their characteristic resonance-like behaviour occurs at significantly different frequencies. [6 marks]

   A material with only electronic and ionic contributions to the total susceptibility has a constant electronic contribution $\chi_e = 3.8$ well below the UV frequency regime and a static (relative) permittivity $\epsilon_s = 10.0$. At a frequency of 1.3×10^{12} Hz it is found that the ionic contribution to the susceptibility has the value $\chi_I = 0.0 - 30.0i$. Calculate the value of the real part of the permittivity at frequency 1.4×10^{12} Hz. [14 marks]