QUEEN'S UNIVERSITY BELFAST

PHY2002
Exam Time Table
Code PHY2002

Use lined, single-sided A4 paper with a black or blue pen.
Write your student number at the top of every page.

Any non-graphical calculator, except those with pre-programmable memory, may be used in this examination

LEVEL 2
Examination contributing to the Degrees of Bachelor of Science (BSc) and Master in Science (MSci)

PHY2002 - EXAM
Physics of the Solid State
Monday, 3rd August 2020, 09.30 - 13.30

Examiners: Prof S Matthews, Dr P van der Burgt
and the Internal Examiners
Dr J Greenwood (j.greenwood@qub.ac.uk)

Answer ALL TEN questions in Section A for 4 marks each.
Answer ONE question in Section B for 30 marks.
Answer ONE question in Section C for 30 marks.
You have FOUR hours to complete and upload this paper.

Contact the module coordinator if you have queries/problems at m.gregg@qub.ac.uk and copy to mpts@qub.ac.uk

By submitting the work, you are declaring that:
1. The submission is your own original work and no part of it has been submitted for any other assignments;
2. You understand that collusion and plagiarism in an exam are major academic offences, for which a range of penalties may be imposed, as outlined in the Procedures for Dealing with Academic Offences.

THE QUEEN'S UNIVERSITY OF BELFAST
DEPARTMENT OF PHYSICS AND ASTRONOMY

PHYSICAL CONSTANTS

Speed of light in a vacuum	$c = 3.00 \times 10^{8}\ \mathrm{ms}^{-1}$
Permeability of a vacuum	$\mu_0 = 4\pi \times 10^{-7}\ \mathrm{Hm}^{-1}$ $\approx 1.26 \times 10^{-6}\ \mathrm{Hm}^{-1}$
Permittivity of a vacuum	$\varepsilon_0 = 8.85 \times 10^{-12}\ \mathrm{Fm}^{-1}$
Elementary charge	$e = 1.60 \times 10^{-19}\ \mathrm{C}$
Electron charge	$= -1.60 \times 10^{-19}\ \mathrm{C}$
Planck Constant	$h = 6.63 \times 10^{-34}\ \mathrm{Js}$
Reduced Planck Constant	$\hbar = 1.05 \times 10^{-34}\ \mathrm{Js}$
Rydberg Constant for hydrogen	$R_\infty = 1.097 \times 10^{7}\ \mathrm{m}^{-1}$
Unified atomic mass unit	$1u = 1.66 \times 10^{-27}\ \mathrm{kg}$ $1u = 931\ \mathrm{MeV}$
1 electron volt (eV)	$= 1.60 \times 10^{-19}\ \mathrm{J}$
Mass of electron	$m_e = 9.11 \times 10^{-31}\ \mathrm{kg}$
Mass of proton	$m_p = 1.67 \times 10^{-27}\ \mathrm{kg}$
Mass of neutron	$m_n = 1.67 \times 10^{-27}\ \mathrm{kg}$
Molar gas constant	$R = 8.31\ \mathrm{JK}^{-1}\mathrm{mol}^{-1}$
Boltzmann constant	$k = 1.38 \times 10^{-23}\ \mathrm{JK}^{-1}$
Avogadro constant	$N_A = 6.02 \times 10^{23}\ \mathrm{mol}^{-1}$
Gravitational constant	$G = 6.67 \times 10^{-11}\ \mathrm{Nm}^2\mathrm{kg}^{-2}$
Acceleration of free fall on the Earth's surface	$g = 9.81\ \mathrm{ms}^{-2}$

SECTION A

Use a section A answer book

Answer ALL ten questions from this section (four marks each)

1 The cubic crystal system has five point groups: 23, 432, $\mathrm{m}\bar{3}$, $\bar{4}3\mathrm{m}$ and $\mathrm{m}\bar{3}\mathrm{m}$. Explain, with reference to the specific crystallographic axes, the general convention (in the Hermann-Maugin notation) used to described the symmetry of this crystal system, and comment on why all point groups have '3' in the second position. **[4]**

2 Sketch a FCC structure, indicate its lattice points (point coordinates) and demonstrate that a FCC crystal can accommodate 4 atoms. **[4]**

3 Using a real space unit cell, draw the reciprocal space unit cell for an orthorhombic crystal system ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$). Consider the following lattice parameters: $a = 8$ Å, $b = 4$ Å and $c = 12$ Å. **[4]**

4 Explain what is meant by the term "heat capacity" and state how the variation in heat capacity as a function of temperature can be used to explicitly determine the enthalpy and entropy of a system. **[4]**

5 Explain how the free energy variation with temperature can be used to distinguish first from second order phase transition behaviour. Sketch how the order parameter for the phase transition will vary with temperature in both cases. **[4]**

6 With reference to the enthalpy change induced when a mechanical mixture of two different atomic types is forced into a solid solution, discuss whether ordering and exsolution are mutually exclusive processes. **[4]**

7 Show how Landau theory can be used to predict transformation plasticity. **[4]**

8 The Fermi Energy, E_F, for a free electron gas at $T = 0\ \mathrm{K}$ is given as:

$$E_F = \frac{\hbar^2}{2m_e}(3\pi^2 n_e)^{\frac{2}{3}},$$

where m_e is the free electron mass and n_e is the number of electrons per unit volume.

Zinc is a metal with $E_F = 9.4\ \mathrm{eV}$, a relative atomic mass of 65.4, and a mass density of $\rho = 7.13\ \mathrm{x}\ 10^3\ \mathrm{kgm}^{-3}$. Estimate how many electrons each zinc atom contributes to the free electron gas. **[4]**

9 When describing semiconductor transport, the behaviour of a 'nearly-full' band of electrons can be equivalently described in terms of positively charged 'holes'. Examine the cases of a full and nearly-full band of electrons to demonstrate how this comes about, using equations to support your answer. **[4]**

10 With the aid of a schematic energy band diagram of a p-n junction, explain what 'drift' and 'diffusion' currents are and how they are related in equilibrium conditions. What happens when a 'forward' bias is applied across the junction? **[4]**

SECTION B

Use a section B answer book

Answer 1 of the 2 questions in this section

11 (a)(i) What is a stereogram and what is the advantage of using this in crystallography? **[3]**

(ii) Explain what the Ewald sphere is and how can it be used to determine the crystal orientations in an observed diffraction pattern. **[3]**

(iii) Why is the entire reciprocal lattice not imaged when a diffraction experiment is carried out on a single crystal? **[3]**

(iv) Explain the difference between a transmission Laue photograph and a Bragg-Brentano (single crystal) Scan. **[4]**

(b) $BaTiO_3$ possesses a perovskite structure with a space group $P4mm$ (tetragonal), with lattice parameters $a = 4.004$ Å and $c = 4.201$ Å, and the following motif:

Ba: 0.5, 0.5, 0
Ti: 0, 0, 0.5
O: 0, 0, 0; 0.5, 0, 0.5; 0, 0.5, 0.5

(i) Draw an accurate structure plan of 2 x 2 unit cells, viewed along [100] and describe the $BaTiO_3$ structure in terms of linked coordination polyhedra. **[4]**

(ii) Draw an accurate reciprocal lattice section a^*- c^* and determine the magnitudes of a^*, c^* and γ^*. **[3]**

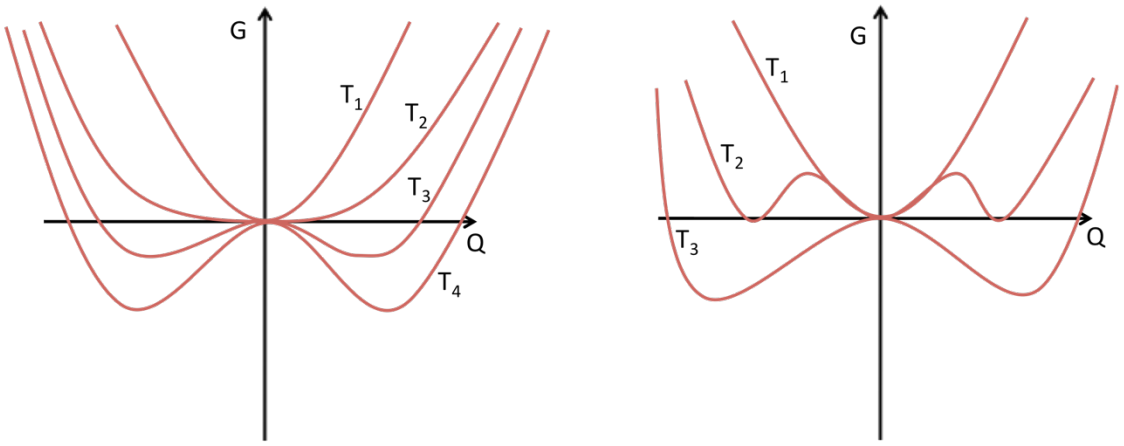
(iii) A single crystal of $BaTiO_3$ is placed in a diffractometer, and rotated with respect to the incident X-ray beam about the a^*- c^* reciprocal lattice (with a Cu-Kα source, λ = 1.54 Å). Using the Ewald sphere and the reciprocal calculate the rotation angle at which the (002) reflection is observed. . **[6]**

(iv) X-rays from a Mo-Kα (λ = 0.71 Å) source are diffracted from a $BaTiO_3$ single crystal. Assuming that $n = 1$, calculate the interplanar distance for (101) and the angle that gives rise to this reflection. **[4]**

SECTION B

12(a) **(i)** What is meant by the term *order parameter* in describing phase transitions in solid state materials? **[4]**

(ii) Consider the two plots of free energy (G) as a function of order parameter (Q) and temperature (T) in figure 12.1 below (where $T_1 > T_2 > T_3 > T_4$). Plot the form of the development of the order parameter as a function of temperature for both (a) and (b) under equilibrium and hence assign the likely 'order' of the phase transitions. **[6]**



(a) (b)

Figure 12.1

(b) The optical activity associated with a thin wafer of SiO_2 was monitored as a function of temperature by noting the angle through which plane polarised light incident on the wafer was rotated on arrival at the detector. The results of rotation angle against temperature are given in Table 12.1.

(i) If at 700°C the phase transformation resulting in optical activity is complete, use the information in Table 12.1 to construct a plot of the order parameter against temperature. **[6]**

[QUESTION 12 CONTINUED OVERLEAF]

[QUESTION 12 CONTINUED]

(ii) By plotting the logarithm of the order parameter against the logarithm of a suitable function of temperature, decide whether the phase transition is 1st order, 2nd order or tricritical. **[6]**

(iii) The transformation may be well described by a Landau free energy expansion. State a suitable Landau free energy expression and assign the coefficients as being positive, negative or zero. **[8]**

Temperature / ^{0}C	Angle of Rotation of Light / degrees
900	0
880	0
860	0
850	0
840	47.9
820	51.1
800	53.6
780	55.5
760	57.1
740	58.4
720	59.4
700	60

Table 12.1

SECTION C

Use a section C answer book

Answer 1 of the 2 questions in this section

13 **(a)** Describe and demonstrate the importance of the harmonic approximation and the time independent Schrodinger equation to the development of Einstein's model for the heat capacity of solids. **[10]**

(b) **(i)** With reference to both the dispersion relations of phonons (angular frequency of lattice vibrations as a function of wavenumber) and the thermal coefficient of expansion, discuss the validity of the statement "crystalline solids are nothing more than balls and springs". **[5]**

(ii) Describe what is meant by the term: "density of states". **[2]**

(iii) By demonstrating that the allowed wavenumbers associated with lattice vibrations in a 3D crystal are evenly distributed in reciprocal space, defend the notion that the density of phonon k-states inevitably increases as the wavenumber of the phonon increases. Hence, develop an expression for the density of states as a function of wavenumber. **[8]**

(c) Describe the phenomenon of Umklapp scattering and outline its relevance in determining the thermal conductivity of solid materials as a function of temperature. **[5]**

SECTION C

14 (a) The Fermi-Dirac distribution is given as:

$$f(E) = \frac{1}{1 + e^{\left[\frac{E-\mu}{kT}\right]}},$$

where $f(E)$ is the state occupancy probability, μ is the Fermi level, E is energy, and T is temperature.

(i) Sketch the Fermi-Dirac distribution at $T = 0$ K, label the Fermi energy (E_F), and explain how its form can be rationalised qualitatively in the context of electrons in a metal. Also, sketch the case for an elevated temperature $T > 0$ K. **[4]**

(ii) For semiconducting materials, explain how suitable choice of dopant species can lead to p- and n-type conduction and include schematic energy band diagrams with Fermi energy at $T = 0$ K labelled for each case. Sketch a plot of how the Fermi level is expected to change with temperature for the p-type scenario, indicating any limiting values on the energy axis. **[5]**

(iii) For the following two situations, use the Fermi-Dirac function to determine the probability that a state of energy E_C at the conduction band edge in a semiconductor is occupied at a temperature T:
$T = 300$ K and $E_C - \mu = 0.33$ eV, and
$T = 10$ K and $E_C - \mu = 0.1$ eV.

If the material is germanium, with a bandgap of 0.66 eV, indicate for each scenario if the semiconductor is likely to behave as 'intrinsic', 'n-type doped', or 'p-type doped' and justify your choice. **[6]**

[QUESTION 14 CONTINUED OVERLEAF]

[QUESTION 14 CONTINUED]

(b) A schematic electron energy band structure for a crystalline solid is shown below. Electron energy (E) is plotted versus electron wavevector (k) along the [100] and [111] directions. The energy axis is plotted such that the zero corresponds to the highest filled energy state at a temperature of $T = 0$ K.

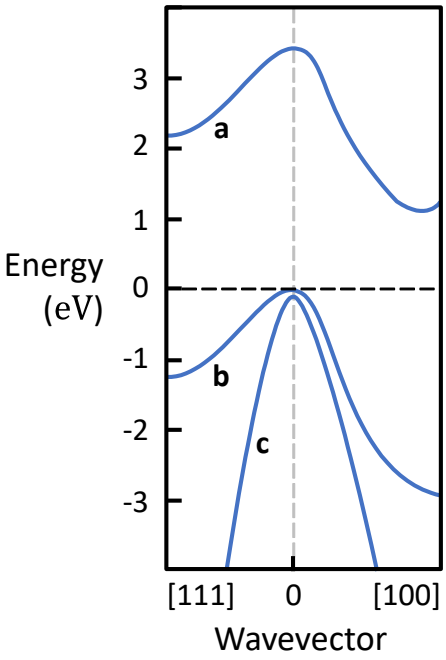


Figure 14.1: Schematic electron energy band structure.

(i) What do the solid lines (in blue) represent in the Figure 14.1 plot? **[1]**

(ii) What information in the figure lets us know that we are dealing with an insulator/semiconductor and not a metal? **[2]**

(iii) Does this material have a direct or indirect bandgap? Rationalise your answer. **[2]**

(iv) Estimate the size of the band gap and comment on whether the material is more likely to behave as an insulator or semiconductor at room temperature. **[2]**

(v) At elevated temperatures, identify whether each band ('a', 'b', and 'c') contributes either an electron current or a 'hole' current to conduction and rationalise your choices. **[5]**

(vi) Qualitatively, how is electron effective mass determined from an E-k plot for a given k value? Hence, rationalise whether carriers in band 'b' or 'c' are expected to have the larger effective mass near $k = 0$. **[3]**

END OF EXAMINATION