

Chapter #4: Vibrations in a Crystal

Lecture 6: Phonon

Introduction

<https://www.youtube.com/shorts/AHtehJ0DQWY>

The vibrational energy of a crystal lattice is **quantized** in a way similar to the quantization of electromagnetic radiation.

Classical vs Quantum Description

	Classical Mechanics	Quantum mechanics
Light	Electromagnetic wave $\vec{E} = E_0 e^{i(\vec{q} \cdot \vec{r} - \omega t)} \hat{r}$	Light has energy $\hbar\omega$. The virtual particle of light is called a "photon".
Crystal vibration	Back-and-forth wave $\vec{u}_q(\vec{R}_l^0) = u_0 e^{i(\vec{q} \cdot \vec{R}_l^0 - \omega t)} \hat{r}$	Vibration in a crystal has energy $\hbar\omega$. The virtual particle of vibration is called "phonon".

Definition of Phonon

Therefore, the **quantized unit of energy** associated with a vibrational (sound) wave inside a crystal is called a:

☞ **Phonon**

Phonon Energy

The energy of a phonon is given by:

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega \quad (1)$$

Where:

- n: represents an integer quantum number
-

◇ Ground State Energy

When: n=0

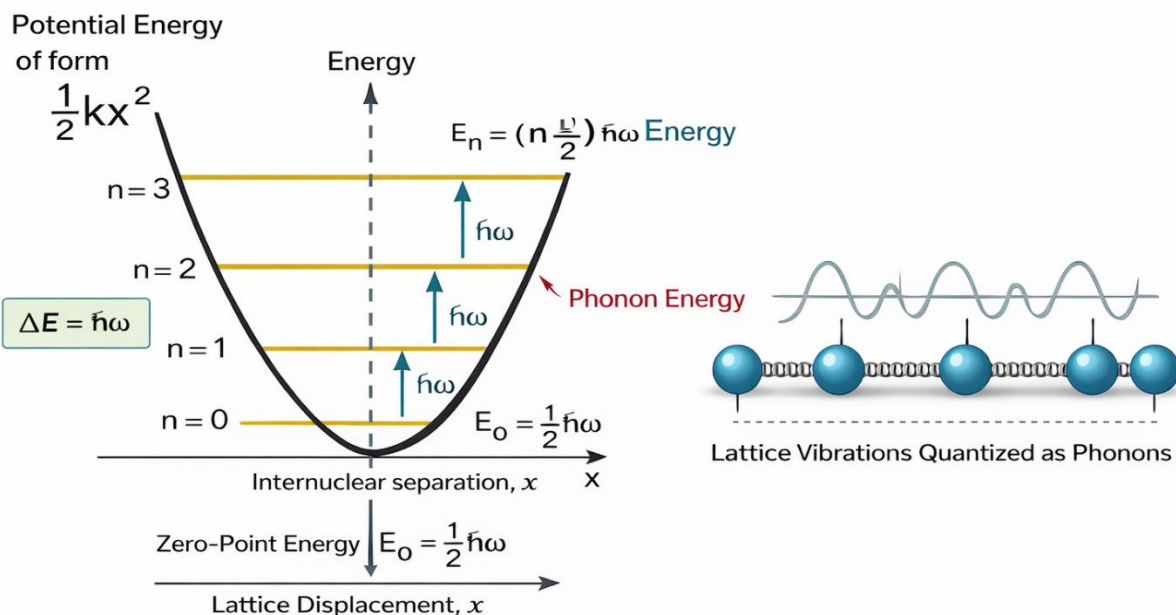
$$E_0 = \frac{1}{2} \hbar \omega$$

👉 This means:

The oscillator still has motion even in the ground state (n=0)
(This is called *zero-point energy*)

- Energy in electromagnetic waves is carried in quanta called **photons**.
- Energy associated with vibrations of a crystal lattice is carried in quanta called **phonons**.

Quantum Harmonic Oscillator and Phonons



📺 In this figure:

- Each horizontal line → energy level
- Distance between lines → $\hbar \omega$
- Arrow → creation/annihilation of phonon (similar to photon emission/absorption in atoms).

📺 As shown in *the figure*, the harmonic oscillator has discrete energy levels:

- $n=0, 1, 2, 3, \dots$
- Each level is separated by $\hbar \omega$
- Each normal mode of lattice vibration behaves like a quantum harmonic oscillator.

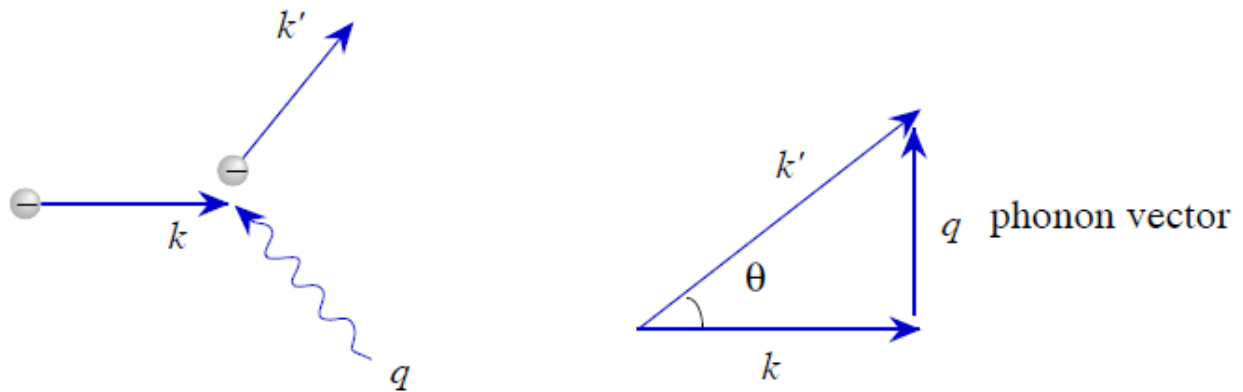
- A phonon corresponds to the transition between two adjacent energy levels.
- ω here is the same frequency from the dispersion relation $\omega(q)$ discussed in the last three lectures.

Phonon Interactions

Phonons can interact with other particles, such as:

- Photons
- Neutrons
- Electrons

Elastic Scattering



In the case of **elastic scattering** of an X-ray photon inside a crystal:

$$\vec{k}' = \vec{k} + \vec{G} \quad (2)$$

◇ Where:

- \vec{k} : incident photon wave vector
- \vec{k}' : scattered photon wave vector
- \vec{G} : reciprocal lattice vector

👉 This is the **diffraction condition** (Bragg condition in reciprocal space)

Inelastic Scattering

When scattering is **inelastic**, the selection rule becomes:

$$\vec{k}' \pm q = \vec{k} + \vec{G} \quad (3)$$

More precisely,

When a phonon is involved:

- Energy changes:

$$E_f = E_i \pm \hbar\omega$$

- Momentum (more precisely, crystal momentum) changes:

$$k_f = k_i \pm q$$

◇ Where:

- q : phonon wave vector
-

◇ Interpretation of Signs:

- (+): phonon is **created**
 - (-): phonon is **annihilated**
-


 As illustrated in *the figures*:

- Momentum conservation involves:
 - photon
 - phonon
 - reciprocal lattice
-

Physical Meaning

- In elastic scattering → no energy exchange
- In inelastic scattering → energy is exchanged with the lattice.

- Elastic → no phonon
- Inelastic → phonon created or destroyed

 This is how phonons are **experimentally observed**.

Option:

You can also find more discussion on phonon and dispersion relation by watching this lecture:

<https://www.youtube.com/watch?v=UnHqQw834Z0>