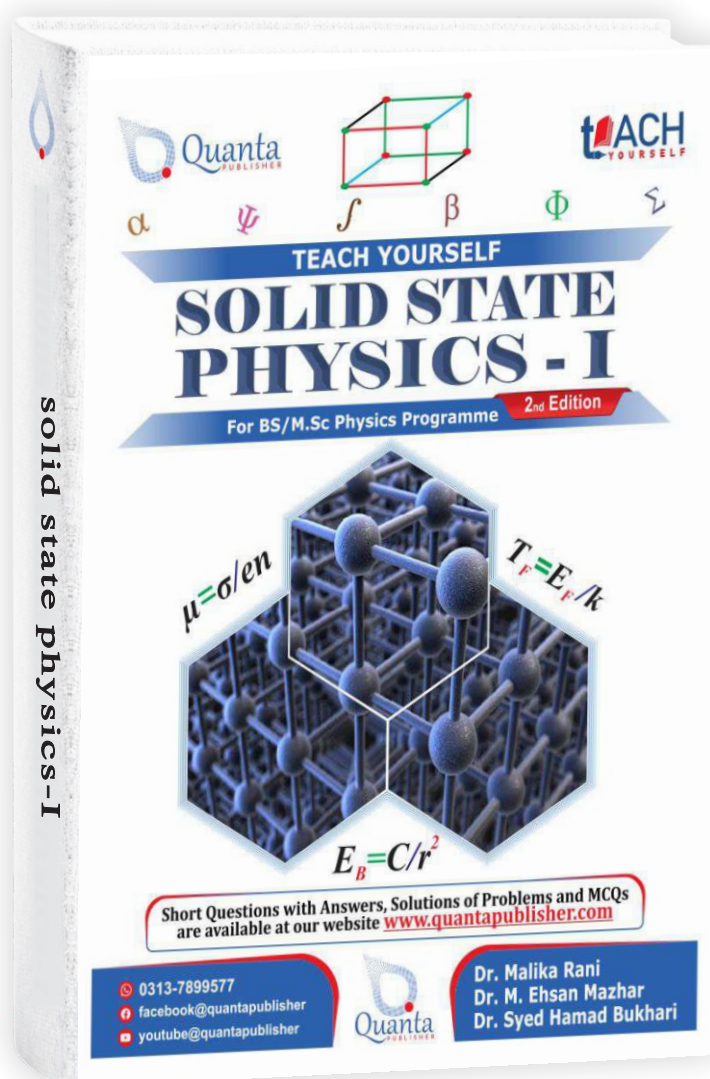




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SOLID STATE PHYSICS - I

2nd Edition

For **BS/M.Sc Physics** students of all Pakistani Universities/Colleges

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Contents

1	Crystal Structure	1
1.1	Introduction to Solids	1
1.2	Crystal Structure	3
1.3	Fundamental Types of Lattices	7
1.4	Symmetry Operations In Crystals	13
1.5	Crystal Binding and Periodic Arrays of Atoms	19
1.6	Index System for Crystal Planes	21
1.7	Interplaner Distances	23
1.8	Simple Crystal Structure	25
1.9	Review Questions and Problems	34
2	Reciprocal Lattice	35
2.1	Electron Diffraction	35
2.2	Neutron Diffraction	36
2.3	X-ray Diffraction	37
2.4	Bragg's Law	37
2.4.1	Experimental Methods of X-Ray Diffraction	39
2.4.2	Laue's Expression for the Amplitude of Scattered Waves	43
2.5	Reciprocal Lattices and Reciprocal Lattice Vectors	45
2.5.1	Bragg's Diffraction Condition in Terms of Reciprocal Lattice	49
2.5.2	Brillouin Zone	50
2.5.3	Ewald's Construction and Ewald's Sphere	52
2.6	Fourier Analysis of The Basis	54
2.7	Review Questions and Problems	55
3	Crystal Binding and Elastic Constants	57
3.1	Classifications of Solids	57
3.2	Ionic Radii	61
3.3	II-VI and III-V Compounds	63
3.4	Analysis of Elastic Strain	64
3.5	Elastic Compliance and Stiffness Constants	67
3.6	Elastic Wave in Cubic Crystal	70
3.7	Review Questions and Problems	73

4	Cohesive Energy	75
4.1	The Lenard Jones Potential	75
4.2	Cohesive Energy of Solid	77
4.3	The Madelung Constant	80
4.3.1	Equilibrium Density and Energy	82
4.4	Bulk Modulus	84
4.5	Cohesion in Covalent Crystals	85
4.6	Review Questions and Problems	86
5	Crystal Vibrations: Phonon-I	88
5.1	Lattice Vibrations	88
5.2	Vibration of Crystal with Monoatomic Basis	88
5.3	Vibration of Crystal with Diatomic Primitive Basis	92
5.4	Quantization of Elastic Waves (Phonons)	100
5.4.1	Review of Quantum Oscillator	101
5.5	Phonon Momentum and Phonon Scattering	104
5.6	Lattice Optical Properties In The Infrared Region	106
5.7	Review Questions and Problems	107
6	Thermal Properties: Phonon-II	109
6.1	Phonon Heat Capacity / Classical Model	109
6.1.1	Planck Distribution	110
6.2	Einstein Model for Density of State	112
6.3	Debye Model for Density of States	114
6.4	Anharmonic Crystal Interactions	118
6.5	Thermal Conductivity	118
6.6	Umklapp Processes	120
6.7	Review Questions and Problems	121
7	Crystal Imperfections	123
7.1	Types of Imperfections	123
7.1.1	Point Imperfections	123
7.1.2	Line Imperfections	127
7.1.3	Surface Imperfections	129
7.1.4	Volume Imperfections	132
7.2	Review Questions and Problems	133
8	Electrical Properties Of Metals	134
8.1	Classical Free Electron Theory	134
8.1.1	Density of States in One Dimension	137
8.1.2	Three Dimensional Case	137
8.1.3	Density of States in Three Dimensions	138
8.2	Effect of Temperature on Fermi-Dirac Distribution	141
8.3	Properties of the Electron Gas	142
8.4	Electrical Conductivity and Ohm's Law	143
8.5	Thermal Conductivity of Metals	145
8.6	Ratio of Thermal to Electrical Conductivity	147
8.7	Motion in Magnetic Fields	147
8.8	Hall Effect	150
8.9	Review Questions and Problems	152

Chapter 1

Crystal Structure

1.1 Introduction to Solids

Solids

Solids are the forms of matter in which atoms or molecules are strongly bound and maintain a definite volume and shape unless changed by applying an external forces.

Solids State Physics

Solid state physics is the study to investigate the physical properties of atomic or molecular matter in the solid form. These physical properties include crystal structure, bonding, thermal, electrical and magnetic properties.

Classification of Solids

On the basis of structure, solids are classified into three categories:

↔ Crystalline solids ↔ Non-crystalline or amorphous solids

Crystalline Solids

When the constituent atoms of a solid are arranged in a definite, regular and repeated geometric pattern throughout the entire three dimensional network then the formed solid is a crystalline solid. Examples of crystalline solid include diamond, metals, rock salts, quartz, sugar, ice etc. Structure of crystals has particular arrangement of particles and primary to understand. This arrangement of particles is in a very ordered fashion as shown in Fig.(1.1). These particles are arranged in a repeating pattern of a three-dimensional network. This network is known as a crystal lattice whose smallest unit is a unit cell. If you see the X-ray of a crystal this distinct arrangement of the unit cells whose repetition

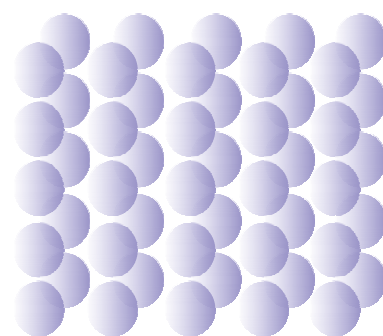


Fig. 1.1. The schematic picture of crystalline solids.

Chapter 2

Reciprocal Lattice

2.1 Electron Diffraction

Similar to X-rays, a beam of electron can also be used to characterize the crystal structure. A beam of electron emitted from a hot wire (as a result of thermionic emission) is accelerated through vacuum under a very large electrode potential V and is then passed through a collimator before it gets diffracted by the specimen to be studied. The energy E acquired by these electrons will depend on accelerating voltage V , thus

$$E = eV \quad (2.1)$$

where e is charge on electron. According to de-Broglie hypothesis, the wavelength of the moving electrons can be given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad (2.2)$$

Since, the $K.E$ of the electron is given as

$$E = \frac{1}{2}mv^2 \quad ; \quad v = \sqrt{\frac{2E}{m}}$$

Now, from Eq.(2.2), we get

$$\lambda = \frac{h}{m\sqrt{\frac{2E}{m}}} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2meV}} \quad \because \text{using Eq.(2.1)}$$

Where m is the mass of electron. Putting $m = 9.11 \times 10^{-31}$ kg and $e = 1.6 \times 10^{-19}$ C, the wavelength λ will be

$$\lambda = \frac{12.24}{\sqrt{V}} \text{ \AA}$$

Thus, wavelength of moving electron is inversely proportional to the square root of the accelerating voltage and hence can be varied easily to get the desired wavelength of electron beam. Thus, if we apply the accelerating voltage V such that the wavelength of the electron beam become equal to the order of atomic distances, then we can use electron beam diffraction.

Chapter 3

Crystal Binding and Elastic

Constants

3.1 Classifications of Solids

Ionic Crystal

“A class of crystal consisting of a lattice of ions held together by electrostatic interactions; they exhibit strong absorption of infrared radiation and have planes along which they cleave easily”. An ionic crystal consists of ions bound together by electrostatic attraction which are arranged in a regular, geometric structure. Examples of such crystals are the alkali halides, which include:

- ↔ Potassium fluoride (KF) ↔ Potassium chloride (KCl) ↔ Potassium bromide (KBr)
- ↔ Potassium iodide (KI) ↔ Sodium fluoride (NaF)
- ↔ Other combinations of Sodium, Cesium, Rubidium, or Lithium ions with Halogens ions such as Fluoride, Bromide, Chloride or Iodide.

These solids tend to be quite hard and have high melting points, reflecting the strong forces between oppositely-charged ions. The exact arrangement of ions in a lattice varies according to the size of the ions in the crystal.

A Case Study: NaCl

The properties of NaCl reflect the strong interactions that exist between the ions. It is a good conductor of electricity when molten (melted state), but very poor in the solid state. When melted, the mobile ions carry charge through the liquid. NaCl crystals are characterized by strong absorption of infrared (IR) radiation, and have planes along which they cleave easily. Structurally, each ion in sodium chloride is surrounded by six neighboring ions of opposite charge. The resulting crystal lattice is of a type known as **face centered**

Chapter 4

Cohesive Energy

4.1 The Lenard Jones Potential

Proposed by Sir John Edward Lennard-Jones, the Lennard-Jones potential describes the potential energy of interaction between two non-bonding atoms or molecules based on their distance of separation. The potential equation accounts for the difference between attractive forces (dipole-dipole, dipole-induced dipole, and London interactions) and repulsive forces.

Introduction

Imagine two rubber balls separated by a large distance. Both objects are far enough apart that they are not interacting. The two balls can be brought closer together with minimal energy, allowing interaction. The balls can continuously be brought closer together until they are touching. At this point, it becomes difficult to further decrease the distance between the two balls. In order to

bring the balls any closer together, increasing amounts of energy must be added. This is because eventually, as the balls begin to invade each other's space, they repel each other; the force of repulsion is far greater than the force of attraction. This scenario is similar to that which takes place in neutral atoms and molecules and is often described by the Lennard-Jones potential.

The Lennard-Jones Potential

The Lennard-Jones model consists of two parts; a steep repulsive term, and smoother attractive term, representing the London dispersion forces. Apart from being an important

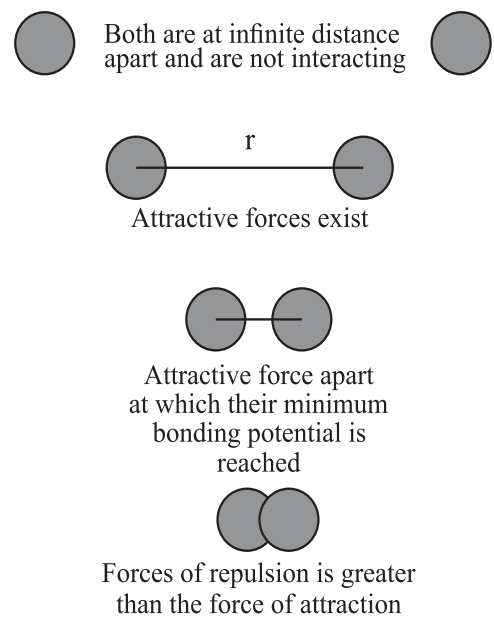


Fig. 4.1. The interaction between two balls at different positions

Chapter 5

Crystal Vibrations: Phonon-I

5.1 Lattice Vibrations

A lattice may be regarded as a regular arrangement of atoms in which atoms are joined by elastic massless springs. The motion of any single atom is shared by all atoms. The lattice can vibrate freely in its normal mode or it may experience forced vibrations. The normal mode vibrations are produced due to its internal energy while forced vibrations produced due to effect of dynamical external forces. The external forces may be of mechanical or electromagnetic type in nature. Normal mode vibrations give informations like thermal properties such as specific heat and thermal conductivity while forced vibrations give informations such as acoustical and optical properties of solid.

5.2 Vibration of Crystal with Monoatomic Basis

Consider one dimensional linear chain of identical atoms each of mass m . Let a be the lattice parameter. At equilibrium, each atom is in its equilibrium lattice position given by $\dots (n - 1), n, (n + 1), \dots$ as shown in Fig.(5.2). We assume that the atoms are simultaneously owing to mutual interaction between them. Therefore, when a longitudinal wave is propagated through the lattice, the entire planes of atoms move in phase with displacement parallel to wave vector \vec{K} . Planes of atoms in equilibrium (dashed lines) and displaced atoms (solid lines) during the passage of longitudinal wave is shown in Fig.(5.1). The atomic displacements are perpendicular for the transverse wave propagation as shown in Fig.(5.3).

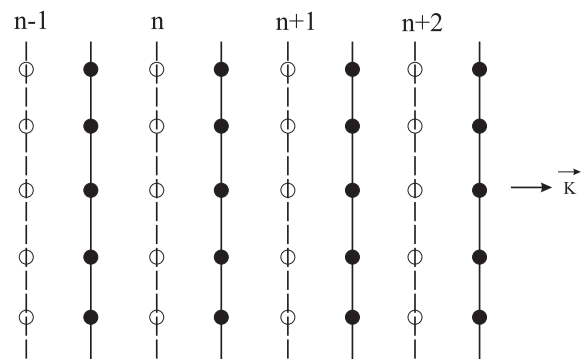


Fig. 5.1. The schematic picture which shows the planes of atoms in equilibrium (dashed lines) and displaced atoms (solid lines) during the passage of longitudinal wave

Chapter 6

Thermal Properties: Phonon-II

6.1 Phonon Heat Capacity / Classical Model

Heat capacity is a materials property which converts absorbed energy into a unit increase in temperature. Knowing the heat capacity of a material can help you answer questions like

↪ If we shine a laser of known power and frequency onto a given crystalline solid (and I know the optical absorptivity of that material for that frequency of light), how much will the region exposed to the laser beam heat up?

↪ If we put a copper pan on a hot plate (powered by known voltage and current) what is the maximum temperature it can reach in 5 minutes?

In this derivation, we will consider the heat capacity at constant volume, defined as

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V$$

Where U is the internal energy and T is the temperature. There is also heat capacity at constant pressure (C_P) which is given by the temperature derivative of the enthalpy

$$H = U + PV$$

The two types of heat capacity are related to each other by the thermodynamic relation

$$C_P - C_V = 9\alpha^2 BVT$$

where α is the coefficient of linear thermal expansion, V is the volume, and B is the bulk modulus. The total energy (U) of phonons at a given temperature is given by:

$$\sum_K \sum_p \langle n_{K,p} \rangle \hbar \omega_{K,p}$$

Where

↪ The sum over K is summing up all available momentum states (e.g. momentum is quantized, so we consider each discrete value and look at the frequency ω at that value according to the dispersion relation).

Chapter 7

Crystal Imperfections

7.1 Types of Imperfections

The perfectly regular crystal structures that have been considered up to now are called ideal crystals in which atoms are arranged in a regular way. In actual crystals, however, imperfections or defects are always present and their nature and effects are very important in understanding the properties of crystals. These imperfections affect the properties of crystals such as mechanical strength, chemical reactions, electrical properties etc., to a great extent. Imperfections are found in all crystals unless some special means are used to reduce them to a low level. The crystallographic defects are classified as follows:

1- Point Defects or Zero Dimensional Defects

- | | |
|----------------------------|---------------------------|
| 1. Vacancy | 2. Schottky imperfections |
| 3. Interstitialcy | 4. Frenkel defect |
| 5. Compositional defects | |
| → Substitutional impurity. | → Interstitial impurity. |
| 6. Electronic defects | |

2-Line Defects or One Dimensional Defects

- | | |
|----------------------|-----------------------|
| 1. Edge dislocation. | 2. Screw dislocation. |
|----------------------|-----------------------|

3-Surface Defects or Plane Defects or Two Dimensional Defects

- | | |
|----------------------|---------------------|
| 1. Grain boundaries. | 2. Tilt boundaries. |
| 3. Twin boundaries. | 4. Stacking fault. |

4-Volume Defects or three dimensional Defects

7.1.1 Point Imperfections

↔ Point defects are imperfect point like regions in a crystal.

↔ The typical size of a point defect is one or two atomic diameters.

Chapter 8

Electrical Properties Of Metals

8.1 Classical Free Electron Theory

Introduction

↪ In solid states and condensed matter physics, the density of state (DOS) function describes the number of state that are available in a system at each energy level.

↪ In general it is statistical average over space and time domains of many states occupied by the system.

↪ The DOS is directly proportional to the dispersion relation properties of the system.

↪ High DOS at a specific energy level means many states are available for occupation.

↪ DOS is essential part to determine the carrier concentrations and energy distributions of carriers within a semiconductor.

↪ In order to determine the actual number of electrons in a given energy state, it is necessary to know the number of states in a system which have energy in specific range and probability function.

↪ The actual number of electrons ($N(E)$) in an energy range E and $(E+dE)$ at any temperature are

$$N(E)dE = D(E)F(E)dE,$$

where $D(E)$ and $F(E)$ are density of states¹ and Fermi-Dirac distribution function respectively.

Fermi Energy of a Free Electron Gas

Consider a free electron of mass m confined in a box of length L . Assume the potential energy everywhere within the box to be zero i.e $v = 0$. At the two ends of the box, the electron is prevented from leaving the box by a very high potential energy barrier, as shown in the Fig. (8.1). The Schrödinger time independent equation in one-dimension is

¹ State is an allowed solution which satisfies the boundary conditions



1 Crystal Structure	01	3.6 Elastic Wave in Cubic Crystal.....	70
1.1 Introduction to Solids	01	3.7 Review Questions and Problems.....	73
1.2 Crystal Structure.....	03	4 Cohesive Energy.....	75
1.3 Fundamental Types of Lattices	07	4.1 The Lenard Jones Potential.....	75
1.4 Symmetry Operations In Crystals.....	13	4.2 Cohesive Energy of Solid.....	77
1.5 Crystal Binding & Periodic Arrays of Atoms... 19		4.3 The Madelung Constant.....	80
1.6 Index System for Crystal Planes.....	21	4.3.1 Equilibrium Density and Energy.....	82
1.7 Interplaner Distances	23	4.4 Bulk Modulus.....	84
1.8 Simple Crystal Structure.....	25	4.5 Cohesion in Covalent Crystals.....	85
1.9 Review Questions and Problems.....	34	4.6 Review Questions and Problems.....	86
2 Reciprocal Lattice	35	5 Crystal Vibrations: Phonon-I.....	88
2.1 Electron Diffraction	35	5.1 Lattice Vibrations.....	88
2.2 Neutron Diffraction.....	36	5.2 Vibration of Crystal with Monoatomic Basis....	88
2.3 X-ray Diffraction	37	5.3 Vibration of Crystal with Diatomic Primitive.....	92
2.4 Bragg's Law.....	37	5.4 Quantization of Elastic Waves (Phonons).....	100
2.4.1 Experimental Methods of X-Ray Diffraction	39	5.4.1 Review of Quantum Oscillator.....	101
2.4.2 Laue's Expression for the Amplitude of		5.5 Phonon Momentum and Phonon Scattering....	104
Scattered Waves.....	43	5.6 Lattice Optical Properties In The Infrared.....	106
2.5 Reciprocal Lattices and Reciprocal Lattice		5.7 Review Questions and Problems.....	107
Vectors	45	6 Thermal Properties: Phonon-II.....	109
2.5.1 Bragg's Diffraction Condition in Terms of		6.1 Phonon Heat Capacity / Classical Model.....	109
Reciprocal Lattice.....	49	6.1.1 Planck Distribution.....	110
2.5.2 Brillouin Zone	50	6.2 Einstein Model for Density of State.....	112
2.5.2 Ewald's Construction and Ewald's Sphere		6.3 Debye Model for Density of States.....	114
52		6.4 Anharmonic Crystal Interactions.....	118
2.6 Fourier Analysis Of The Basis.....	54	6.5 Thermal Conductivity.....	118
2.7 Review Questions and Problems.....	55	6.6 Umklapp Processes.....	120
3 Crystal Binding and Elastic Constants	57	6.7 Review Questions and Problems.....	121
3.1 Classifications of Solids	57	7 Crystal Imperfections	123
3.2 Ionic radii	61	7.1 Types of Imperfections.....	123
3.3 II-VI and III-V Compounds.....	63	7.1.1 Point Imperfection.....	123
3.4 Analysis of Elastic Strain.....	64	7.1.2 Line Imperfections.....	127
3.5 Elastic Compliance and Stiffness Constants.....	67	7.1.3 Surface Imperfections.....	129
		7.1.4 Volume Imperfections.....	132
		7.2 Types of Imperfections.....	133
		8 Electrical Properties Of Metals.....	134
		8.1 Classical Free Electron Theory.....	134
		8.1.1 Density of States in One Dimension.....	137
		8.1.2 Three Dimensional Case.....	137
		8.1.3 Density of States in Three Dimensions..	138
		8.2 Effect of Temperature on Fermi-Dirac.....	141
		8.3 Properties of the Electron Gas.....	142

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