

Any calculator, except one 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
Physics of the Solid State

Duration: 3 hours plus additional 1 hour for upload of work

Friday 7th of May 2021
09:30 AM – 1:30 PM

Examiners: Prof S Matthews, Prof F. Peters
and the internal examiners
Dr S Sim (s.sim@qub.ac.uk)

Answer ALL questions in Section A for 4 marks each.
Answer ONE question from Section B for 30 marks.
Answer ONE question from Section C for 30 marks.

If you have any problems or queries, contact the School Office at
mpts@qub.ac.uk or 028 9097 1907, and the module coordinator
m.gregg@qub.ac.uk

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

PHYSICAL CONSTANTS

Speed of light in a vacuum	$c = 3.00 \times 10^8 \text{ ms}^{-1}$
Permeability of a vacuum	$\mu_0 = 4\pi \times 10^{-7} \text{ Hm}^{-1}$ $\approx 1.26 \times 10^{-6} \text{ Hm}^{-1}$
Permittivity of a vacuum	$\epsilon_0 = 8.85 \times 10^{-12} \text{ Fm}^{-1}$
Elementary charge	$e = 1.60 \times 10^{-19} \text{ C}$
Electron charge	$= -1.60 \times 10^{-19} \text{ C}$
Planck Constant	$h = 6.63 \times 10^{-34} \text{ Js}$
Reduced Planck Constant	$\hbar = 1.05 \times 10^{-34} \text{ Js}$
Rydberg Constant for hydrogen	$R_\infty = 1.097 \times 10^7 \text{ m}^{-1}$
Unified atomic mass unit	$1u = 1.66 \times 10^{-27} \text{ kg}$ $1u = 931 \text{ MeV}$
1 electron volt (eV)	$= 1.60 \times 10^{-19} \text{ J}$
Mass of electron	$m_e = 9.11 \times 10^{-31} \text{ kg}$
Mass of proton	$m_p = 1.67 \times 10^{-27} \text{ kg}$
Mass of neutron	$m_n = 1.67 \times 10^{-27} \text{ kg}$
Molar gas constant	$R = 8.31 \text{ JK}^{-1} \text{ mol}^{-1}$
Boltzmann constant	$k = 1.38 \times 10^{-23} \text{ JK}^{-1}$
Avogadro constant	$N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$
Gravitational constant	$G = 6.67 \times 10^{-11} \text{ Nm}^2 \text{ kg}^{-2}$
Acceleration of free fall on the Earth's surface	$g = 9.81 \text{ ms}^{-2}$

SECTION A

Use a section A answer book

Answer all 10 questions from this section

- 1 Explain the difference between a *crystal lattice* and a *crystal structure*. [4]
- 2 For a FCC unit cell, determine the lattice positions and the relationship between the atomic radius (r) and the lattice parameter (a). [4]
- 3 Consider the structure 'A' in Fig. 1, indicate and list the symmetry operations present in the molecule shown below, indicate the direction of the symmetry operation and the corresponding point group. [4]

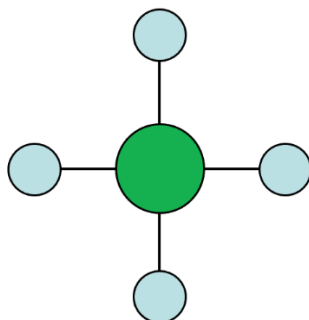


Figure 1. Structure 'A'.

- 4 Define the term "*heat capacity*"; justify and explain how it can be used to determine both the enthalpy and entropy of a system at finite temperature. [4]
- 5 Explain what is meant by "*order parameter*" and "*Landau free energy*" and justify why the Landau free energy function usually contains order parameter terms with even exponents only. [4]
- 6 With reference to bond energies, explain why a solid solution of two elements may either *exsolve* or *order* on cooling, but not, in general, do both. [4]

- 7 Explain how the conservation of energy and momentum can lead to a situation where two phonons, with notionally positive momenta, can coalesce to create a new phonon with a negative momentum. What is this process called? **[4]**
- 8 State the defining characteristics of an acoustic phonon. Sketch a frequency-wavenumber function typical of acoustic phonons in the first Brillouin Zone and use it to illustrate that the density of wavenumber states as a function of energy increases as the energy of the acoustic phonons increase. **[4]**
- 9 Sketch the form of the electrical resistivity as a function of temperature (T) for a typical elemental metal from room temperature down to $T = 0$ K. Describe how the form is rationalised in an electron wave picture with reference to the terms identified in Matthiessen's rule. **[4]**
- 10 Give an argument to explain why the Fermi level (μ) in an intrinsic semiconductor should be positioned centrally in the energy band gap, rather than at the valence band edge.

Where is μ typically found in n- and p-type doped semiconductors when they are operating in the 'extrinsic' regime and why does μ move towards the mid-gap as temperature is increased? **[4]**

SECTION B

Use a section B answer book

Answer 1 of the 2 questions in this section

- 11 (a)(i) Sketch a hexagonal unit cell (either in 3D or 2D) and demonstrate that the hexagonal lattice can be represented by an alternative (and smaller) primitive unit cell. [3]
- (ii) Nickel Arsenide (NiAs) adopts a hexagonal structure, with a space group $P6_3/mmc$ and unit cell parameters: $a = 4.152 \text{ \AA}$ and $c = 5.813 \text{ \AA}$. Explain the meaning of 'P' and '6₃'. [3]

- (iii) The motif (or basis) for NiAs is

Ni: $(0, 0, 1/2)$ and $(0, 0, 0)$

As: $(1/3, 2/3, 3/4)$ and $(2/3, 1/3, 1/4)$

Draw a structure plan of 2x2 unit cells viewed down the [001] axis and describe the structure in terms of a coordination polyhedra. [4]

- (b)(i) The naturally occurring mineral *jadeite* ($\text{NaAl}(\text{SiO}_3)_2$) is monoclinic with the following lattice parameters: $a = 9.42 \text{ \AA}$, $b = 8.56 \text{ \AA}$, $c = 4.8 \text{ \AA}$ and $\beta = 107.6^\circ$. Sketch the primary axes of the real and reciprocal space lattices for *jadeite*, showing their relative orientation, and calculate the magnitudes of the reciprocal lattice parameters a^* , b^* , c^* and β^* . [4]
- (ii) Using a suitable portion of the reciprocal lattice, calculate the interplanar spacing for the plane (101). [3]
- (iii) Calculate the zone axis common to both the (101) and (400) planes in *jadeite*. [3]
- (iv) A single crystal of *jadeite* is irradiated with Cu K α X-rays (wavelength = 1.54 \AA) along the a axis, in a static configuration. Demonstrate diagrammatically that the Ewald sphere for this wavelength intersects the reciprocal lattice point 002, and show that the 008 reciprocal lattice point could never satisfy the Bragg diffraction condition for this wavelength. [6]
- (v) Crystal diffraction experiments can be carried out by using neutrons, electron and X-rays. Consider a single crystal diffraction experiment on the *jadeite* crystal using electrons accelerated at 300 kV (wavelength = 2.24 pm) and X-rays (wavelength $\sim 100 \text{ pm}$), incident on the same direction. Using this information, discuss how the Ewald sphere will change in each case and how different the resulting diffraction patterns will be. [4]

SECTION B

- 12 (a)(i)** Explain what is meant by the terms: *free energy*, *enthalpy* and *entropy* and present the simplest form of a thermodynamic equation that relates these three entities together. [4]
- (ii)** Consider a system composed of “A” and “B” atoms, which forms a solid solution at high temperatures, but then displays phase segregation (exsolution) on cooling. Sketch the form of the free energy of mixing in such a system, as a function of A-B composition, at a number of different temperatures and use these sketches to describe and rationalize the manner in which equilibrium phase segregation proceeds on cooling. [8]
- (b) (i)** Phase transitions can be classified as being either *first order*, *second order* or *tricritical*. Define these terms and present the expected development of the primary order parameter associated with each type of phase transition as a function of temperature. [6]
- (ii)** Show how Landau theory successfully predicts the existence of these three classifications of phase transition. [6]
- (iii)** Explain what *transformation plasticity* is and demonstrate how Landau theory predicts its occurrence. [6]

SECTION C

Use a section C answer book

Answer 1 of the 2 questions in this section

13 (a)(i) By considering the interatomic potential energy as a function of bond length, explain what is meant by the term “*Harmonic Approximation*” and comment on how it allows crystals to be modelled as arrays of “balls and springs”. **[3]**

(ii) Explain and demonstrate how a “balls and springs” model of a 1D monatomic chain allows the dispersion relation of acoustic vibrational modes to be predicted. **[6]**

(iii) When a “balls and springs” model of a 1D diatomic chain is considered, equations of motion generate a more complex functional relationship between vibrational angular frequency (ω) and wavenumber (k), in which there are two solutions:

$$\omega^2 = \frac{\mu(M_A + M_B)}{M_A M_B} \pm \frac{\mu \sqrt{(M_A + M_B)^2 - 4M_A M_B (\sin ka)^2}}{M_A M_B}$$

where: μ is the effective spring constant of the “springs”; M_A and M_B are the masses of the two types of “balls”, and a is the equilibrium interatomic spacing. Using the above expression, determine the angular frequencies of the two vibrational modes at both the centre and boundary of the first Brillouin Zone. Use these values to help sketch the dispersion relation for both branches. **[9]**

(b) (i) The Harmonic Approximation is also key for Einstein’s development of a heat capacity model. Briefly explain this statement and comment on how the Harmonic Approximation informs the quantisation of allowed energy states for each vibrating atom. **[4]**

[QUESTION 13 CONTINUED OVERLEAF]

[QUESTION 13 CONTINUED]

- (ii) Einstein modelled the internal energy (U) due to atomic vibrations as:

$$U = 3N\langle n \rangle \hbar \omega$$

Explain the meaning of the terms used in this expression and rationalise how their product should give a sensible approximation for the internal energy. How is this expression then used to determine the heat capacity (you do not have to derive the heat capacity explicitly – rather, state how it could be derived)? **[4]**

- (iii) Einstein's model for the heat capacity assumed that the number of vibrational states associated with a given energy level would be the same, irrespective of the energy associated with that state. Demonstrate that this notion is flawed. **[4]**

SECTION C

14(a) The time independent Schrödinger equation in 1D is given as:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \quad \text{Equation 14.1}$$

where $\psi(x)$ is the eigenfunction, E is energy, and $V(x)$ is a potential energy function.

- (i) For a 'free electron gas', what approximation can be made for the $V(x)$ term? **[1]**
 - (ii) Show that an oscillatory function, such as $\psi(x) = e^{ikx}$, is a solution to Equation 14.1 for a free electron gas. Show that the derived energy-wavevector ($E - k$) relationship is parabolic and sketch this function. **[5]**
 - (iii) When an electric field is applied across a metal a current is established. How is this rationalised in terms of changes in the energy-wavevector distribution of the electron population when the field is applied? Support your answer with sketches of $E - k$ diagrams for the scenarios before and after the field is applied. **[5]**
- (b)**
- (i) Describe how the introduction of the periodic lattice potential affects your free electron gas $E - k$ dispersion from part **(a)** and support this with an illustration. In the wave picture, what is happening to electrons having wavevector $k = \pm\pi/a$? **[5]**
 - (ii) How can this modified $E - k$ dispersion be used to explain the existence of insulating behaviour under an applied field? **[3]**
 - (iii) How can the existence of semiconducting behaviour at elevated temperatures be explained using this modified $E - k$ picture? Include a sketch with your answer. What experimental measurement can be used to verify intrinsic semiconducting behaviour in a material? **[4]**
 - (iv) What feature of the $E - k$ diagram is primarily responsible for the difference in the room temperature conductivity between an insulator (e.g. diamond) and a semiconductor (e.g. silicon)? **[1]**

[QUESTION 14 CONTINUED OVERLEAF]

[QUESTION 14 CONTINUED]

- (c)(i) What is the purpose of introducing the concept of the 'effective mass', m^* ? Use the form of the parabolic $E - k$ dispersion discussed in (a)(ii) to derive a general expression for m^* . **[3]**
- (ii) Measurements of the effective mass m^* are made in two semiconducting samples, 'X' and 'Y'. In the conduction band, m^* is measured to be $2m_0$ in 'X' and $0.5m_0$ in 'Y'. Which of the below hypothetical band structures (A or B) shown in Figure C14.1 is likely to represent sample 'X'? Explain your reasoning. **[3]**

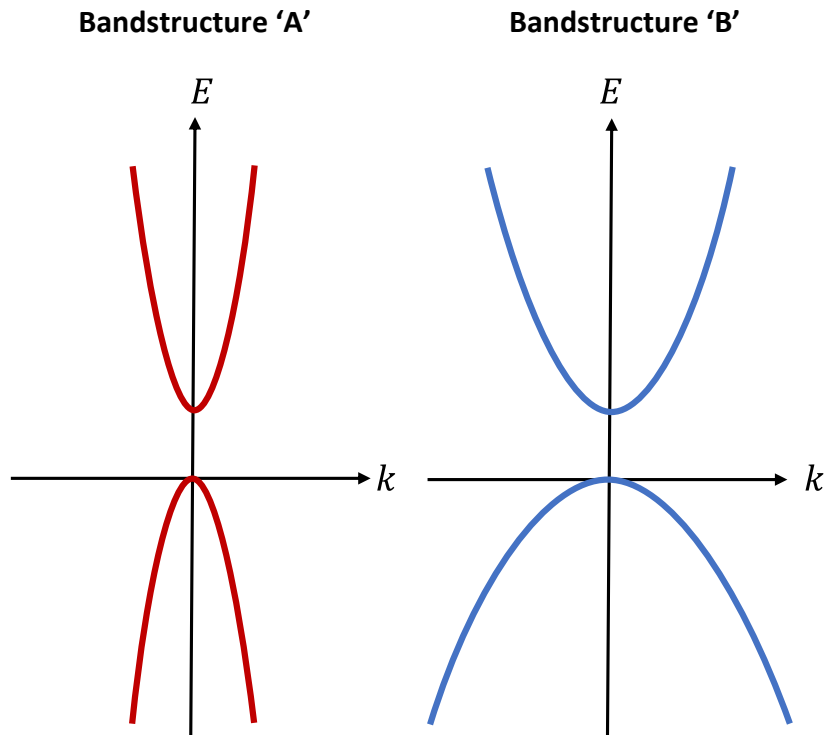


Figure C14.1 Two hypothetical bandstructures A and B (both are plotted with the same scale for E and k)

END OF EXAMINATION