University of Durham

EXAMINATION PAPER

May/June 2012 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. DIELECTRICS and ORGANIC ELECTRONICS

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:

Speed of light:
Boltzmann constant:

Electron mass:

Gravitational constant:

Proton mass: Planck constant:

Permittivity of free space:

Magnetic constant:

Molar gas constant: Avogadro's constant:

Gravitational acceleration at Earth's surface:

Stefan-Boltzmann constant:

Astronomical Unit:

Parsec:

Solar Mass:

Solar Luminosity:

 $e = 1.60 \times 10^{-19} \text{ C}$

 $c = 3.00 \times 10^8 \,\mathrm{m\,s^{-1}}$

 $k_{\rm B} = 1.38 \times 10^{-23} \; {\rm J \, K^{-1}}$

 $m_{\rm e} = 9.11 \times 10^{-31} \text{ kg}$

 $G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$

 $m_{\rm p} = 1.67 \times 10^{-27} \text{ kg}$

 $h = 6.63 \times 10^{-34} \text{ J s}$

 $\epsilon_0 = 8.85 \times 10^{-12} \text{ F m}^{-1}$

 $\mu_0 = 4\pi \times 10^{-7} \; \mathrm{H} \, \mathrm{m}^{-1}$

 $R = 8.31 \times 10^3 \text{ J K}^{-1} \text{ kmol}^{-1}$

 $N_{\rm A} = 6.02 \times 10^{26} \ \rm kmol^{-1}$

 $q = 9.81 \text{ m s}^{-2}$

 $\sigma = 5.67 \times 10^{-8} \; \mathrm{W} \; \mathrm{m}^{-2} \; \mathrm{K}^{-4}$

 $AU = 1.50 \times 10^{11} \text{ m}$

 $pc = 3.09 \times 10^{16} \text{ m}$

 $M_{\odot} = 1.99 \times 10^{30} \text{ kg}$

 $L_{\odot} = 3.84 \times 10^{26} \text{ W}$

SECTION A. SEMICONDUCTORS

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

- 1. (a) Describe how the band gaps of typical compound semiconductors vary with the atomic weight and the ionicity of the constituent elements and indicate the manner in which this consequently tends to affect the conduction band effective mass of direct gap semiconductors. [4 marks]
 - (b) Given that a particular alloy of the semiconductor A_xB_{1-x} has a band gap of 0.9 eV at 0 K, estimate the specific alloy composition given that semiconductor A has a band gap of 1.52 eV, semiconductor B has a band gap of 0.42 eV and the bowing parameter b is 0.40 eV. [4 marks]
 - (c) A single, spherical, parabolic energy band has a density of states that is proportional to $m^{3/2}$ where m represents an appropriate effective mass for that energy band. Discuss the issues which we must consider in order to evaluate the density of states effective mass in the conduction band and the top of the valence band in a typical indirect gap semiconductor. [4 marks]
 - (d) The electron energy as a function of wavevector in a 2-D semiconductor is of the form

$$E(\underline{k}) = A\left(0.2k_x^2 + 0.5k_y^2\right)$$

where A is a constant. If an electric field is applied in the (1,1) direction what is the resultant direction of acceleration of an electron in this energy band? [4 marks]

(e) Describe the impact ionisation process in direct gap semiconductors with the help of an appropriate diagram. What is the inverse process called? [4 marks]

- 2. (a) What is the significance of N_c , the effective density of states in the conduction band of a semiconductor? Without giving a detailed derivation, write down an expression for the electron carrier concentration, n, in terms of N_c and state what approximations are employed to derive this expression. [4 marks]
 - (b) A doped semiconductor with a band gap $E_g=1.3$ eV has electron and hole carrier concentrations of 1.2×10^{16} m⁻³ and 3.7×10^{10} m⁻³ respectively at 300 K. Calculate the value of the intrinsic carrier concentration at the same temperature and name the law that you have employed. [4 marks]
 - (c) Given that $N_c = 2.1 \times 10^{23} \text{ m}^{-3}$ at 300 K what is the position of the Fermi level relative to the top of the valence band and what is the effective density of states in the valence band for the above doped semiconductor? [6 marks]
 - (d) If the impurity energy level of the dopant employed in the above semiconductor is 6 meV from the appropriate band edge estimate the occupation of this level. Hence confirm that the impurity is nearly fully ionised at 300 K. [6 marks]

- 3. (a) Imagine that electron transport in a semiconductor is impeded by two scattering processes, one in which the lifetime/relaxation time is proportional to the temperature, T, and the other in which it is proportional to 1/T. Make a sketch, with an accompanying explanation, of the form of the mobility for the individual processes and their combined effect to give the overall electron mobility as a function of temperature for this semiconductor. [6 marks]
 - (b) It is found that the semiconductor has a mobility of 0.27 m 2 V $^{-1}$ s $^{-1}$ at 100 K and 0.41 m 2 V $^{-1}$ s $^{-1}$ at 465 K. Find the value of the mobility at 200 K. [6 marks]
 - (c) In order to optimize the performance of a particular device made from the above semiconductor it must operate at a temperature corresponding to the highest available mobility. At what temperature should the device operate? [6 marks]
 - (d) Usually, what are the two most important mobility-limiting scattering processes in doped semiconductors? [2 marks]

SECTION B. MAGNETIC PROPERTIES

Answer Question 4 and either Question 5 or Question 6.

- 4. (a) Briefly describe the vortex state of a Type II superconductor and indicate how this state develops as the applied magnetic field is increased from the lower critical field, B_{C1} , to the upper critical field, B_{C2} . [4 marks]
 - (b) A ferromagnetic material consists of atoms that each have total angular momentum J=5/2 and Landé g factor of g=2. The number of atoms per unit volume is 2×10^{28} m⁻³. Calculate the spontaneous magnetization that occurs at T=0 K and, given that the spontaneous magnetization falls to a tenth of its zero temperature value at T=1 K, calculate the spontaneous magnetization at T=0.25 K. State any assumptions that you make and take the Bohr magneton to be $\mu_{\rm B}=9.27\times 10^{-24}$ J T⁻¹. [4 marks]
 - (c) What is the Barkhausen effect and how would it be identified in a magnetic hysteresis curve? [4 marks]
 - (d) Make a sketch of the temperature dependence of the magnetic susceptibility of an antiferromagnet. Indicate the Néel temperature, T_N , on your sketch and briefly explain why the magnetic susceptibility is anisotropic below T_N . [4 marks]
 - (e) What is magnetocrystalline anisotropy and how does it affect the induced magnetization of a ferromagnet in the presence of an applied magnetic field? [4 marks]

- (a) What is meant by L-S (or Russell-Saunders) coupling and under what conditions is it applicable? [2 marks]
 - (b) The magnetization of a paramagnet consisting of isolated atoms in their ground state with total angular momentum J is given by the Brillouin function,

$$M = M_s \left[\frac{(2J+1)}{2J} \coth\left(\frac{2J+1}{2J}y\right) - \frac{1}{2J} \coth\left(\frac{y}{2J}\right) \right]$$

where M_s is the saturated magnetization value, $y = g\mu_B JB/(k_B T)$, B is the flux density and g is the Landé g-factor which is given by the expression,

$$g = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}.$$

Use the expression for M to derive Curie's law, stating any assumptions that you make. [5 marks]

[Hint:
$$\coth x \simeq \frac{1}{x} + \frac{x}{3}$$
 for $x \to 0$]

- (c) Use Hund's rules to determine the ground state and excited total angular momentum states of an isolated Ti²⁺ ion which has a 3d² electronic structure. Calculate the total magnetic moments of each of these states in terms of μ_B . [5 marks]
- (d) The spin-orbit coupling constant of the Ti^{2+} ion is $\lambda = 4.5$ meV. Calculate the energies, $E_{SO}(J)$ of the total angular momentum states determined in part (c). [4 marks]
- (e) Sketch the form of the temperature dependence of the inverse paramagnetic susceptibility of a solid of non-interacting Ti²⁺ ions, measured at low magnetic fields. Note that the probability of thermal occupation of the energy levels, determined in part (d), is proportional to $(2J+1) \exp(-E_{SO}(J)/k_BT)$. [4 marks]

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- 6. (a) What is a ferromagnetic magnon? [2 marks]
 - (b) Consider an atom with a spin S within a two dimensional ferromagnetic solid with each atom surrounded by four identical neighbours. The spins are Heisenberg exchange coupled with an exchange constant, J_{ex} . It is possible to describe this interaction in terms of an 'exchange field' acting on an atom given by $|\underline{B}_{ex}| = (2J_{ex}/(g\mu_{\rm B}))\sum_i S_i$ where g is the Landé g-factor, the Bohr magneton $\mu_{\rm B} = 9.27 \times 10^{-24}$ J T⁻¹ and the sum is over all other spins. In Weiss' molecular field theory the interactions between the magnetic moments is described by an 'internal field'. State the form of the 'internal field' and show that the molecular field constant, $N_W = 2zJ_{ex}/(g^2\mu_{\rm B}^2\mu_0N)$, where z is the coordination number and N is the number of atoms per unit area. State any assumptions that you make. [5 marks]
 - (c) A two dimensional organic solid has a square lattice of molecules each with a free radical of spin of S=1/2. The lattice constant of the solid is a=0.5 nm. If the exchange constant has the value $J_{ex}=0.30$ meV, calculate the 'internal field' experienced by a magnetic moment at T=0 K and determine the Curie temperature using the molecular field result $T_C=2zJ_{ex}S(S+1)/(3k_{\rm B})$. [3 marks]
 - (d) If the solid described in part (c) is ferromagnetic then magnons may be expected to be thermally excited below T_C . Given that, in the long wavelength limit, the magnon dispersion relation of a two dimensional ferromagnet has the form $\omega \approx (2J_{ex}Sa^2/\hbar)k^2$, show that the total number of magnons excited at a temperature T is given by

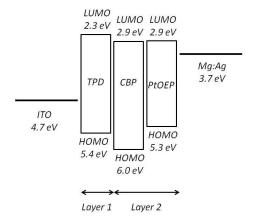
$$\sum_{k} n_{k} = \left(\frac{A}{8\pi}\right) \frac{k_{\rm B}T}{J_{ex}Sa^{2}} \int_{0}^{\infty} \frac{dx}{\exp(x) - 1}$$

where $x = \hbar \omega / k_{\rm B} T$ and A is the total area of the solid. Take the 2D density of magnon states to be $D(\omega)d\omega = (A/4\pi^2)2\pi kdk$ and state any assumptions that you make. [5 marks]

(e) Use the form of $\sum_k n_k$ given in part (d) to obtain an expression for the decrease in the value of spontaneous magnetization, ΔM_{sp} , upon increasing temperature from T=0 K. Estimate the value of ΔM_{sp} at some very small but arbitrary temperature above zero and comment upon your result. [5 marks]

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

- 7. (a) What is the essential property which must be satisfied for a structure to exhibit piezoelectric behaviour? Give an example of a structure with zero initial dipole moment which exhibits this property and demonstrate how it does so with the use of appropriate diagrams. [4 marks]
 - (b) A 50 μ m square PZT pyroelectric detector of thickness $d=2~\mu$ m is subject to an infra-red radiation energy flux $F=5.3~\mathrm{J~m^{-2}~s^{-1}}$ and as a result, a pyroelectric current of $1\times10^{-12}~\mathrm{A}$ is measured in an external circuit. Given that PZT has a density $\rho=7.5\times10^3~\mathrm{kg~m^{-3}}$ and a specific heat capacity $c=350~\mathrm{J~kg^{-1}~K^{-1}}$, estimate the minimum value of the pyroelectric coefficient of PZT. [4 marks]
 - (c) Consider the schematic energy diagram shown below of a phosphorescent organic light emitting device (OLED) containing two organic layers. Layer 1 is a thin film of TPD and layer 2 is a film of CBP doped with 6 percent PtOEP. The luminescence of the device peaks at 652 nm. Explain the role of each organic layer and electrode material on the device function. What is the purpose of dispersing PtOEP into CBP?



Caption: Schematic energy diagram of a bilayer phosphorescent OLED showing the electrode work functions and the HOMO and LUMO energies of the organic materials.

[4 marks]

- (d) The fluorescence quantum yield of a luminescent polymer film spin-coated on a quartz substrate is 0.4, and the fluorescence emission decays with 350 ps lifetime. Determine the natural radiative decay rate constant, and the non-radiative decay rate constant of the luminescent polymer. When mixed with a suitable red emitting dopant, the fluorescence lifetime of the polymer host decreases to 10 ps, due to host-guest energy transfer. Determine the emission quenching rate constant. [4 marks]
- (e) Why are singlet excitons more useful than triplet excitons in OLED devices? Explain the mechanism that allows the use of organic emitting phosphors, e.g. organic heavy metal complexes, and provides an important strategy for harvesting triplet excitons in OLEDs. [4 marks]

8. A dielectric material has a complex relative permittivity which depends on the angular frequency, ω , according to

$$\epsilon^*(\omega) = A + \frac{B}{(1 + i\omega C)}.$$

Explain the significance of the constants A, B and C in terms of the standard Debye equation model and state the frequency regime in which it is most likely to be applicable. [5 marks]

Define the loss tangent and obtain an expression for it in terms of A, B, C and ω . [7 marks]

Show that the peak in the loss tangent occurs at a frequency given by

$$\omega = \frac{1}{C} \left(\frac{A+B}{A} \right)^{1/2}$$

[4 marks]

If the material has a relative permittivity of 10 at zero frequency, an approximately constant relative permittivity of 4 at high frequency and $C = 1 \times 10^{-4}$ s, at what frequency does the loss tangent peak occur? [4 marks]

9. (a) Consider an organic solar cell device fabricated with a donor-acceptor bilayer heterojunction. Describe the device structure and the mechanism of photoinduced charge generation in this type of device. In particular discuss the merits and disadvantages of this particular device architecture, and explain the different routes that are open to the device engineer to optimise material characteristics and device nanostructures to achieve maximum device efficiencies. Highlight the important roles of light absorption, exciton dissociation and recombination, and charge transport. [8 marks]

Absorption of light on the active layer of an organic solar cell creates singlet excitons, with few triplet excitons potentially being formed due to intersystem crossing in the organic material. Triplets are not normally used for charge generation, even in situations where a longer exciton lifetime is expected to be beneficial for charge generation. Answer the following questions concerning the possibility of using the triplet state as the precursor for photoinduced charge generation.

- (b) Why is the concept of using the triplet state as the donor for photoinduced charge generation difficult to realize in organic solar cells with the bulk heterojunction architecture? [3 marks]
- (c) The triplet yield in organic materials is normally low, less than 10% in most conjugated polymers for example; this limits the number of triplets that are created by direct light absorption. Explain which strategies are available to increase the number of triplets created in films of organic materials. [3 marks]
- (d) Increasing the number of triplets in the active layer of a solar cell, might give rise to triplet-triplet annihilation (TTA). How is TTA going to affect the use of triplets in photoinduced charge generation? [3 marks]
- (e) The open circuit voltage, V_{oc} , in an organic solar cell device is governed by the energy of the charge separated state, E_{CT} , formed at the interface between donor and acceptor materials. Discuss how do you expect V_{oc} to be affected by using triplets instead of singlet states as precursors for photoinduced charge generation. [3 marks]