SOLID STATE PHYSICS 1

- February 2005 -

Do not forget to write your full name and student number on each sheet.
Please use separate sheets for each of the four problems.

Planck's constant	$\hbar$	$1.055\text{x}10^{-34}$ Js
Boltzmann's constant	k_B	$1.38\text{x}10^{-23}$ J K^{-1}
Permittivity of free space	ε_0	$8.85\text{x}10^{-12}$ F m^{-1}
Permeability of free space	μ_0	$4\pi\text{x}10^{-7}$ H m^{-1}
speed of light	c	$3.0\text{x}10^{8}$ m s^{-1}
elementary charge	e	$1.60\text{x}10^{-19}$ C
mass of the electron	m	$9.11\text{x}10^{-31}$ kg
Bohr magneton	μ_B	9.27x10-24 J T^{-1}

I. The following questions should be answered very briefly (2-3 sentences at most); [2 points for each correct response].

a) What are the two structures of ionic crystals of the type X^+Y^- which have coordination numbers of six and eight respectively? (Description and sketch)

b) What is the necessary condition for a structural phase transition to occur?

c) In a crystal with 3 atoms in the primitive cell, how many branches does the phonon dispersion relation have?

d) What is the difference between the Fermi velocity and the drift velocity of free electrons in solids?

e) What does the excitation of a magnon correspond to?

f) Apply Hund's rule to find the angular momentum quantum number, the spin quantum number and the total angular + spin momentum quantum number for Dy^{3+} in the configuration $4f^9 5s^2 p^6$. Give also the spectroscopic notation of the ground state.

g) What feature of the density of states of electrons is characteristic of semimetal?

h) What happens when sufficiently high magnetic field is applied to a superconductor? How are H_c and T_c related?

i) What is an Umklapp scattering of electrons by phonons and what property of the metal is determined by this property?

j) What is a colour centre?

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II. The potential energy for a pair of inert gas atoms separated by a distance r may be written as the Lennard-Jones potential:

$$U_{pair}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

(a) Explain the physical origin of these two terms. [2 points]

(b) Find the equilibrium atomic separation (r_0) of a pair of atoms and $U_{pair}(r_0)$. [2 points]

FCC$_{12}$ = 12.13

(c) Sketch $U_{pair}(r)$ clearly labelling σ and ε. [2 points]

FCC$_6$ = 14.45

(d) Write down the cohesive energy of an inert gas whose N atoms interact via the Lennard-Jones potential. [2 points]

(e) The lattice sums $A_6 = \sum_j' p_{ij}^{-6}$ and $A_{12} = \sum_j' p_{ij}^{-12}$ where $p_{ij}r$ is the distance between reference atom I and any other atom j are given in the table below for bcc and fcc crystal structures. Calculate which structure is energetically preferred.

[6 points]

(f) An ionic solid can be modelled by a line of 2N ions of alternating charge ±q, interacting electrostatically. There is also a repulsive potential energy of $\frac{A}{r^n}$ between nearest neighbours only.

Show that at the equilibrium separation r_0 the cohesive energy of this solid is

$$U(r_0) = \frac{-2Nq^2}{4\pi\varepsilon_0 r_0}\ln 2\left(1-\frac{1}{n}\right)$$ [6 points]

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III. Consider a cubic solid with atoms of mass M separated by a distance a. Planes of atoms are coupled by a force constant C_p between planes s and s+p.

(a) By considering the equation of motion of atoms in plane s, show that the dispersion relation ω(k) for a travelling wave perpendicular to the plane is given by:

$$\omega^2 = \frac{2}{M}\sum_p C_p(1-\cos pka)$$ [5 points]

(b) Sketch the dispersion relation for the case $C_2 = C_1/2$ and $C_p=0$ for p>2.

[5 points]

(c) For a solid with $C_1=15\ Nm^{-1}$, M = 6.44 x 10-25 kg, a = 0.485 nm and force constants as in (b) above, calculate

i. the velocity of sound;

ii. the frequency at the Brillouin zone boundary;

iii. the energy and the crystal momentum of a phonon associated with the maximum frequency.

[10 points] 20

IV. Given the following expressions for a 1 dimensional conduction and valence band

$E_{val}(k) = - W (1 + coska)$ (W > 0)

$E_{cond}(k) = E_g + D (1 - coska)$ (D > 0)

(a) Assume the valence band to be filled, is this material an insulator or a conductor at temperature T = 0? [2 points]

(b) Given that E_g/k_B = 1000K, are we dealing with a direct or indirect gap semiconductor? Explain the difference. [2 points]

(c) Assume we have a semiconductor made of Si. Do we have to dope this material with B or with N in order to obtain an electron conductor?

[2 points]

(d) Draw the bandstructure and point out the Fermi level for these two cases.

[2 points]

(e) Given W = 0.1 eV and D = 1 eV, calculate the effective mass for the electrons and for the holes.

[2 points]

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