One hour thirty minutes

A list of Constants is enclosed

UNIVERSITY OF MANCHESTER

Fundamentals of Solid State Physics

5th June 2018

2.00 p.m. – 3.30 p.m.

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

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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) Two electrons in a He atom occupy different single-particle wavefunctions $\psi_\alpha(\underline{r}_1)$ and $\psi_\beta(\underline{r}_2)$. Write down symmetric and antisymmetric two-particle wavefunctions. For a system of two interacting electrons, state which two-particle wavefunction gives rise to the lower energy state, and briefly justify your answer.

[5 marks]

b) A magnetic field of 20 T is applied to a lithium atom with electron configuration $(1s)^2(2s)^1$. What is the energy splitting between adjacent states in the presence of the field? How would you expect your answer to change for a helium atom with electron configuration $(1s)^2$?

[5 marks]

c) Briefly explain the process by which NaCl absorbs light of frequency 1.14 x 10^{13} Hz and calculate the interatomic force constant for the bond between the sodium and chlorine ions.
(Atomic mass of Na = 23 u; atomic mass of Cl = 35.5 u.)

[5 marks]

d) Using the free electron model of a metal, and given that the density of states per unit volume is $g(\varepsilon) = \dfrac{\sqrt{2m^3\varepsilon}}{\pi^2\hbar^3}$, show that the Fermi energy ε_F is proportional to $n^{2/3}$ where n is the electron density.

[5 marks]

e) Sketch graphs of the resistivity *vs.* absolute temperature for two samples of the same metal with different impurity contents, and indicate the important features.

[5 marks]

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2.

a) Describe the sequence of steps in a Hartree calculation of the states of a multi-electron atom.

[6 marks]

b) What is meant by a self-consistent potential?

[2 marks]

c) Hartree theory assumes that the potential arising from the other electrons is central. Why is that assumption justified for filled sub-shells?

[2 marks]

d) State Hund's Rules which prescribe the angular momentum quantum numbers S, L and J in the ground state of a partly full sub-shell, and give brief physical arguments to make the first two rules plausible. What is the effect which gives rise to the third rule?

[6 marks]

e) A Cr^{3+} ion has three 3d electrons. What are S, L and J in the ground state of this ion? Write your answer in spectroscopic notation.

[4 marks]

f) Magnetic anisotropy arises for magnetic ions in solids as a result of the orbital angular momentum interacting with neighbouring atoms. Yb^{3+} ions have thirteen 4f electrons, and Lu^{3+} ions have fourteen 4f electrons. Would you expect greater magnetic anisotropy from materials containing Yb^{3+} or Lu^{3+} ions? Explain your answer.

[5 marks]

3.

a)

i. Sketch a graph of the confining potential for an independent oscillator in Einstein's model of specific heat and indicate the allowed energies in terms of the frequency of the oscillator.

[3 marks]

ii. In the context of the energy states described above, define the Einstein temperature.

[3 marks]

iii. Sketch a graph of the measured molar heat capacity at constant volume (C_V) versus T for diamond, which has an Einstein temperature of 1325 K.

[3 marks]

b) Using the Einstein model for specific heat show that

$$C_V = 3R \frac{\theta_E^2 \exp\left(\frac{\theta_E}{T}\right)}{T^2 \left[\exp\left(\frac{\theta_E}{T}\right) - 1\right]^2} ,$$

where R is the universal gas constant, θ_E is the Einstein temperature and T is the absolute temperature. State any simplifying assumptions.
You may take the occupation function for phonons to be

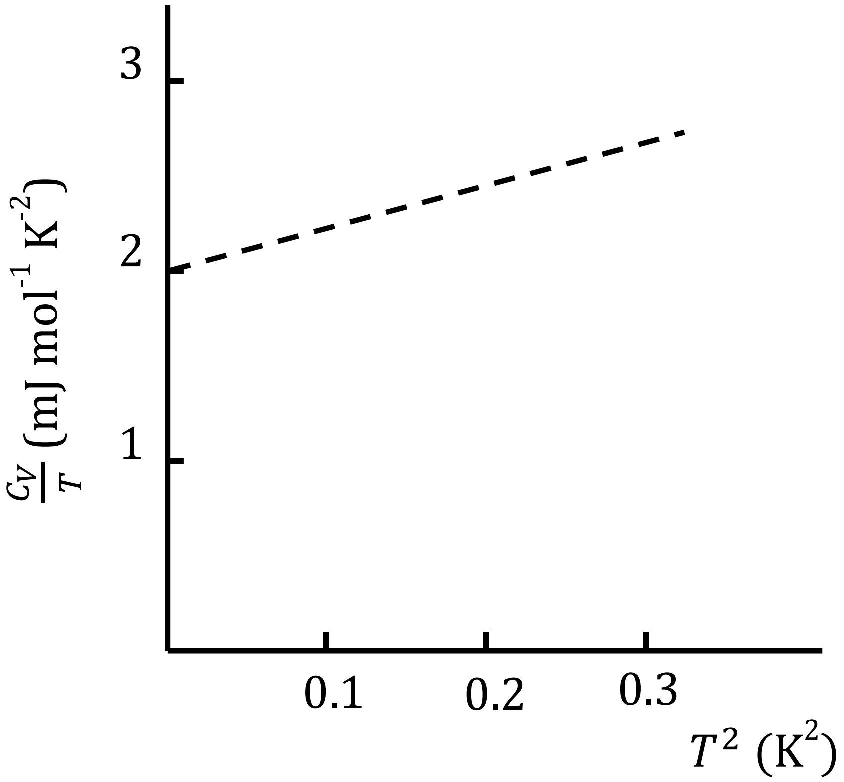
$$f(\varepsilon, T) = \frac{1}{\exp\left[\frac{\varepsilon}{k_B T}\right] - 1} .$$

[8 marks]

c) Compare the expression for C_V in part b) with your sketch of the experimental finding in part a) iii, both in the low and high temperature limits.

[3 marks]

d) Shown overleaf is a plot of experimental data for the metal potassium.



The contribution to the molar heat capacity of the free electrons in a metal is given by

$$\frac{\pi^2}{2} R \frac{T}{T_F} ,$$

where T_F is the Fermi temperature.
Using data from the graph calculate the Fermi temperature for electrons in potassium.

[5 marks]

P.T.O.

4.

a) Briefly describe the main characteristics of the bonding in silicon.

[3 marks]

b) Silicon has a fcc lattice and a basis of two Si atoms. The (200) Bragg reflection in first order is observed for an X-ray wavelength of 1.54 Å at a scattering angle (2θ) of 33.0°. Calculate the density of silicon. (Atomic mass of Si = 28 u.)

[7 marks]

c) The electron density, n, in a semiconductor is given by

$$n = 2\left(\frac{2\pi m_e^* k_\mathrm{B} T}{h^2}\right)^{\frac{3}{2}} \exp\left(\frac{\varepsilon_F - E_C}{k_\mathrm{B} T}\right),$$

where m_e* is the electron effective mass, ε_F is the Fermi energy and E_C is the energy of the conduction band edge.
Assuming that the effective masses of electrons in the conduction band and of holes in the valence band of Si are equal, calculate the hole density in the valence band of intrinsic Si at 1000 K.
(The band gap of Si is 1.1 eV, and m_e* =1.06 m_e.)

[5 marks]

d) Extrinsic doping can be achieved in Si by substituting phosphorus (P) atoms onto Si lattice sites. Draw a schematic energy level diagram to illustrate the band structure at T = 0 K of Si doped with P 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 P-doped Si is 25 meV. Assuming the semiconductor is in the impurity range, estimate the carrier density due to the dopant atoms at 300 K. Comment on your answer in comparison with your answer to part c).

[5 marks]

END OF EXAMINATION PAPER