UNIVERSITY OF ESWATINI

FACULTY OF SCIENCE AND ENGINEERING

DEPARTMENT OF PHYSICS

MAIN EXAMINATION 2019/2020

TITLE OF PAPER:	SOLID STATE PHYSICS
COURSE CODE:	P412/PHY412
TIME ALLOWED:	THREE HOURS

USEFUL INTSRUCTIONS:

1. There are five questions in this paper, and each question carries a total of 25 marks. Answer any four questions in your preferred order.
2. Additional materials included in this paper are a list of useful constants, particle masses and some conversion factors.

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THIS PAPER CONSISTS OF 8 PAGES WITH COVER PAGE AND THE ADDITIONAL ATTACHED MATERIAL

Question One [25 marks]

(a) (i) What is meant by the phrase *crystalline solid*? (1)

(ii) What special feature enabled certain elements to form into solids? (1)

(b) Van der Waals forces are in charge of interactions between the chemically saturated units in molecular crystals. Fig. 1.1 shows two 1-D harmonic oscillators used to illustrate the nature of van der Waals forces.

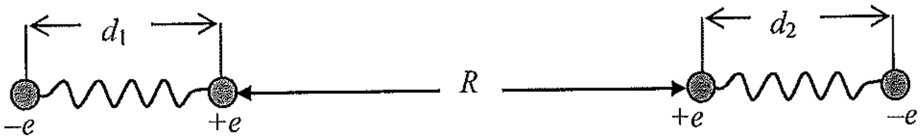

Figure 1.1

(i) Show that for separations $R >> d_i$, the total energy of the vibrating dipoles is given by the following expression:

$$E = \frac{1}{2M}\left(P_1^2 + P_2^2\right) + \frac{k}{2}\left(d_1^2 + d_2^2\right) + 2Ke^2\frac{d_1 d_2}{R^3} \qquad (15)$$

(ii) In a short summary, interpret all terms in the above expression. (5)

(iii) Cite any three shortfalls of the above modeling of van der Waals forces. (3)

Question Two [25 marks]

(a) With the aid of unit cell diagrams, define the following crystal symmetry structures.

(i) Triclinic Symmetry. (1)

(ii) Monoclinic Symmetry. (1)

(iii) Orthorhombic Symmetry. (1)

(iv) Trigonal Symmetry. (1)

(v) Hexagonal Symmetry. (1)

(b) (i) Copper crystallizes as a face-centered cubic crystal structure with the radius of each atom given by $r = 128\,\text{pm}$. Calculate its density in g/cm^3. (5)

{**Hint**: The atomic weight of copper is $M = 63.54$ g/mol .}

(ii) Calculate the number of cations, anions, and formula units per unit cell in each of the following solids.

1. The cesium chloride ($CsCl$) unit cell. (2)
2. The rutile (TiO_2) unit cell. (3)

(iii) Graphite forms extended two-dimensional layers.

1. Draw the smallest possible rectangular unit cell for a layer of graphite. (2)
2. How many carbon atoms are in the unit cell? (2)
3. What is the coordination number of carbon in a single layer of graphite? (1)

(c) (i) Define the following terms/phrases.

1. Lattice. (1)
2. Bravais lattice. (1)
3. Primitive unit cell. (1)
4. Wigner-Seitz primitive cell. (2)

Question Three [25 marks]

(a) (i) Define the following terms/phrases.

1. Lattice vibrations (1)
2. Phonons (1)

(ii) The many-particle Schrödinger wave equation, which is given by $H_c\psi = i\hbar\partial\psi/\partial t$, where H_c is the crystal *Hamiltonian*. With a clear description of all parameters involved, write down the general form of the wave function ψ. (3)

(iii) The Hamiltonian for such a many-body problem is given by

$$H_c = -\sum_i \left(\hbar^2/2m\right)\nabla_i^2 - \sum_l \left(\hbar^2/2M_l\right)\nabla_l^2 + (1/2){\sum_{i,j}}'' \left(e^2/4\pi\varepsilon_0|\boldsymbol{r}_i - \boldsymbol{r}_j|\right) - \sum_{i,l}\left(e^2 Z_l/4\pi\varepsilon_0|\boldsymbol{r}_i - \boldsymbol{R}_l|\right)$$
$$+ (1/2){\sum_{l,l''}}'' \left(e^2 Z_l Z_{l''}/4\pi\varepsilon_0|\boldsymbol{R}_l - \boldsymbol{R}_{l''}|\right)$$

1. State the role played by each of the parameters m, M_l, Z_l, and e. (4)
2. State the significance of each of the terms in the above expression. (5)

(iv) State the physical content of the *Born-Oppenheimer approximation* both in words and in expression form. (5)

(b) Fig. 3.1 shows the two-atom lattice used to connect with real lattice vibrations. Here, γ is the spring constant, a is the equilibrium separation of atoms, x_1 and x_2 are coordinates that measure the displacements of atoms 1 and 2 from equilibrium, and m is the mass of each atom.

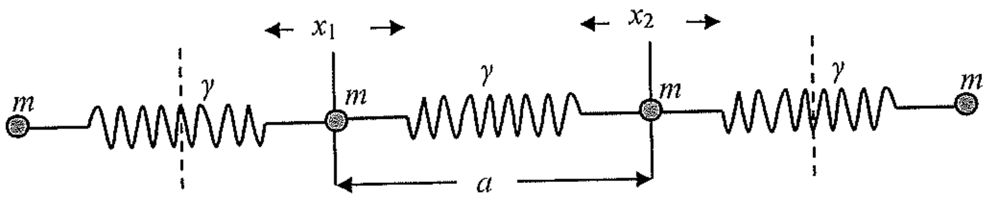

Figure 3.1

Derive the secular equation and give values of the eigenfrequencies that satisfy it. (6)

Question Four [25 marks]

(a) What is meant by the acoustic mode and optic mode in relation to classical diatomic lattices? (4)

(b) Fig. 4.1 is a schematic used to illustrate the linear diatomic lattice.

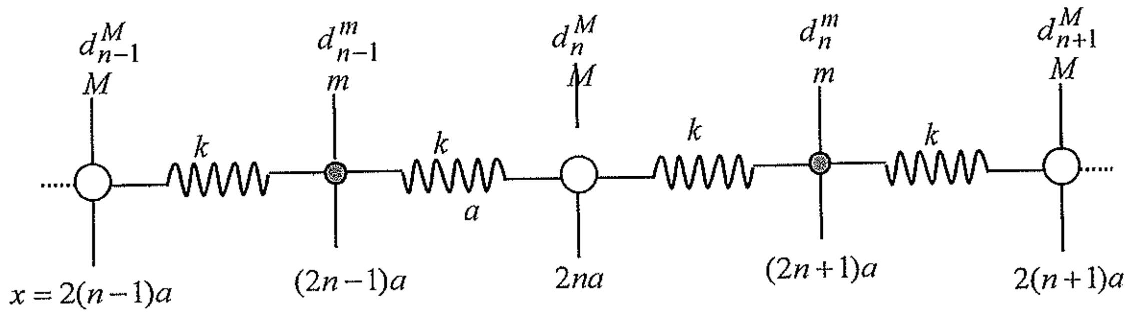

Figure 4.1

1. If $K_1 = k/m$ and $K_2 = k/M$, show that the equations of motion for the above lattice system are given by $\ddot{d}_n^m = K_1\left(d_{n+1}^M - d_n^m\right) + K_1\left(d_n^M - d_n^m\right) = -K_1\left(2d_n^m - d_{n+1}^M - d_n^M\right)$ as well as $\ddot{d}_n^M = K_2\left(d_n^m - d_n^M\right) + K_2\left(d_{n-1}^m - d_n^M\right) = -K_2\left(2d_n^M - d_n^m - d_{n-1}^m\right)$. (4)

2. If the normal mode solutions $d_n^m = A\exp\left[i\left(qx_n^m - \omega t\right)\right]$ and $d_n^M = B\exp\left[i\left(qx_n^M - \omega t\right)\right]$ are sought, show that $\begin{bmatrix} \omega^2 + 2K_1 & -2K_1\cos qa \\ -2K_2\cos qa & \omega^2 + 2K_2 \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ (4)

(c) (i) What is meant by a lattice defect? (2)

(ii) What is meant by the direct lattice? (2)

(iii) If (a_1, a_2, a_3) are the primitive vectors of a 3-dimensional lattice, and if (b_1, b_2, b_3) are three vectors chosen in such a way that $a_i \cdot b_j = \delta_{ij}$, define the reciprocal lattice in equation form. (3)

(d) (i) If Fig. 4.2 illustrates the notation used for 3-dimensional lattices, what role is played by the vectors l and b? (2)

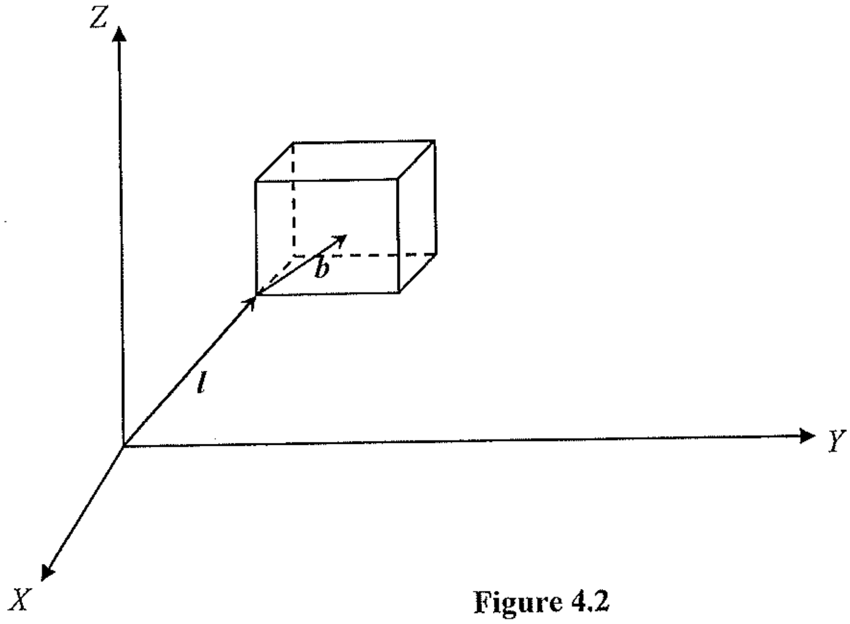

Figure 4.2

(ii) If $\boldsymbol{p}_{lb}$ is the momentum of the atom located at $\boldsymbol{l}+\boldsymbol{b}$ with mass m_b, write an expression for the Hamiltonian. (4)

Question Five **[25 marks]**

(a) (i) If in the Debye approximation for the specific heat, the number of phonons in mode (q, p) is given by the expression $\bar{n}_{q,p} = \frac{1}{\exp(\hbar\omega_{q,p}/kT) - 1}$, write expressions for the average energy per mode and the thermodynamic average energy. (4)

(ii) Use the above results to deduce an expression for the specific heat at constant volume. (4)

(iii) If in the Debye model, the total density of states is represented by the summation expression $D(\omega) = \sum_p D_p(\omega)$, define the quantity $D_p(\omega)$. (2)

(b) (i) In a box of length L_x, width L_y, and height L_z, write down an expression for the dispersion relation with a full description. (4)

(ii) If the volume of the crystals is $V = L_x L_y L_z$, write an expression for the number of states in a sphere of radius ω in ω space. (4)

(iii) With a full description, write an expression for the *density of states* for some mode p. (3)

(iv) With a full description thereof, write an expression the total density of states based on above. (4)

Fundamental Constants

Quantity	Symbol	Value
Elementary charge	e	1.6022×10^{-19} C
Speed of light in vacuum	c	2.9979×10^{8} m/s
Permeability of vacuum	μ_0	$4\pi\times10^{-7}$ N·A^{-2}
Permittivity of vacuum	ε_0	8.8542×10^{-12} F·m^{-1}
Planck constant	h	6.6261×10^{-34} J·s
		4.1357×10^{-15} eV·s
Avogadro constant	N_A	6.0221×10^{23} mol^{-1}
Boltzmann constant	k	1.3807×10^{-23} J·K^{-1}
Stefan-Boltzmann constant	σ	5.6704×10^{-8} W·m^{-2}·K^{-4}
Atomic mass unit	u	1.66053886×10^{-27} kg
		931.494061 MeV/c^2

Particle masses

	Mass in units of		
Particle	**kg**	**MeV/c^2**	**u**
Electron	9.1094×10^{-31}	0.5110	5.4858×10^{-4}
Proton	1.6726×10^{-27}	938.27	1.00728
Neutron	1.6749×10^{-27}	939.57	1.00866
Deuteron	3.3436×10^{-27}	1875.61	2.01355
α particle	6.6447×10^{-27}	3727.38	4.00151

Conversion factors

$1\,\text{MeV/c} = 5.344\times10^{-22}\ \text{kg}\cdot\text{m/s}$

$1\,\text{u} = 1.66054\times10^{-27}\ \text{kg}$

$1\ \text{Ci} = 3.7\times10^{10}\ \text{Bq}$

$1\,\text{eV} = 1.6022\times10^{-19}\ \text{J}$

Useful Combinations of Constants

$$\hbar = h/2\pi = 1.0546\times10^{-34}\ \text{J}\cdot\text{s} = 6.5821\times10^{-16}\ \text{eV}\cdot\text{s}$$

$$hc = 1.9864\times10^{-25}\ \text{J}\cdot\text{m} = 1239.8\ \text{eV}\cdot\text{nm}$$

$$\hbar c = 3.1615\times10^{-26}\ \text{J}\cdot\text{m} = 197.33\ \text{eV}\cdot\text{nm}$$

$$\frac{1}{4\pi\varepsilon_0} = 8.9876\times10^{9}\ \text{N}\cdot\text{m}^2\cdot\text{C}^{-2}$$

Compton wavelength $\lambda_C = \dfrac{h}{m_e c} = 2.4263\times10^{-12}$ m

$$\frac{e^2}{4\pi\varepsilon_0} = 2.3071\times10^{-28}\ \text{J}\cdot\text{m} = 1.4400\times10^{-9}\ \text{eV}\cdot\text{m}$$

Rydberg constant $R_\infty = 1.09737\times10^{7}$ m^{-1}