## FACULTY OF SCIENCE

## DEPARTMENT OF PHYSICS APK

PHY003B
SOLID STATE PHYSICS OPEN-BOOK EXAM

DATE: Mon 15 NOVEMBER 2021
INTERNAL MODERATOR
EXTERNAL MODERATOR
DURATION: 2 HOURS

SESSION: 08:30-10:30
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Prof. A. QUANDT
(WITS , 011-717-6956)

THIS PAPER CONSISTS OF 5 PAGES INCLUDING THIS COVER
Instructions
ATTEMPT ALL FOUR QUESTIONS
Section B (Solid State Physics)
103 marks available, 90 marks or more is $100 \%$

You have 120 minutes for writing (08:30-10:30) plus 60 minutes for scanning and packaging the pdf files. Send to me by e-mail by 11:30 as a pdf file (grhearne@uj.ac.za). Filename should be student-number-surname.pdf. There is a penalty of $25 \%$ for a late submission after $11: 30$, and a further $25 \%$ penalty if submission is after $12: 30$, etc.

## Be academically honest and abide by the rules at all times geven while writing online assessments.

While writing your assessment you may not:

1. Provide assistance to another student
2. Receive assistance from another student or any third party.
3. Use unauthorized material or sources except the one that is expressly permitted by your lectures or the university.
4. Plagiarize or submit plagiarized material.

> You willbe held accountable for dishonest behavior duling assessment.

## Section B: SOLID STATE PHYSICS, 103 marks available

## QUESTION B1 [crystallography, 22 marks ]

(a) A real-space lattice has primitive lattice vectors given by: $\vec{a}_{1}=a \bar{i} \quad \vec{a}_{2}=b \bar{j} \quad \vec{a}_{3}=c \bar{k} \quad$ where $\overline{\mathrm{i}}, \overline{\mathrm{j}}, \overline{\mathrm{k}}$ are unit vectors in the cartesian axes. The real space lattice may is designated $\vec{R}=n_{1} \vec{a}_{1}+n_{2} \vec{a}_{2}+n_{3} \vec{a}_{3}$, where $n_{1}, n_{2}, n_{3}$ are integers. The lengths of the primitive lattice vectors have the relation $a>b>c$.
(i) Define what is meant by the reciprocal lattice $\vec{G}$ of $\vec{R}$ above and specify its primitive lattice vectors in terms of the unit vectors in the cartesian axes.
(ii) Make a sketch of the real space and reciprocal space lattices. For the purpose of illustrations, you may use two-dimensions only.
(iii) What does each reciprocal lattice point indicate in terms of Bragg planes.
(b) The crystal structure of fluorite $\left(\mathrm{CaF}_{2}\right)$ has a face-centered cubic (fcc) Bravais lattice, and a basis consisting of Ca ions at $(0,0,0)$ and F ions at $\pm(1 / 4,1 / 4,1 / 4)$, referred to the conventional unit cell with lattice constant $a$.
(i) Make a sketch of the cubic unit cell projected down the z -axis onto the $\mathrm{z}=0$ plane. Indicate the $z$ coordinate next to each ion.
(ii) After showing your ( $\mathrm{x}, \mathrm{y}, \mathrm{z}$ ) coordinate system, identify on separate diagrams the set of planes with Miller indices (110), (020) and (400).

## QUESTION B2 [lattice vibrations, 24 marks]

Heat capacity of a layered lattice. Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers, so that the motion of atoms is restricted to the plane of a layer. We are interested to find the phonon heat capacity of this 2D system. Proceed as follows:
(a) There are both an in-plane (longitudinal) and out-of-plane (transverse) modes of vibration. First find the density of $k$ states $\rho(k)$ in 2D. Then show that in the Debye approximation the density of frequency states is
$g(\omega)=A \frac{\omega}{\pi v_{s}^{2}}$, where $A$ is the area of a layer and $v_{\mathrm{s}}$ is the velocity of sound in the crystal.
(b) Now write down final expressions for the vibrational energy uptake of the 2 D system using the information from (a).
(c) Show that phonon heat capacity $\mathrm{C}_{\text {vib }}$ in the low-temperature limit is proportional to $T^{2}$.


## QUESTION B3 [conduction electrons, 29]

(a) Explain what is meant by the Fermi energy and the Fermi surface in $k$-space of a metal.
(b) By using the density of $k$-states $g(k)$, show that the Fermi wavevector in terms of the number density $N / V$ of a gas of electrons in 3-D is $k_{F}=\left(3 \pi^{2} N / V\right)^{1 / 3}$. Then use this to write down the expression for the Fermi energy $E_{F}$ in terms of the fermion number density. Note, there is an upspin and down-spin electron associated with each $k$ state.
(c) Using your findings in (b) and the density of energy states (not the density of $k$ states), show that the kinetic energy of the free electron gas at absolute zero temperature is $E=\frac{3}{5} N E_{F}$.
(d) Now find the expression for the degeneracy pressure $P$ of the free electron gas at absolute zero temperature.

Information given: The plane-wave solution to the Schrodinger equation for free electrons subject to boundary conditions of a crystal of dimensions ( $L_{X}, L_{Y}, L_{Z}$ ), indicates that the allowed $k$-values are:
$k_{X}=\frac{2 \pi p}{L_{X}} ; \quad k_{Y}=\frac{2 \pi q}{L_{Y}} ; \quad k_{Z}=\frac{2 \pi r}{L_{Z}} \quad p, q, r$ are integers.

## QUESTION B4 [semiconductors, 28 marks]

(a) In a fully labelled energy versus wave-vector (dispersion) plot, depict the valence band and the conduction band for a semiconductor with a gap of 1 eV and whose electrons and holes have effective masses $m_{e}^{*}=(0.1) m$ and $m_{h}^{*}=(0.5) m$, where $m$ is the bare electron mass.
(b) Show in terms of your plot in (a) above what is meant by a hole and explain how it leads to conduction if there is p -type doping. Also show how your $\varepsilon-k$ dispersion plot is modified by such p-type doping.
(c) By using the group velocity $v_{g}=d \omega / d k$ of the electron or hole wavepacket, derive the expression for the momentum of an electron or hole in terms of its wavevector $\boldsymbol{k}$.
(d) The effective mass of the electron or hole $m^{*}=\hbar^{2}\left(d^{2} \varepsilon / d k^{2}\right)^{-1}$. Show how this expression is derived by considering the acceleration and momentum of the charge carrier.
(e) Use the expressions for the number of thermally excited electrons and holes in an intrinsic semiconductor to show that the chemical potential $\mu$ lies in the middle of the gap at low temperatures. Explain the meaning of having $\mu$ midway in a region of forbidden energy states.

