

Department of Physics

PH956 Advanced Nanoscience 2

August 9, 2022

9:30 am – 12:30 pm – 3 hours

**Attempt ALL questions in Section A (40%) and
ALL questions from Section B (60%)**

Calculators must not be used to store text and/or formulae nor be capable of communication. Invigilators may require calculators to be reset.

Physical constants

Speed of light	$c = 3.00 \times 10^8 \text{ m s}^{-1}$	Bohr radius	$a_0 = 5.29 \times 10^{-11} \text{ m}$
Free space permittivity	$\epsilon_0 = 8.85 \times 10^{-12} \text{ F m}^{-1}$	Compton wavelength	$\lambda_C = 2.43 \times 10^{-12} \text{ m}$
Free space permeability	$\mu_0 = 4\pi \times 10^{-7} \text{ H m}^{-1}$	Avogadro's number	$N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$
Electrostatic constant	$k_E = 8.99 \times 10^9 \text{ m F}^{-1}$	Boltzmann's constant	$k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$
Electron mass	$m_e = 9.11 \times 10^{-31} \text{ kg}$	Universal Gas constant	$R = 8.31 \text{ J mol}^{-1} \text{ K}^{-1}$
Electron charge size	$e = 1.60 \times 10^{-19} \text{ C}$	Gravity acc. on earth	$g = 9.81 \text{ m s}^{-2}$
Planck's constant	$h = 6.63 \times 10^{-34} \text{ J s}$	Gravitational constant	$G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$
Wien's law constant	$b = 2.90 \times 10^{-3} \text{ m K}$	Stefan-Boltzmann	$\sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$
Rydberg constant	$R_\infty = 1.10 \times 10^7 \text{ m}^{-1}$	Atomic mass unit	$u = 1.66 \times 10^{-27} \text{ kg}$

Section A – Attempt ALL questions in this section

1. Carbon atoms convert their electronic structure to hybridised states in a range of solids and molecules.
 - a) Prove that the angle between any two hybridised orbitals of an sp^1 carbon atom is 180° . [4]
 - b) Given that the single electron energies for the $3s$ and $3p$ orbitals of a carbon atom are ε_s and ε_p , estimate the energy difference between the atomic ground state and the sp^1 hybridised state for the *isolated* atom. [6]
2. For a one-dimensional chain of atoms aligned along the x direction, which have both s and p orbitals on each site, derive an expression for the energies of the *two* bands consisting of p_y and p_z orbitals in a tight-binding model of this system. [10]
3. A common crystalline structure of boron has 12 atoms in its unit cell and is a three dimensional crystal.
 - a) Explain how many branches of acoustic and optical phonons should be present for this material. [4]
 - b) For which magnitude of the crystal momentum, \mathbf{k} , can the optical and acoustic phonons always be unambiguously distinguished? [2]
 - c) Are phonons either a) bosons, b) fermions or c) neither? [2]

PLEASE TURN OVER

4. The vibrational dispersion relation for a one dimensional crystal with a single atom in its unit cell is of the form

$$\omega(k) \propto \left| \sin \left(\frac{ka}{2} \right) \right|.$$

- a) Based on this dispersion, show that the form of the density of states for this system is

$$g(\omega) = \frac{1}{a\pi\sqrt{\omega_m^2 - \omega^2}}$$

where ω_m is the frequency at the Brillouin zone boundary. [4]

- b) Comment on the density of states at the zone boundaries. [2]

The identity $\cos[\arcsin(x)] = \sqrt{1 - x^2}$ may be useful.

5. The electron and hole masses of Cu_2O are $1.0 m_e$ and $0.7 m_e$ respectively. Given that the dielectric constant of this material is $\epsilon_r = 10.0$ and its band gap is 2.170 eV, at which characteristic energies would you expect optical emission for a low temperature photoluminescence experiment where above band-gap light is used for excitation? Assume that the binding energy of the $1s$ state of hydrogen is 13.61 eV. [6]

PLEASE TURN OVER

Section B – Attempt ALL questions in this section

6. Ideal boson systems undergo a phase transition at a critical temperature T_c when the density of particles is given by

$$\frac{N}{V} = 2.261 \left(\frac{mk_B T_c}{2\pi\hbar^2} \right)^{3/2}$$

where there are N particles of mass m in a volume V , with all values in standard units.

- a) Calculate the expected Bose-Einstein condensation temperature for spin-0 excitons in AgBr when the exciton density is 10^{24} m^{-3} . The electron and hole masses are $0.285 m_e$ and $1.105 m_e$ respectively. [5]
- b) The dielectric constant, ϵ_r , of AgBr is 10.60. On the basis of the radius of the $n = 1$ exciton (where n is the principal quantum number), decide whether Bose-Einstein condensation could occur for the exciton density in part a). [5]
7. In the original BCS theory of superconductivity, fermions form a condensate at low temperatures.
- a) What is the general type of interaction between electrons that is necessary to cause this condensate state to be stable? Give a formula for the form of this interaction. [4]
- b) What are the main features of the single particle states which make up the wavefunction of the condensate? [6]
- c) Explain the difference between type I and II superconductors with reference to the parameter κ in the Ginzburg-Landau phenomenological model. [5]
- d) Why was the 2001 discovery of materials that were simultaneously ferromagnetic and superconducting surprising? [5]

PLEASE TURN OVER

8. Topological insulators (TI) and the quantum-Hall insulating (QHI) state are superficially similar, as both possess topologically protected edge states, but these are distinct different states of matter.
- a) Sketch the general form of the bulk density of states for these two states of matter, labelling significant features. [10]
 - b) Are the surfaces of examples of these two types of materials conductive or insulating? [2]
 - c) Provide a further sketch of the band energies at the surface of these two materials. [6]
 - d) Qualitatively describe the effect disorder or impurities on the surface will have on your answer in part b). [6]
 - e) Both the TI and QHI states of matter are labelled by topological invariants, but with different physical origins. Briefly outline the physical nature of these invariants and comment on any differences in their possible values for these two types of system. [6]

END OF PAPER

(Dr. B. Hourahine)