ONE HOUR THIRTY MINUTES

A list of constants is enclosed

UNIVERSITY OF MANCHESTER

Fundamentals of Solid State Physics

31st May 2017

09:45 a.m. – 11:15 a.m.

Answer **ALL** parts of question 1 and **TWO** other questions.

Electronic calculators may be used, provided that they cannot store text.

The numbers are given as a guide to the relative weights of the different parts of each question.

P.T.O.

1.

a) A plutonium (Pu^{3+}) ion has five 5f electrons. What are the orbital, spin and total angular momenta in the ground state of the ion? Write the answer in spectroscopic notation.

[5 marks]

b) A magnetic field of 18 T is applied to a hydrogen atom in the ground state. What is the energy splitting between adjacent states in the presence of the field? How would you expect your answer to change for a ground state neon atom with electron configuration $(1s)^2(2p)^6$?

[5 marks]

c) Using a molecular orbital energy level diagram, explain why the bond length of the H_2^+ molecular ion is larger than that of the H_2 molecule. Do you expect the bond length for the three-electron species H_2^- to be smaller or larger than that for H_2? Briefly justify your answer.

[5 marks]

d) Use the Drude model to derive an expression for the electrical conductivity of a metal, defining the terms you use.

[5 marks]

e) Sketch the dispersion relation $\varepsilon(k)$ for a nearly free electron interacting with a one-dimensional lattice, over the range $-\frac{2\pi}{a} \leq k \leq +\frac{2\pi}{a}$, where a is the spacing of the atoms.

[5 marks]

P.T.O.

2.

a) Write down two spatial wavefunctions that represent two identical electrons in terms of one-electron wavefunctions. In each case say whether the wavefunction is symmetrical or antisymmetrical when the particles are exchanged.

[4 marks]

b) The combined spin eigenfunctions of the total spin for two electrons are:

$$\chi_{s1} = \chi_1^+ \chi_2^+,$$
$$\chi_{s2} = \frac{1}{\sqrt{2}}\left(\chi_1^+ \chi_2^- + \chi_1^- \chi_2^+\right),$$
$$\chi_{s3} = \chi_1^- \chi_2^-,$$
$$\chi_a = \frac{1}{\sqrt{2}}\left(\chi_1^+ \chi_2^- - \chi_1^- \chi_2^+\right).$$

The operators for the z-components of the individual spins have the following eigenstates, $\chi_1^+, \chi_1^-, \chi_2^+, \chi_2^-$:

$$\hat{S}_{1z}\chi_1^+ = \frac{\hbar}{2}\chi_1^+;\ \hat{S}_{1z}\chi_1^- = -\frac{\hbar}{2}\chi_1^-;\ \hat{S}_{2z}\chi_2^+ = \frac{\hbar}{2}\chi_2^+;\ \hat{S}_{2z}\chi_2^- = -\frac{\hbar}{2}\chi_2^-.$$

By applying the operator for the z-component of the total spin, $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$, show that these eigenfunctions are also eigenfunctions of the z-component of the total spin, and calculate the M_S quantum numbers for each combined spin eigenfunction.

[8 marks]

c)

The table below shows the energies of a number of energy eigenstates of a helium atom. In each case, one electron is in the $n = 1, \ell = 0$ state. The combined spin state, n and ℓ for the other electron are shown below.

Combined spin state	n	ℓ	Energy / eV
singlet	1	0	-79.2
triplet	2	0	-59.7
singlet	2	0	-58.5
triplet	2	1	-58.2
singlet	2	1	-57.7

P.T.O.

Explain:

(i) why the ground state ($n = 1$, $\ell = 0$) energy is not $-8E_R$;

[3 marks]

(ii) why there is no state which is a triplet with $n = 1$, $\ell = 0$;

[3 marks]

(iii) why the energy depends on ℓ ;

[3 marks]

(iv) why the energies depend on the overall spin symmetry, and why the singlet energies are higher than those of the corresponding triplets.

[4 marks]

3.

a) Cubic gallium nitride (GaN) has a fcc lattice and a basis of one gallium atom (69.7 amu) and one nitrogen atom (14.0 amu). The (200) Bragg reflection in first order is observed for an X-ray wavelength of 1.54 Å at a scattering angle (2θ) of 40.0°. Calculate the density of cubic gallium nitride.

[7 marks]

b) The electron density n in the conduction band of an *intrinsic* semiconductor can be written as

$$n = N_C e^{\frac{-(E_C - \varepsilon_F)}{k_B T}},$$

where N_C is the effective density of states in the conduction band, and all other symbols have their conventional meaning.

Calculate n at a temperature of 300 K for GaN, given that the band gap is 3.2 eV and the value of N_C is 4 x 10^{25} m^{-3}.

[3 marks]

c) Sketch a graph showing a typical variation of log(n) where n is the free electron concentration for an n-type semiconductor as a function of the inverse of the absolute temperature. Indicate three important ranges on your graph and explain why the different ranges exist.

[5 marks]

d) Extrinsic n-type doping can be achieved in GaN by substituting silicon (Si) atoms onto Ga lattice sites. Draw a schematic energy level diagram to illustrate the band structure at T = 0 K of GaN doped with Si atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

e) The dopant ionisation energy in Si-doped GaN is 20 meV. Assuming the semiconductor is in the impurity range, estimate the carrier density due to the dopant atoms at 300 K. You may use the value of N_C given in part (b). Comment on your answer in comparison with your answer to part (b).

[5 marks]

P.T.O.

4.

a) Sketch the form of a typical experimental plot of the molar heat capacity for a monatomic solid at constant volume, C_v, versus absolute temperature, measured from near absolute zero to room temperature.

[2 marks]

b) State the law of equipartition of energy. Using the first law of thermodynamics show for a monovalent solid that C_v is equal to $3R$ where R is the universal gas constant.

[7 marks]

c) Describe the Einstein model of specific heat, and explain why it predicts that C_v should depend on temperature as opposed to the prediction based on the equipartition of energy. In your answer briefly discuss the relevance of the Einstein temperature.

[7 marks]

d) The Einstein temperature of diamond (atomic mass = 12 amu) is 1300 K and that of lead (atomic mass = 207 amu) is 60 K. Calculate the ratio of the spring constants of the C – C and Pb – Pb bonds. Illustrate on a diagram the relative values of the ground state vibrational energies of the C and Pb atoms, together with the confining potentials for both C and Pb.

[4 marks]

e) Briefly describe the shortcomings of the Einstein model, and explain how the Debye model rectifies them.

[5 marks]

END OF EXAMINATION PAPER