

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

Wednesday 11th of August 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
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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 Consider the 2D lattice shown in Figure A. Identify and draw one primitive and one non-primitive unit cell. [4]

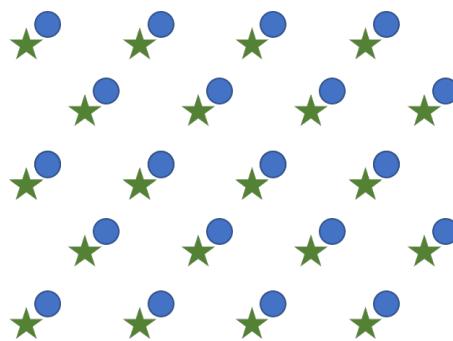


Figure A. 2D Lattice

- 2 Determine the indices for the direction and plane shown in the cubic unit cell in Fig. B. [4]

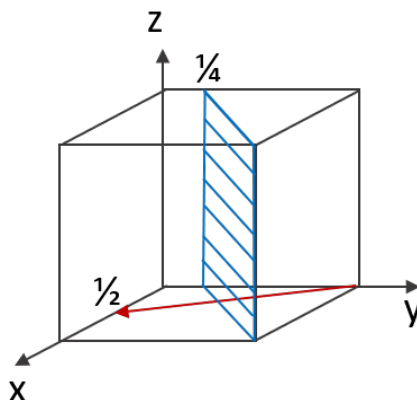


Figure B. Cubic unit cell showing a direction (red arrow) and a plane (in blue).

- 3 Explain the difference between point group and space group. [4]
- 4 Explain what is meant by the terms *internal energy*, *entropy* and *heat capacity*; in addition, show how the heat capacity can be used to quantify both the internal energy and the entropy of a system. [4]

SECTION A

- 5 Phase transitions can generally be classified as *first order*, *second order* or *tricritical*. Briefly explain how these classifications relate to discontinuities in either the gradient or curvature of the free energy as a function of temperature. [4]
- 6 Materials which have mixed chemical composition often exist as solid solutions at high temperature, but then either order or exsolve on cooling. Briefly discuss the thermodynamics responsible for these behaviours. [4]
- 7 The potential energy, as a function of the interatomic bond length, is often represented by a parabola. Explain why this parabolic representation is often sensible, but also give an example of a material property for which the parabolic energy approximation fails. [4]
- 8 Explain why the thermal conductivity of solids, as a function of temperature, often shows a distinct maximum. [4]
- 9 Explain the difference between 'direct' and 'indirect' band gap semiconductors, illustrating your answer with energy band diagram sketches. Perform a calculation to determine if infra-red light of wavelength $\lambda = 3 \mu\text{m}$ incident on PbTe would be expected to lead to electron-hole pair creation (PbTe is a direct bandgap semiconductor with a bandgap $\Delta E = 0.32 \text{ eV}$). [4]
- 10 Explain how a current is established in a metal under an applied electric field in the energy band picture. [4]

SECTION B

Answer 1 of the 2 questions in this section

11

- (a) The cubic crystal system contains the highest number of point groups (and space groups).
- (i) Explain the general convention (in the Hermann-Mauguin notation) used to describe the symmetry of this crystal system and comment on the defining symmetry operation. Describe the symmetry operations in the cubic point group 432. [4]
 - (ii) Explain what a stereogram is and what the advantage is of using this in crystallography. [3]
 - (iii) Draw a stereogram for a primitive crystal system with orthogonal axes, viewed down along [001]. By adding triads along the body diagonals, what new symmetry element is automatically generated and in what directions? [4]
- (b) Gallium nitride (GaN), in the form known as wurtzite, has a space group $P6_3mc$ (hexagonal crystal system), with lattice parameters $a = 3.21 \text{ \AA}$ and $c = 5.24 \text{ \AA}$.
- (i) Explain what the element 'P' means and what the symmetry element ' 6_3 ' describes. [4]
 - (ii) Sketch the relationship between the real and reciprocal lattice axes for GaN, and determine the magnitudes of a^* , c^* and γ^* . [4]
 - (iii) Using the reciprocal lattice, calculate the spacing between the (210) planes in wurtzite GaN. [3]
 - (iv) What is the Ewald Sphere and how can it be used, in conjunction with the reciprocal lattice, to determine the orientations in which constructive interference of scattered radiation occurs? [4]
 - (v) Explain why the entire reciprocal lattice is not imaged when a diffraction experiment is carried out on a single crystal. [4]

SECTION B

12

- (a) (i) In the context of solid-state phase transitions, explain what is meant by *the order parameter* and *the Landau Free Energy*. [4]

- (ii) Explain why it is usually the magnitude, rather than the sign, of the order parameter that is important in defining the Free Energy of a state. Hence, comment on the fact that basic Landau Free Energy expressions usually only consider order parameter terms with even exponents. [6]

- (b) Consider the following Landau Free Energy (G) expression, as a function of order parameter (Q), conjugate external field (H) and temperature (T):

$$G = \frac{a}{2}(T - T_c)Q^2 + \frac{b}{4}Q^4 + \frac{c}{6}Q^6 - H \cdot Q \quad \text{equation 12.1}$$

where T_c is the Curie Temperature and a , b and c are scalar constants.

- (i) Explain the origin of the $(T - T_c)$ prefactor. [5]

- (ii) In the absence of an applied field (i.e. $H = 0$), sketch graphically the manner in which the Landau Free Energy, implied by equation 12.1, develops on cooling through T_c for two different cases: firstly, when $b > 0$ and $c = 0$ and secondly, when $b < 0$ and $c > 0$. [5]

- (iii) With two further sketches, show how the Landau Free Energy functions for these two cases are altered whenever a finite external field is applied (i.e. $H \neq 0$). [4]

- (iv) Using equation 12.1 as a starting point, develop an expression for the susceptibility of the order parameter to the applied field and hence discuss the phenomenon of transformation plasticity. [6]

SECTION C

Answer 1 of the 2 questions in this section

13

- (a) (i) Explain why it is often reasonable to consider atomic dynamics, induced by thermal excitation in crystalline materials, using “ball and spring” models. [4]
- (ii) Consider a 1D chain of atoms, in which all atoms possess the same mass and for which interatomic bonds are well represented by Hookean springs. Explain the physics associated with the development of the frequency (ω) – wavevector (k) dispersion relation for this system. [6]
- (iii) When a similar chain of atoms contains two distinct atomic types (of differing mass), in alternating positions along the chain length, the frequency-wavevector dispersion relation becomes more complex: two functions emerge as solutions. Sketch the form of both of these allowed $\omega - k$ functions within the first Brillouin Zone. Label them, as optic or acoustic modes, and describe the key properties of each. [5]
- (b) (i) While a classical view of vibrating atoms predicts the dispersion relations found in crystalline materials reasonably well, it fails in rationalising the temperature variation of heat capacity. Considering Einstein’s model, discuss how treating atoms as quantum objects helps. [8]
- (ii) Einstein’s model for heat capacity did not consider variations in the “density of states”, as a function of frequency. Explain what the phrase “density of states” means and discuss the notion that it generally increases as frequency increases. [7]

SECTION C

14

- (a) (i) For a *free electron gas* in 3 dimensions, confined to a cubic volume (V) with side of length L , the total number of electron states (up to some magnitude of wavevector k) can be shown to be:

$$N = \frac{Vk^3}{3\pi^2} \quad \text{equation 14.1}$$

Carefully explain how equation 14.1 comes about, by consideration of the distribution of states in k -space. [4]

- (ii) Write out an integral expression involving the density of states $D(E)$ and a statistical distribution $f(E)$ that allows the total number of electrons N over some energy range to be determined. What statistical function for $f(E)$ should be used for the free electron gas? [2]

- (iii) For a free electron gas, the density of states is given as:

$$D(E) = \frac{V}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}}, \quad \text{equation 14.2}$$

where m_e is electron mass.

Explain what assumptions can be made about the energy distribution of electrons at $T = 0$ K and hence introduce suitable limits of integration into your expression for (ii). Evaluate the integral to show that the Fermi Energy E_F is obtained as:

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

where n is the number of valence electrons per unit volume. [6]

- (iv) Determine E_F for aluminium which gives 3 valence electrons per atom to the free electron gas. Aluminium has a mass density of 2700 kgm^{-3} and a relative atomic mass of 27. Give your answer in units of eV. [5]

[QUESTION 14 CONTINUES ON NEXT PAGE]

SECTION C

[QUESTION 14 CONTINUED]

(b) (i) How does the introduction of a periodic lattice potential affect the free electron gas picture and how can insulating behaviour now be predicted? Support your answer with sketches of dispersion plots. [5]

(ii) When describing intrinsic semiconducting behaviour, the carrier density n can be shown to vary as $n = Ce^{-\Delta E/k_b T}$, where C is a temperature dependent prefactor, ΔE is the energy band gap, and T is temperature.

To obtain this expression, what assumptions are made for the form of the conduction band dispersion and for the statistical distribution of electrons in the energy band? How can the latter approximation be justified? [3]

(iii) In semiconductors, under an applied field, a current contribution is also expected from the valence band at finite temperatures. Give an analysis which shows that the valence band contribution to current can be described in terms of positively-charged 'holes'. [5]

END OF EXAMINATION