# JIMMA UNIVERSITY

## COLLEGE OF NATURAL SCIENCE

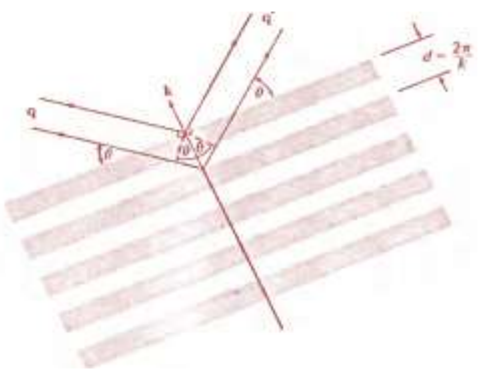
## DEPARTMENT OF PHYSICS

### Assignment for 2nd year BSc stream

Course title *solid state physics I* code Phy2062

**Attempt each of the following questions by showing your steps neatly.**

1. Why you study crystal structures?
2. a) Explain the basics difference between primitive cell and Wigner Seitz cell. b) Discuss the Brillion Zone.
3. Calculate the packing fractions for Simple cubic (SC), Base centered cubic (Bcc), and Face centered cubic (Fcc) crystal structures.
4. Consider the plane with (100), and (001), the lattice is FCC, and the indices refer to conventional cubic cell. What are the indices of these planes when referred to primitive axis of (fig 1: "Kittle Introduction to solid state physics")?
5. Show that $\frac{c}{a}$ ratio for ideal hexagonal close packed structure is $\left(\frac{8}{3}\right)^{1/2} = 1.633$. Now what happen to the crystal structure if $\frac{c}{a}$ is significantly larger than this value?
6. Explain the Bragg's law of diffraction. What is the basis for Bragg's law? Consider the figure below. If the angle of incidence equal angle of reflection, what can you conclude about the magnitude of q and q'? Where is the direction of q'- q?



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7. Show that the electron number density, n(r) is both periodic and real.
8. If the primitive translation vector of BCC lattice are

   $a_1 = \frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z})$ , $a_2 = \frac{1}{2}a(\hat{x}-\hat{y},+\hat{z})$, $a_3 = \frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$ then show that the primitive translation vectors of reciprocal lattice are

   $b_1 = \frac{2\pi}{a}(\hat{y}+\hat{z})$ , $b_2 = \frac{2\pi}{a}(\hat{x}+\hat{z})$, $b_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$.
9. In the crystal structure of diamond the basis consist of 8 atoms when the cell is taken as conventional cell.
   a) Find the structural factor S of this basis.
   b) Find the zeroth of structural factor S and show that the allowed reflections of diamond structures satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is integer or else all indices are odd.
10. Consider a plan ***hkl*** in the crystal lattice.
    a) Prove that the reciprocal lattice vector G = $hb_1 + kb_2 + lb_3$ is perpendicular to this plan.
    b) The distance between two adjacent parallel planes of the lattice is $d$(hkl) $= {}^{2\pi}/_{|G|}$
    C) Show for simple cubic lattice that $d^2 = \frac{a}{(h^2+k^2+l^2)}$.
11. What is the importance of x-ray diffraction?
12. Discus the crystal structure of inert gases and compare with the crystal structure of alkali metals.
13. Let the interaction energy between two atoms be given by:

    E(r) = $\frac{-A}{r^2} + \frac{B}{r^8}$

    If the atoms form a stable molecule with an inter-nuclear distance of 0.4 nm and a dissociation energy of 3eV, calculate *A* and *B*.
14. Using λ =2.05x$10^{-8}$ erg and $\rho = 0.326$Å the Madelung constant,$\alpha = 2ln2$, calculate cohesive energy for KCl in the zinc blend, ZnS structure. Compare with the value calculated for KCl in the NaCl structure.
15. Explain the basic properties of Ionic, covalent and Metallic bonds.

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I. Attempt each of the following questions by elaborating and showing your steps carefully. (15%)

1. Explain the relations between;

a) Transverse acoustic phonon and transverse optical phonon,

b) Longitudinal acoustic phonon and longitudinal optical phonon.

2. If there are 3 atoms in the primitive cell, then what are the total number of acoustic & optical phonon branches respectively?

3. Consider the normal mode of a linear chain in which the force constants between nearest neighbor atoms are alternatively C and 10C. Let the masses be equal and the nearest neighbouring distance be $\frac{a}{2}$. Find

a) $\omega(k)$ at k = 0 and K = $\frac{\pi}{a}$.

b) Sketch the dispersion relation for this problem.

4. In the phonon dispersion relation, $\omega = \left(\frac{4c}{M}\right)^{\frac{1}{2}} \left|sin\frac{1}{2}ka\right|$

a) If the product, Ka is small enough what will happen to the $\omega$?

b) When the wave vector is long enough, what happens to the relations between $\omega$ and K?

c) What will happen to the dispersion relation when the sine term is replaced by the cosine term?

d) Determine the zeroth of $\omega = \left(\frac{4c}{M}\right)^{\frac{1}{2}} \left|sin\frac{1}{2}ka\right|$.

5. I) what are the similarities and difference between Photons and Phonons?

II) Compare and contrast the dispersion relations of Photons and Phonons?

III) Explain some of experimental techniques to determine such dispersion relations?

6. Consider a longitudinal wave, $u_s = ucos(\omega t - sKa)$ , Which propagate in monatomic linear lattice of atoms of mass, M, spacing $a$, and the nearest neighbor interaction C,

a) Show that the total energy of the wave is

$$E = \frac{1}{2} M \sum_s \left(\frac{du_s}{dt}\right)^2 + \frac{1}{2} C \sum_s (u_s - u_{s+1})^2$$

Where, s runs over all integers.

b) By substitution of $u_s$ in this expression show that the time averaged total energy per atom is

$$\frac{1}{4} M\omega^2 u^2 + \frac{1}{2} C(1 - coska)u^2 = \frac{1}{2} M\omega^2 u^2 .$$

7. Explain the Debye's Model of specific heat Capacity of solids at low temperature limits and high temperature limit. Compare and contrast this Model with Dulong Petit law.

8. Explain the Van Hove Singularity points in the density of States. What is the Physical interpretation of these points?

9. Einstein's model of solids gives the expression for the specific heat

$$C_v = 3N_o K \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\frac{\theta_E}{T}}}{\left(e^{\frac{\theta_E}{T}} - 1\right)^2}$$

Where, $\theta_E = \frac{\hbar v_E}{K}$ and $\theta_E$ is called the characteristic temperature. Show that

(a) At high Temperature, Dulong Petit law is reproduced. (b) But at very low temperatures, the $T^3$ law is not given.

10. ***Zero point lattice displacement and strain.*** (a) In the Debye approximation, show that the mean square displacement of an atom at absolute zero is

$$\langle R^2 \rangle = \frac{3\hbar\omega_D{}^2}{8\pi^2 \rho v^3}$$

Where, v is the velocity of sound. Start from the result (4.29) summed over the independent lattice modes

$$\langle R^2 \rangle = \left(\frac{\hbar}{2\rho V}\right) \sum \omega^{-1} .$$

We have included a factor of ½ to go from mean square amplitude to mean square displacement. (b) Show that $\sum \omega^{-1}$ and $\langle R^2 \rangle$ diverge for a one-dimensional lattice, but that the mean square strain is finite. Consider $\langle \left(\frac{\partial R}{\partial x}\right)^2 \rangle = \frac{1}{2} \sum k^2 \, {u_o}^2$ as the mean square strain, and show that it is equal to $\frac{\hbar {\omega_D}^2 L}{4MNv^3}$ for a line N of atoms each of mass ***M***, counting longitudinal modes only. Notice that the divergence of $R^2$ is not significant for any physical measurement.

11. **Heat capacity of layer lattice*;*** (a) Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that, the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to $T^2$.

b) Suppose instead, as in many layer structures, that adjacent layers are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures?