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Subject: Physics

Production of Courseware

e-Content for Post Graduate Courses

Paper No. : Solid State Physics

Module : Quantization of Lattice vibrations

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Description of Module	
Subject Name	Physics
Paper Name	Solid State Physics
Module Name/Title	Quantization of Lattice vibrations
Module Id	

Contents of this Unit

Learning Outcomes

After studying this module, you shall be able to

- Quantize the Hamiltonian of collection of N harmonic oscillators in **ID.**
- Introduce the quantum mechanical operators satisfying commutation relations.
- Write expression for displacement of the j^{th} ion and corresponding momentum.
- Know about the energy transported by an elementary excitation of quasiparticle termed as Phonons.
- Write expression for displacement and momentum for ion in **3D.**
- Arrive at three-dimensional quantized Hamiltonian.
- Learn about the lowest vibrational state and its corresponding energy known as zero point energy.

1. INTRODUCTION

In module I, we discussed Lattice vibrations from the point of view of classical mechanics. The agreement between classical and quantum mechanics of harmonic Oscillations is very good for high temperatures. However at low temperatures, the differences between classical and quantum mechanical results increases substantially. A classical mode may have arbitrary amplitude while a quantum-mechanical mode has discrete amplitude. The energy of mode $\vec{k}$, polarization $\hat{\epsilon}_{\vec{k}}$ is allowed to have values

$$\hbar\omega_{\vec{k},\hat{\epsilon}_{\vec{k}}}\left(n+\frac{1}{2}\right) \tag{2.1}$$

where $n \geq 0$ is an integer. For a single quantum mode of wavenumber $\vec{k}$, polarization $\hat{\epsilon}_{\vec{k}}$, n=1. In the present module, we will focus on the quantum understanding of lattice vibrations.

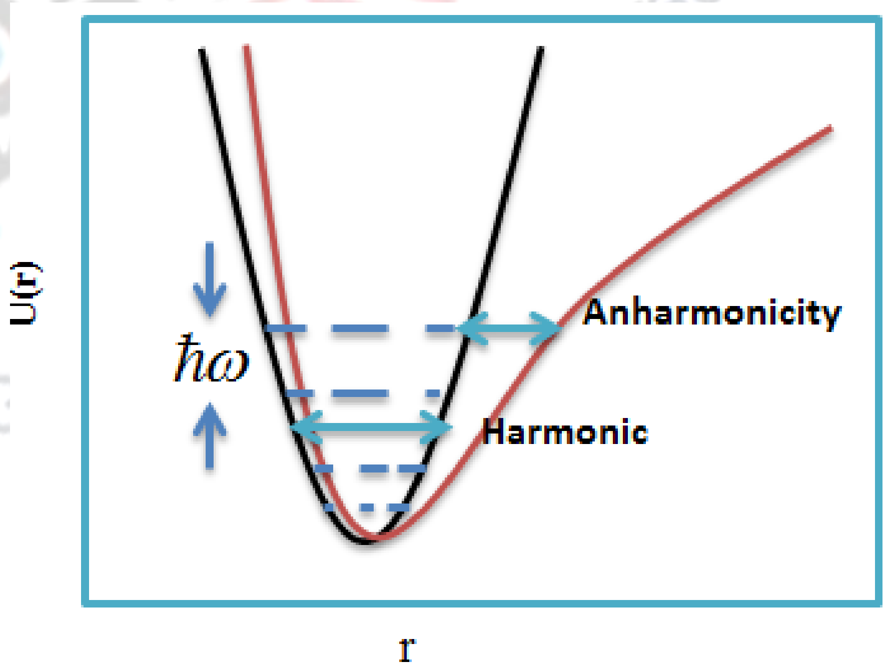

Figure 1.1 *A phonon is quantum (ħω) of crystal vibration energy, analogous to photon*

2. QUANTIZATION OF LATTICE VIBRATIONS IN ID

When dealing with small vibrations in classical mechanics, the Hamiltonian of a collection of N harmonic Oscillators (as in the case of Lattice vibrations), in terms of normal coordinates p_k and q_k can be written as

$$H = \sum_k H_k = \sum_k \left[\frac{p_k p_k^*}{2M} + \frac{1}{2} M \omega_k^2 q_k q_k^* \right] \tag{2.2}$$

We now quantize the Hamiltonian equation (2.2). In the process of quantization, we replace the dynamical variables q_k and p_k by the quantum-mechanical operators $\hat{q}_k$ and $\hat{p}_k$ which satisfy the commutation relation

$$[\hat{p}_k, \hat{q}_{k'}] = -i\hbar \delta_{k,k'} \tag{2.3}$$

Hence, the corresponding quantum-mechanical Hamiltonian is written as,

$$H_k = \frac{\hat{p}_k \hat{p}_k^\dagger}{2M} + \frac{1}{2} M \omega_k^2 \hat{q}_k \hat{q}_k^\dagger \tag{2.4}$$

Here $\hat{p}_k^\dagger$ and $\hat{q}_k^\dagger$ are the Hermitian conjugate of $\hat{p}_k$ and $\hat{q}_k$ respectively. Note that the Hamiltonian H_k is Hermitian. Now taking motivation from the study of quantum mechanics of harmonic Oscillator, we introduce the two operators $\hat{a}_k$ and $\hat{a}_k^\dagger$ defined in the following way,

$$\hat{q}_k = \left(\frac{\hbar}{2M\omega_k} \right)^{1/2} (\hat{a}_k + \hat{a}_{-k}^\dagger) \tag{2.5}$$

$$\hat{p}_k = i\left(\frac{\hbar m\omega_k}{2}\right)^{1/2}(\hat{a}_k^{\dagger} - \hat{a}_{-k}) \tag{2.6}$$

The operators $\hat{a}_k$ and $\hat{a}_k^{\dagger}$ satisfy the following Commutation relations

$$[\hat{a}_k, \hat{a}_{k'}^{\dagger}] = \delta_{k,k'} \text{ and } [\hat{a}_k, \hat{a}_{k'}] = [\hat{a}_k, \hat{a}_{k'}^{\dagger}] = 0 \tag{2.7}$$

The displacement of the jth ion and its corresponding momentum can be written as

$$\delta\hat{R}_j = \sum_k \left(\frac{\hbar}{2MN\omega_k}\right)^{1/2} e^{ikna}(\hat{a}_k + \hat{a}_{-k}^{\dagger}) \tag{2.8}$$

$$\hat{p}_j = \sum_k i\left(\frac{\hbar\omega_k M}{2N}\right)^{1/2} e^{-ikna}(\hat{a}_k^{\dagger} - \hat{a}_{-k}) \tag{2.9}$$

Note here that the normal coordinates q_k and p_k and related to the jth ion δR_i and its momentum P_i in as,

$$\delta R_j = \frac{1}{\sqrt{N}}\sum_k q_k e^{ikna} \tag{2.10}$$

$$P_j = \frac{1}{\sqrt{N}}\sum_k p_k e^{-ikna} \tag{2.11}$$

Now using the results (2.2)…(2.11), we can now write down the Hamiltonian of the Linear chain of ions as

$$H = \sum_k \hbar\omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) \tag{2.12}$$

with eigenfunctions and eigenvalues as

$$\left| n_1, n_2 \dots n_N \right\rangle = \frac{\left(a_{k_1}^\dagger \right)^{n_1}}{\sqrt{n_1\,!}} \dots\dots\dots \frac{\left(a_{k_N}^\dagger \right)^{n_N}}{\sqrt{n_N\,!}} \left| 0 \right\rangle, \tag{2.13}$$

And

$$E_{n_1, n_2 \dots\dots n_N} = \sum_{j=1}^{N} \hbar\omega_{k_j} \left(n_j + \frac{1}{2} \right) \tag{2.14}$$

Here $|0\rangle = |0_1\rangle |0_2\rangle \dots . |0_N\rangle$ is the ground state of the N independent harmonic Oscillators.

The energy of $\hbar\omega_k$ can be associated with the energy transported by an elementary excitation or a quasiparticle which in Lattice dynamics is termed as phonons. In the quantum ground state, no phonons are present (n_j=0). The state $|n_1, n_2 \dots . n_N\rangle$ indicates n_1 phonons in oscillator with mode k_1, n_2 in k_2 ….. n_N in k_N.

PHONONS

- Packets of sounds found present in the lattice as it vibrates….as the lattice vibration cannot be heard.
- Unlike static lattice model which deals with average position of atoms in a crystal, lattice dynamics extends the concept of crystal lattice to an array of atoms with finite masses that are capable of motion.
- This motion is not random but is the superposition of vibrations of atoms around there equilibrium sites due interaction with neighbour atoms.
- A collective vibration of atoms in the crystal forms a wave of allowed wavelength and amplitude.

- Just as light is a wave motion that is considered as composed of particles called photons. We can think of normal modes in a solid as being particle-like.

Quantum of lattice vibration is called the phonon.

Comparison of Phonon and Photons

PHONONS	**PHOTONS**
Quantized normal modes of lattice vibrations. The energies and momenta of phonons are quantized.	Quantized normal modes of electromagnetic waves. The energies and momenta of photons are quantized
$E_{phonon} = \frac{hv_s}{\lambda}$	$E_{photons} = \frac{hc}{\lambda}$
$P_{phonon} = \frac{h}{\lambda}$ Phonon wavelength: 1nm	$P_{phonon} = \frac{h}{\lambda}$ Photon wavelength(visible): 380-750nm

3. QUANTIZATION OF LATTICE VIBRATIONS IN 3D

Analogous to the one-dimensional Case, we now define the new coordinates $q_{\vec{k},\lambda}$ and $p_{\vec{k},\lambda}$ as

$$\delta\vec{R}_j = \frac{1}{\sqrt{N}}\sum_{\vec{k},\lambda}\hat{\in}_{\vec{k},\lambda}q_{\vec{k},\lambda}e^{i\vec{k}.\vec{R}_{j,0}} \qquad (2.15)$$

$$\vec{P}_j = \frac{1}{\sqrt{N}}\sum_{\vec{k},\lambda}\hat{\in}_{\vec{k},\lambda}\, P_{\vec{k},\lambda}e^{-i\vec{k}.\vec{R}_{j,0}} \qquad (2.16)$$

The three-dimensional Hamiltonian then becomes

$$H=\sum_{\vec{k},\lambda}H_{\vec{k},\lambda}=\sum_{\vec{k},\lambda}\left[\frac{p_{\vec{k},\lambda}p^{*}_{\vec{k},\lambda}}{2M}+\frac{1}{2}M\omega^{2}_{\vec{k},\lambda}q_{\vec{k},\lambda}q^{*}_{\vec{k},\lambda}\right] \quad (2.17)$$

The polarization vectors $\hat{\in}_{\vec{k},\lambda}$ satisfy

$$\hat{\in}_{\vec{k},\lambda}=-\hat{\in}_{-\vec{k},\lambda} \; and \; \hat{\in}_{\vec{k},\lambda}\,.\,\hat{\in}_{k,\lambda'}=\delta_{\lambda\lambda'}$$

Also $$\sum_{j}e^{i(\vec{k}-\vec{k}').\vec{R}_{j,0}}=N\delta_{\vec{k},\vec{k}'} \quad (2.18)$$

and $$\sum_{j}\hat{\in}_{\vec{k},\lambda}\,.\,\hat{\in}_{\vec{k},\lambda'}\,e^{i(\vec{k}-\vec{k}').\vec{R}_{j,0}}=N\delta_{\vec{k},\vec{k}'}\delta_{\lambda,\lambda'} \quad (2.19)$$

we now require that $\vec{P}_i$ and $\delta\vec{R}_i$ to be real,
hence,

$$\vec{P}^{*}_{\vec{k},\lambda}=\vec{P}_{-\vec{k},\lambda} \text{ and } \vec{q}^{*}_{\vec{k},\lambda}=\vec{q}_{-\vec{k},\lambda} \quad (2.20)$$

Here $\vec{P}_{\vec{k},\lambda}=\hat{\in}_{\vec{k},\lambda}P_{\vec{k},\lambda}$ and $\vec{q}_{\vec{k},\lambda}=\hat{\in}_{\vec{k},\lambda}q_{\vec{k},\lambda}$

We now initiate the quantization process by replacing the variables $P_{\vec{k},\lambda}$ and $q_{\vec{k},\lambda}$ by the corresponding quantum-mechanical operators $\hat{P}_{\vec{k},\lambda}$ and $\hat{q}_{\vec{k},\lambda}$ which satisfy the commutation relations

$$\left[\hat{P}_{\vec{k},\lambda},\hat{q}_{\vec{k}',\lambda'}\right]=-i\hbar\delta_{\vec{k},\vec{k}'}\delta_{\lambda,\lambda'} \tag{2.21}$$

As before, we introduce the creation and annihilation operators $\hat{a}^{\dagger}_{\vec{k},\lambda}$ and $\hat{a}_{\vec{k},\lambda}$ defined as follows:

$$\hat{q}_{\vec{k},\lambda}=\left(\frac{\hbar}{2M\omega_{\vec{k},\lambda}}\right)^{1/2}\left(\hat{a}_{\vec{k},\lambda}-\hat{a}^{\dagger}_{-\vec{k},\lambda}\right) \tag{2.22}$$

$$\hat{P}_{\vec{k},\lambda}=i\left(\frac{\hbar M\omega_{\vec{k},\lambda}}{2}\right)^{1/2}\left(\hat{a}^{\dagger}_{\vec{k},\lambda}+\hat{a}_{-\vec{k},\lambda}\right) \tag{2.23}$$

Compare the above results with equations (2.5) and (2.6)

The operators $\hat{a}^{\dagger}_{\vec{k},\lambda}$ and $\hat{a}_{\vec{k},\lambda}$ satisfy,

$$\left[\hat{a}_{\vec{k},\lambda},\hat{a}^{\dagger}_{\vec{k}',\lambda'}\right]=\delta_{\vec{k},\vec{k}'}\delta_{\lambda,\lambda'} \tag{2.24}$$

$$\left[\hat{a}_{\vec{k},\lambda},\hat{a}_{\vec{k}',\lambda'}\right]=\left[\hat{a}^{\dagger}_{\vec{k},\lambda},\hat{a}^{\dagger}_{\vec{k}',\lambda'}\right]=0 \tag{2.25}$$

For the three-dimensional case, the displacement of the j^{th} ion and the corresponding momentum as

$$\delta\vec{R}_j=\sum_{\vec{k},\lambda}\left(\frac{\hbar}{2MN\omega_{\vec{k},\lambda}}\right)^{1/2}\hat{\epsilon}_{\vec{k},\lambda}\,e^{i\vec{k}.\vec{R}_{j,0}}(\hat{a}_{\vec{k},\lambda}-\hat{a}^{\dagger}_{-\vec{k},\lambda}) \tag{2.26}$$

$$\vec{P}_j = i\sum_{\vec{k},\lambda}\left(\frac{\hbar M\omega_{\vec{k}\lambda}}{2N}\right)^{1/2} \hat{\epsilon}_{\vec{k}\lambda}\, e^{-i\vec{k}.\vec{R}_{j,0}}(\hat{a}_{\vec{k}\lambda} + \hat{a}_{-\vec{k}\lambda}) \qquad (2.27)$$

Finally putting together all the previous results, we get the three-dimensional quantized Hamiltonian as

$$H = \sum_{\vec{k}\lambda}\hbar\omega_{\vec{k}\lambda}\left(\hat{a}^{\dagger}_{\vec{k}\lambda}\hat{a}_{\vec{k}\lambda} + \frac{1}{2}\right) \qquad (2.28)$$

4. ZERO-POINT ENERGY

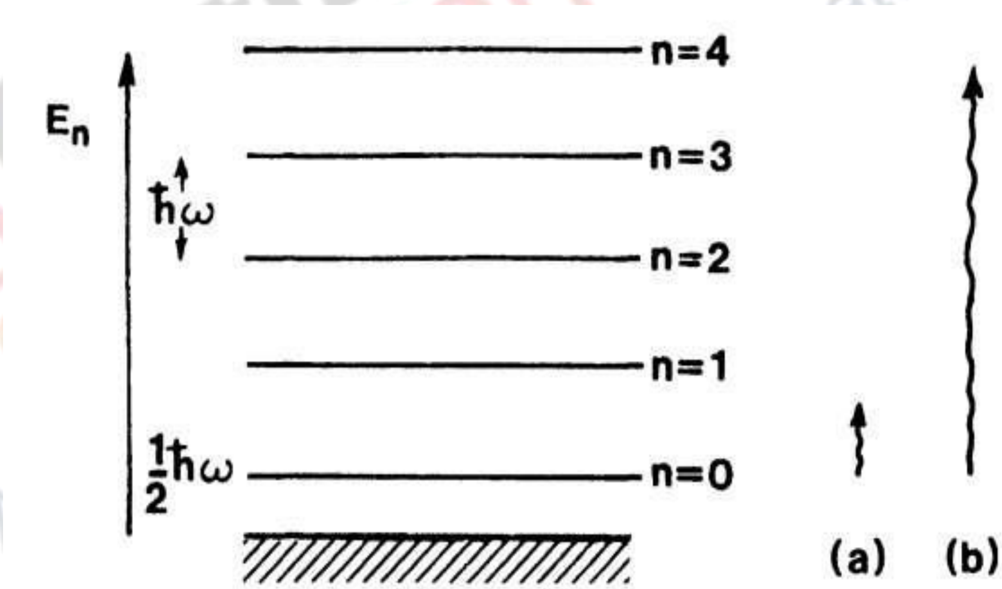

Figure 1.2 *Lowest vibrational state carries energy and is known as zero point energy*

The relation (2.28) demonstrates that the energy of the harmonic oscillator with mode $\vec{k}$ is not zero in the lowest vibrational state (n=0) and this has the value $\frac{1}{2}\hbar\omega_{\vec{k},\lambda}$ .This energy is the lowest vibrational state is known as Zero- point energy. In the quantum picture, the momentum of a phonon is written as $\hbar\vec{k}$.

SUMMARY

In this module you study

- The quantized Hamiltonian obtained during process of quantization is Hermitian.
- How we can write the displacement of j^{th} ion and its corresponding momentum in terms of quantum mechanical operators.
- To obtain the Eigenvalues from the Hamiltonian of the linear chain of ions.
- That no phonons are present in the quantum ground state.
- To obtain the three dimensional quantized Hamiltonian in terms of annihilation and creation operator.
- The energy of the harmonic oscillator is not zero in the lowest vibrational state (zero point energy) and has some value.