THE OPEN UNIVERSITY OF SRI LANKA

DEPARTMENT OF PHYSICS

BACHELOR OF SCIENCE DEGREE PROGRAMME -2015/2016 - LEVEL 05

PYU3173 – SOLID STATE PHYSICS   Final Examination – 2015/2016

TIME: TWO HOURS (2 hrs)   ANSWER <u>FOUR</u> QUESTIONS ONLY

Date: 14-07-2016   Time: 1.00 pm – 3.00 pm

1) (a) In the context of crystallography, what is meant by

(i) lattice

(ii) primitive unit cell

(iii) translation vector

(iv) basis

(v) reciprocal lattice vector **(10 Marks)**

(b) A simple orthorhombic lattice has primitive translation vectors

$$\vec{a} = a\,\hat{i}, \quad \vec{b} = b\,\hat{j}, \quad \vec{c} = c\,\hat{k}$$

Where $\hat{i}, \hat{j}, \hat{k}$ are the usual Cartesian unit vectors and a, b and c are constant. Determine

(i) the volume of the unit cell.

(ii) the reciprocal lattice vectors.

(iii) the volume of the unit cell in the reciprocal lattice.

(6 Marks)

(c) Briefly describe the Bragg's diffraction in crystals and show that the Bragg condition for crystal diffraction on (*hkl*) planes is given by:

$$2d_{hkl} \sin\theta_{hkl} = n\lambda$$

where the symbols have their usual meanings. **(5 Marks)**

A beam of X –rays is incident on a NaCl crystal with lattice spacing 0.282 nm. Determine

(i) the wavelength of X-rays if the first order Bragg reflection takes place at a glancing angle of $8^0 35'$

(ii) the maximum order of diffraction possible.

(4 Marks)

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2) A simple, one dimensional model of a solid consists of a series of two atoms having masses m and M respectively, joined by springs of spring constant β, with an equilibrium separation of a.

(a) Write down an equation of motion for the $2n^{th}$ atom in terms of the displacement of the $2n-1$, $2n$ and $2n+1$ atoms. **(4 Marks)**

(b) Show that the relation between the frequency ω and wave-vector q (the dispersion relation) is

$$\omega^2 = \beta\left(\frac{1}{m}+\frac{1}{M}\right) \pm \beta\sqrt{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{4\sin^2 qa}{mM}}$$ **(10 Marks)**

(c) Sketch the dispersion curve indicting the Optical branch, Forbidden gap and the Acoustic branch clearly. **(5 Marks)**

(d) Show as $q \to 0$, the ω_+ corresponds to Optical branch is given by the relation

$$\omega_+ = \sqrt{2\beta\left(\frac{1}{m}+\frac{1}{M}\right)}$$ and

when $q = \frac{\pi}{2a}$, ω_+ corresponds to Optical branch is given by the relation

$$\omega_+ = \sqrt{\frac{2\beta}{m}}$$ **(6 Marks)**

3) (a) With reasons categorize the following substances according to their bonding nature:

Cu, Zn, Pb, Ni, Mg, Ne, Ar, and NaCl **(5 Marks)**

(b) In a sodium chloride (NaCl) crystal, the ions are positioned on a cubic lattice with each ion surrounded by six nearest neighbours of the other species. The energy of the crystal per pair of ions may be written

$$U(r) = -M\frac{e^2}{4\pi\varepsilon_0 r} + 6\frac{B}{r^n}$$

where the Madelung constant $M = 1.747$, r is the nearest neighbour distance and B and n are parameters.

(i) Sketch the form of this function and explain the physical origin of the two terms.

(ii) Without a detailed derivation, describe how the value of M is calculated.

(iii) The equilibrium nearest neighbour distance in a NaCl crystal is 0.282 nm and the cohesive energy of the crystal is -1.27×10^{-18} J per ion pair. Determine the values of B and n.

(iv) Assuming the harmonic approximation applies, what is the bond force constant in NaCl?

(20 Marks)

4) (a) Write down the assumptions are made in the Debye model for the specific heat of solids? **(5 Marks)**

(b) According to the Debye model, the number of vibrational modes for each polarisation with frequencies between ω and $d\omega$ is given by

$$g(\omega)d\omega = \frac{V\omega^2}{2\pi^2 v^3} d\omega ,$$

where v is the speed of sound and V is the volume of the sample.

Show that the frequency ω_{max} of the highest frequency mode is given by

$$\omega_{max}^3 = \frac{6\pi^2 v^3 N}{V},$$

where N is the number of atoms in the sample. **(10 Marks)**

(c) The Debye temperature θ_D is related to ω_{max} by

$$k_B \theta_D = \hbar \omega_{max} ,$$

where k_B is the Boltzmann constant. What is the Debye temperature of chromium?

Density of chromium is 7190 kg m^{-3}, speed of sound in chromium is 4847 m s^{-1}, relative atomic mass is 52.0 g mol^{-1}.

(10 Marks)

5) (a) By considering the volume of a spherical shell in 'k-space' and the volume occupied by each electron state, show that the free electron density of states is given by

$$g(E) = \frac{V}{2\pi^2 \hbar^3} (2m_e)^{\frac{3}{2}} E^{\frac{1}{2}}$$ **(9 Marks)**

(b) The average energy of a free electron can be written as

$$\langle E \rangle = \frac{1}{N} \int_0^{E_F} E\, g(E)\, dE$$

where N is the total number of free electrons. Show that (at 0 K) the average energy of an electron in a metal is 60% of the Fermi energy (E_F). **(8 Marks)**

(c) Silver has 1 free electron per atom and a face centred cubic structure with conventional unit cell length, a= 0.409 nm. Calculate the Fermi energy of silver at absolute zero. Hence determine the average energy of a free electron in Silver at absolute zero. **(8 Marks)**

Assume that the Fermi energy at absolute zero as $E_F = \frac{\hbar^2}{2m_e}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}$ and the symbols have their usual meanings.

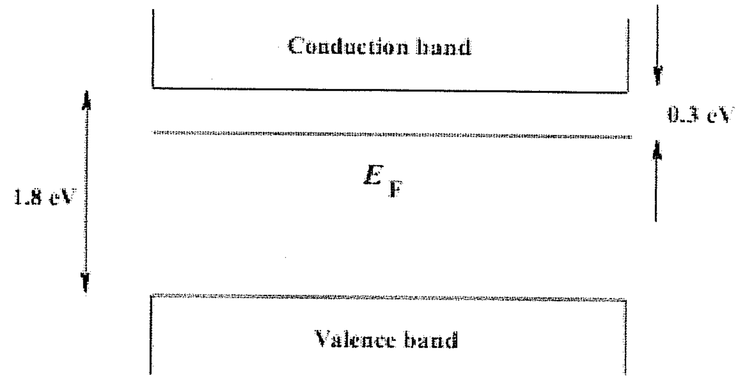
6) (a) The concentrations of conduction electrons (n) and holes (p) in a semiconductor at temperature T are given by

$$n = N_c \exp\left[-\frac{(E_c - E_F)}{k_B T}\right] \quad \text{and} \quad p = N_v \exp\left[-\frac{(E_F - E_v)}{k_B T}\right]$$

respectively. State what is meant by the terms N_c, N_v, E_c, E_v, E_F in these expressions.

(10 Marks)

(b) The figure shows the energy band for a semiconductor, in the region of the band gap.



(i) Would you consider that the semiconductor is an n–type or a p–type? Explain your answer

(ii) Calculate the probability, at 270 K, that an electron occupies an energy state at the bottom of the conduction band.

(iii) Calculate the probability, at 270 K, that there is a vacancy in an energy state at the top of the valence band.

(iv) For this semiconductor, the effective masses are $m_e^* = 0.10 m_e$ and $m_h^* = 0.05 m_e$. Calculate the density of states at the top of the valence band and at the bottom of the conduction band at 270 K.

(v) Hence calculate the concentration of holes at the top of the valence band and of electrons at the bottom of the conduction band.

(15 Marks)

You may assume that the probability of occupancy of a state with energy E is

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]}$$

and that

$N_c = N_v = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}$, where m^* is the effective mass and k_B is the Boltzmann constant.

Physical Constants

electron charge	$e = 1.60\times10^{-19}$ C
electron mass	$m_e = 9.11\times10^{-31}$ kg $= 0.511$ MeV c^{-2}
proton mass	$m_p = 1.673\times10^{-27}$ kg $= 938.3$ MeV c^{-2}
neutron mass	$m_n = 1.675\times10^{-27}$ kg $= 939.6$ MeV c^{-2}
Planck's constant	$h = 6.63\times10^{-34}$ J s
Dirac's constant ($\hbar = h/2\pi$)	$\hbar = 1.05\times10^{-34}$ J s
Boltzmann's constant	$k_B = 1.38\times10^{-23}$ J K^{-1} $= 8.62\times10^{-5}$ eV K^{-1}
speed of light in free space	$c = 299\,792\,458$ m s^{-1} $\approx 3.00\times10^{8}$ m s^{-1}
permittivity of free space	$\varepsilon_0 = 8.85\times10^{-12}$ F m^{-1}
permeability of free space	$\mu_0 = 4\pi\times10^{-7}$ H m^{-1}
Avogadro's constant	$N_A = 6.02\times10^{23}$ mol^{-1}
gas constant	$R = 8.32$ J mol^{-1} K^{-1}
ideal gas volume (STP)	$V_0 = 22.4$ l mol^{-1}
gravitational constant	$G = 6.67\times10^{-11}$ N m^2 kg^{-2}
Rydberg constant	$R_\infty = 1.10\times10^{7}$ m^{-1}
Rydberg energy of hydrogen	$R_H = 13.6$ eV
Bohr radius	$a_0 = 0.529\times10^{-10}$ m
Bohr magneton	$\mu_B = 9.27\times10^{-24}$ J T^{-1}
fine structure constant	$\alpha \approx 1/137$
Wien displacement law constant	$b = 2.898\times10^{-3}$ m K
Stefan's constant	$\sigma = 5.67\times10^{-8}$ W m^{-2} K^{-4}
radiation density constant	$a = 7.55\times10^{-16}$ J m^{-3} K^{-4}
mass of the Sun	$M_\odot = 1.99\times10^{30}$ kg
radius of the Sun	$R_\odot = 6.96\times10^{8}$ m
luminosity of the Sun	$L_\odot = 3.85\times10^{26}$ W
mass of the Earth	$M_\oplus = 6.0\times10^{24}$ kg
radius of the Earth	$R_\oplus = 6.4\times10^{6}$ m

Conversion Factors

1 u (atomic mass unit) $= 1.66\times10^{-27}$ kg $= 931.5$ MeV c^{-2}
1 astronomical unit $= 1.50\times10^{11}$ m
1 eV $= 1.60\times10^{-19}$ J
1 atmosphere $= 1.01\times10^{5}$ Pa
1 Å (angstrom) $= 10^{-10}$ m
1 g (gravity) $= 9.81$ m s^{-2}
1 parsec $= 3.08\times10^{16}$ m
1 year $= 3.16\times10^{7}$ s

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