

Subject: Physics

Production of Courseware

 -Content for Post Graduate Courses

Paper No. : Solid State Physics

Module : Lattice Dynamics in three dimensions



Development Team

Principal Investigator Prof. Vinay Gupta, Department of Physics and Astrophysics,
University of Delhi, Delhi

Paper Coordinator Dr. Aranya .B. Bhattacharjee, School of Physical Sciences,
Jawaharlal Nehru University, New Delhi

Content Writer Dr. Aranya .B. Bhattacharjee, School of Physical Sciences,
Jawaharlal Nehru University, New Delhi

Content Reviewer Dr. Poonam Silotia, Department of Physics and Astrophysics,
University of Delhi, Delhi

Description of Module	
Subject Name	Physics
Paper Name	Solid State Physics
Module Name/Title	Lattice dynamics In Three Dimensions
Module Id	M1

Contents of this Unit

1. Introduction
2. Harmonic Approximation
3. Hamiltonian in harmonic approximation
4. Equation of Motion and Normal Modes
5. Acoustical and Optical Modes

Learning Outcomes

After studying this module, you shall be able to

- Learn the harmonic approximation as applied to understand lattice dynamics.
- Understand the concept of normal modes of a lattice.
- Write Hamiltonian of the system in harmonic approximation.
- Learn how to find out the normal modes of a 3D lattice.
- Obtain acoustical and optical modes.

1. INTRODUCTION

To understand the properties of solid, ions are used as the basis of crystal structure. The delocalized valence electrons move in the force field generated by the lattice of ions. Much of the properties of solid can be understood from the motions of ions and electrons. Some of the properties which can be determined from ion dynamics include Lattice heat capacity, thermal expansion.

In the present module, we will focus on the classical understanding of small ionic vibrations in a three dimensional (3D) Lattice. The small vibrations of the ions are described in terms of normal modes. These small ionic vibrations are called Lattice vibrations and corresponding wave that is generated is called a Lattice Wave. In dealing with ionic vibrations, we will work in the “adiabatic approximation” in which we assume that the electrons remain in their ground state during the ionic motion since the motion of the ions is extremely slow on the scale of electronic motion. Typically the electrons have velocities of about 10^8 cm/sec while ions have velocities of about 10^5 cm/sec.

2. HARMONIC APPROXIMATION

In order to understand lattice dynamics in three dimensions, we consider the crystalline lattice as chains of ions connected to nearest neighbors by springs. This is a highly simplified view of the crystalline lattice but never the less, it is very helpful to understand the basic physics associated with the dynamics provided we assume small deviations of the ions from equilibrium position.

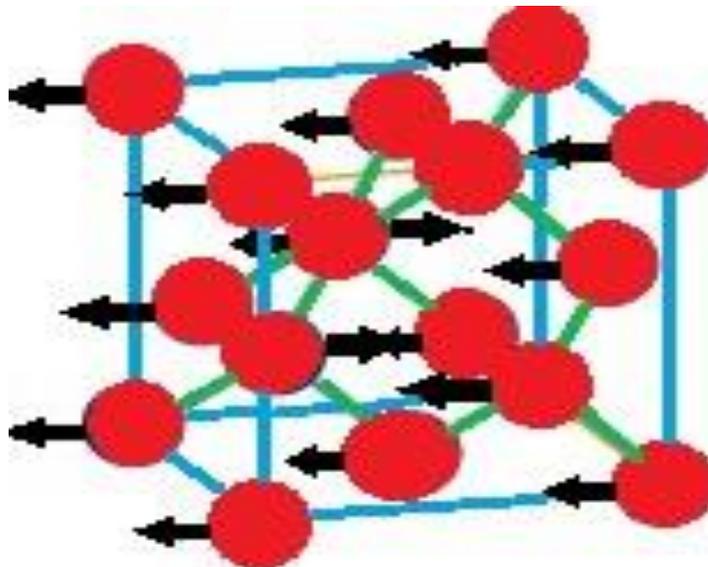


Figure 1.1 3D Lattice showing the vibrations of ions/atoms in the crystal

Under such a situation the restoring forces on the ions are linear. The assumption of a mean equilibrium position of each ion accounts for the crystalline structure of solids. The assumption of small ionic deviations from the mean equilibrium position leads to a simple theory of harmonic approximation. These two assumptions actually connect very well with experiments.

We now explicitly consider a three-dimensional lattice, which possesses N atoms of equilibrium position \bar{R}_{i0} , and a potential energy of the form $V(R_1, R_2, \dots)$.

The Hamiltonian of the system is then written as,

$$H = \sum_i \frac{P_i^2}{2M} + V(R_1, R_2, \dots, R_N) \quad (1.1)$$

The first term of equation (1.1) is the sum of Kinetic energies of all the ions while the second term is the total potential energy of the crystal.

Since the ions are executing small oscillations about its mean position, we write $\bar{R}_i = \bar{R}_{i0} + \delta\bar{R}_i$, where $\delta\bar{R}_i$ is the deviation from the equilibrium position \bar{R}_{i0} of the i^{th} ion.

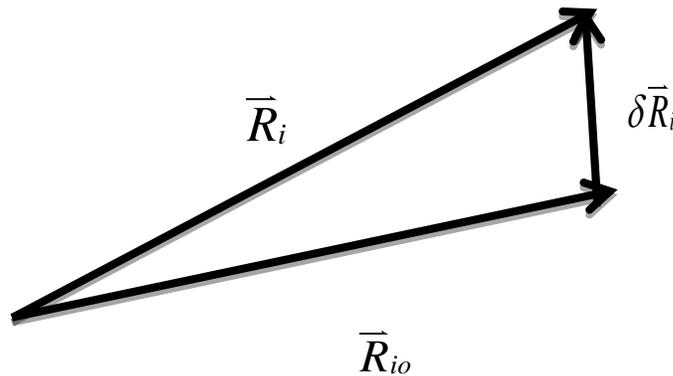


Figure 1.2 The relation $\bar{R}_i = \bar{R}_{i0} + \delta\bar{R}_i$ is depicted in this figure.

At the equilibrium positions $(\bar{R}_{10}, \bar{R}_{20}, \dots, \bar{R}_{N0})$, the potential energy has a minimum $V(\bar{R}_{10}, \bar{R}_{20}, \dots, \bar{R}_{N0})$. If $\delta\bar{R}_i$ is small, then we can expand the potential energy about its equilibrium value to obtain

$$V(\bar{R}_1, \bar{R}_2, \dots, \bar{R}_N) = V(\bar{R}_{10}, \bar{R}_{20}, \dots, \bar{R}_{N0}) + \sum_{i(\alpha=x,y,z)} \left(\frac{\partial V}{\partial R_{i\alpha}} \right)_{R_{i,0}} \delta R_{i,\alpha} + \frac{1}{2!} \sum_{i,j(\alpha,\beta=x,y,z)} \delta R_{i,\alpha} \left(\frac{\partial^2 V}{\partial R_{i,\alpha} \partial R_{j,\beta}} \right)_{R_{i,0}, R_{j,0}} \delta R_{j,\beta} + \dots \quad (1.2)$$

The first term is a constant and can be absorbed to set the zero of the energy. The second term corresponds to the lowest energy state which is a minimum as a function of ion locations. Hence this must vanish due to the fact that the net force on any ion is zero in equilibrium. Hence, the first nonzero correction term is the quadratic term, and further we ignore all the other higher order terms. This is called the harmonic approximation.

The Hamiltonian in the Harmonic approximation is

$$H = \sum_i \frac{P_i^2}{2M} + \frac{1}{2!} \sum_{\alpha,\beta} \delta R_{i\alpha} \left(\frac{\partial^2 V}{\partial R_{i,\alpha} \partial R_{j,\beta}} \right)_{R_{i,0}, R_{j,0}} \delta R_{j,\beta} \quad (1.3)$$

$$= \sum_i \frac{P_i^2}{2M} + \frac{1}{2} \sum_{i,j} \delta\bar{R}_i \cdot C_{ij} \cdot \delta\bar{R}_j \quad (1.4)$$

Here C_{ij} is a three-dimensional tensor for each value of i and j given by

$$C_{ij} = [\bar{\nabla}_{R_i} \bar{\nabla}_{R_j} V(\bar{R}_1, \bar{R}_2, \dots)]_{R_i, R_j} \quad (1.5)$$

If we move along the direction of any of the three primitive vectors of the Bravais lattice, the displacements $\delta\bar{R}_i$ of the ions is periodically repeated. All the points in the crystal are equivalent. The tensor C_{ij} depends only upon $(\bar{R}_{i,0} - \bar{R}_{j,0})$ because if one displaces just two ions by $\delta\bar{R}_i$ and $\delta\bar{R}_j$, keeping all the other ions in their equilibrium positions, the resulting energy can depend only upon their relative locations.

The factor C_{ij} obeys some important symmetry properties useful for studying the normal modes of a crystal. If every ion is given the same displacement ($\delta \bar{R}_i = d$), then the entire crystal will simply be displaced without any change in the crystal energy.

Therefore $\sum_i C_{ij} = 0$

3. Equation of Motion and Normal Modes

The dynamical 3N equations of motion follow from the force on the i^{th} ion i.e. $-\frac{\partial V}{\partial \delta R_i}$,

This leads to

$$M \ddot{\delta R}_i = -\sum_j C_{ij} \delta R_j \quad (1.6)$$

Note that each $C_{i,j}$ is a 3×3 matrix.

Equation (1.6) can be solved by plane waves keeping track of their polarization. We assume a solution of the form

$$\bar{\delta R}_i = \hat{e}_{\bar{K}} q_{\bar{K}} e^{i\bar{K} \cdot \bar{R}_{i,0} - i\omega_K t} \quad (1.7)$$

where $\hat{e}_{\bar{K}}$ is a unit polarization vector and $q_{\bar{K}}$ is the amplitude associated with wave vector \bar{k} .

Substituting the assumed solution (1.7) in the equation of motion (1.6) gives

$$M \omega_K^2 \hat{e}_{\bar{K}} = \sum_j C_{ij} \hat{e}_{\bar{K}} e^{i\bar{K} \cdot (\bar{R}_{j,0} - \bar{R}_{i,0})} \quad (1.8)$$

Equation (1.8) is a vector equation and for each value of \bar{k} , it has three solutions.

We define a tensor, $D(\vec{K}) = -\sum_j e^{i\vec{K}\cdot(\vec{R}_{j,0}-\vec{R}_{i,0})} C_{ij}$. Here $\vec{D}(\vec{k})$ is known as dynamical matrix. Equation

(1.8) can now be rewritten in terms of $\vec{D}(\vec{k})$ as a matrix equation

$$\begin{pmatrix} M\omega_k^2 + D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & M\omega_k^2 + D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & M\omega_k^2 + D_{zz} \end{pmatrix} \begin{pmatrix} \hat{\epsilon}_{kx} \\ \hat{\epsilon}_{ky} \\ \hat{\epsilon}_{kz} \end{pmatrix} = 0 \quad (1.9)$$

The three solutions of equation (1.9) for each of the N allowed values of \vec{k} will yield 3N normal modes. These three solutions for a particular k can be labeled by a polarization index λ . The corresponding eigenvalues will be $\omega_{k\lambda}^2$ and eigenfunctions will be $\hat{\epsilon}_{k\lambda} = (\epsilon_{k\lambda}^x, \epsilon_{k\lambda}^y, \epsilon_{k\lambda}^z)$ with $\lambda = 1, 2, 3$. Since we are dealing with crystals, we have to apply periodic boundary conditions which lead to the condition

$$e^{iK_i N_i a_i} = 1 \quad (1.10)$$

Where $i = 1, 2, 3$ for the three primitive translation directions. Also k_i is the component of \vec{k} along the primitive vector a_i and N_i are integers satisfying $N = N_1 N_2 N_3$. From equation (1.10), the allowed values of \vec{k} are,

$$\vec{k} = 2\pi \left(\frac{n_1}{N_1} \vec{b}_1 + \frac{n_2}{N_2} \vec{b}_2 + \frac{n_3}{N_3} \vec{b}_3 \right), \quad (1.11)$$

where n_1, n_2, n_3 are integers and \vec{b}_i are the reciprocal lattice vectors satisfying $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$. Only \vec{k} values within a single primitive cell of the reciprocal lattice gives distinct solutions. Consequently, we chose independent values of \vec{k} which satisfy equation (1.11) and the condition

$$-\frac{N_i}{2} \leq n_i \leq \frac{N_i}{2} \quad (1.12)$$

Equation (1.12) restricts the \vec{k} values to the first Brillouin zone which is the primitive cell in the reciprocal space. Therefore in the first Brillouin zone, the total number of \vec{k} values is N and there are three normal modes for each \vec{k} value, which gives us $3N$ normal modes. The periodicity of the crystal lattice allows us to find an equivalent \vec{k} value inside first Brillouin zone for those \vec{k} values that lie outside the first Brillouin zone by simply adding a reciprocal lattice vector \vec{G} to \vec{k} .

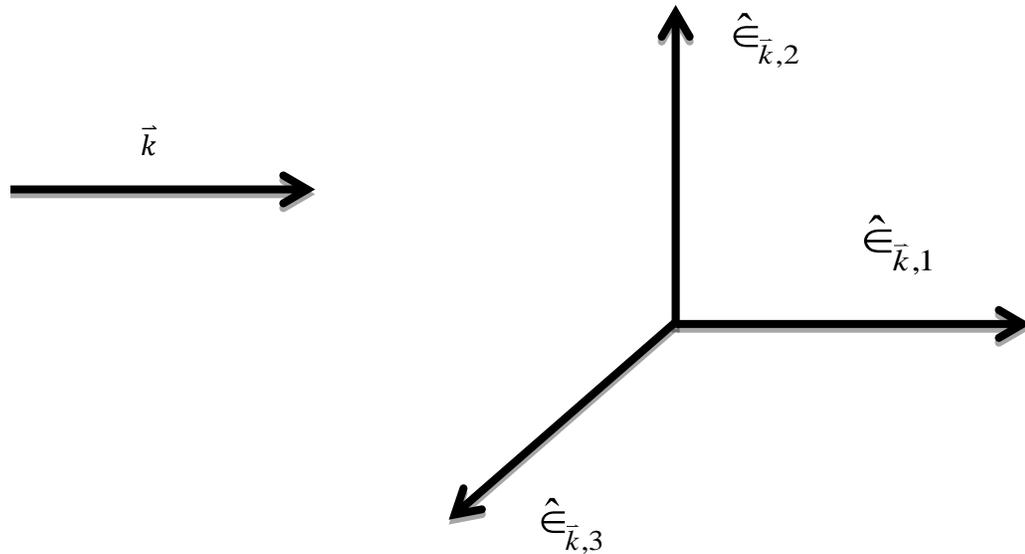


Figure 1.3: Schematic figure illustrating that along the axis of a cubic crystal, there is a longitudinal mode in the direction of wave propagation and two transverse modes perpendicular to the direction of propagation.

For a cubic crystal, when \vec{k} points along an axis, one polarization vector $\hat{\epsilon}_{\vec{k},1}$, points along \vec{k} and other two $\hat{\epsilon}_{\vec{k},2}$ and $\hat{\epsilon}_{\vec{k},3}$ points in the perpendicular direction to \vec{k} . $\hat{\epsilon}_{\vec{k},1}$ is the longitudinal mode while $\hat{\epsilon}_{\vec{k},2}$ and $\hat{\epsilon}_{\vec{k},3}$ are the two transverse modes.

4. Acoustical and Optical Modes

We now analyze the Long-wavelength properties of the 3D lattice. Now from the definition of $\vec{D}(\vec{k})$, it is clear that at $\vec{k} = 0$, the components of $\vec{D}(\vec{k})$ matrix are real. The displacement $\vec{\delta R}_i$ from equation (1.7) for $\vec{k} = 0$ is real and \vec{k} independent. If we use the property $\sum_j C_{ij} = 0$ in equation (1.8), we get $\omega_{k=0,\lambda} = 0$ for all $\lambda = 1, 2, 3$. So these three are the acoustic branches since the frequencies vanish in the long wavelength limit. The remaining $(3N-3)$ are the optical modes.

5.SUMMARY

In this module, you have studied

- What is adiabatic and harmonic approximation in lattice dynamics.
- How to write down the Hamiltonian describing the dynamics of a 3D crystal lattice.
- The concept of normal modes from equations of motion.
- How to find the normal modes from the equation of motion for the lattice displacement.
- Obtain Dynamical matrix equation whose three solutions will yield $3N$ normal modes. The periodicity of crystal lattice will allow us to find equivalent k values.
- What are acoustical and optical modes and what condition determines which modes are acoustical.

