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

▧ Definition of Phonon

A phonon is the quantum of vibrational energy associated with a normal mode of a crystal lattice. It represents an elementary excitation of the quantized lattice vibrations.

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

👉 **Phonon**

▧ Phonon Energy

The energy of a phonon is given by:

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

Where:

- n: represents an integer quantum number

◇ Ground State Energy

When: n=0

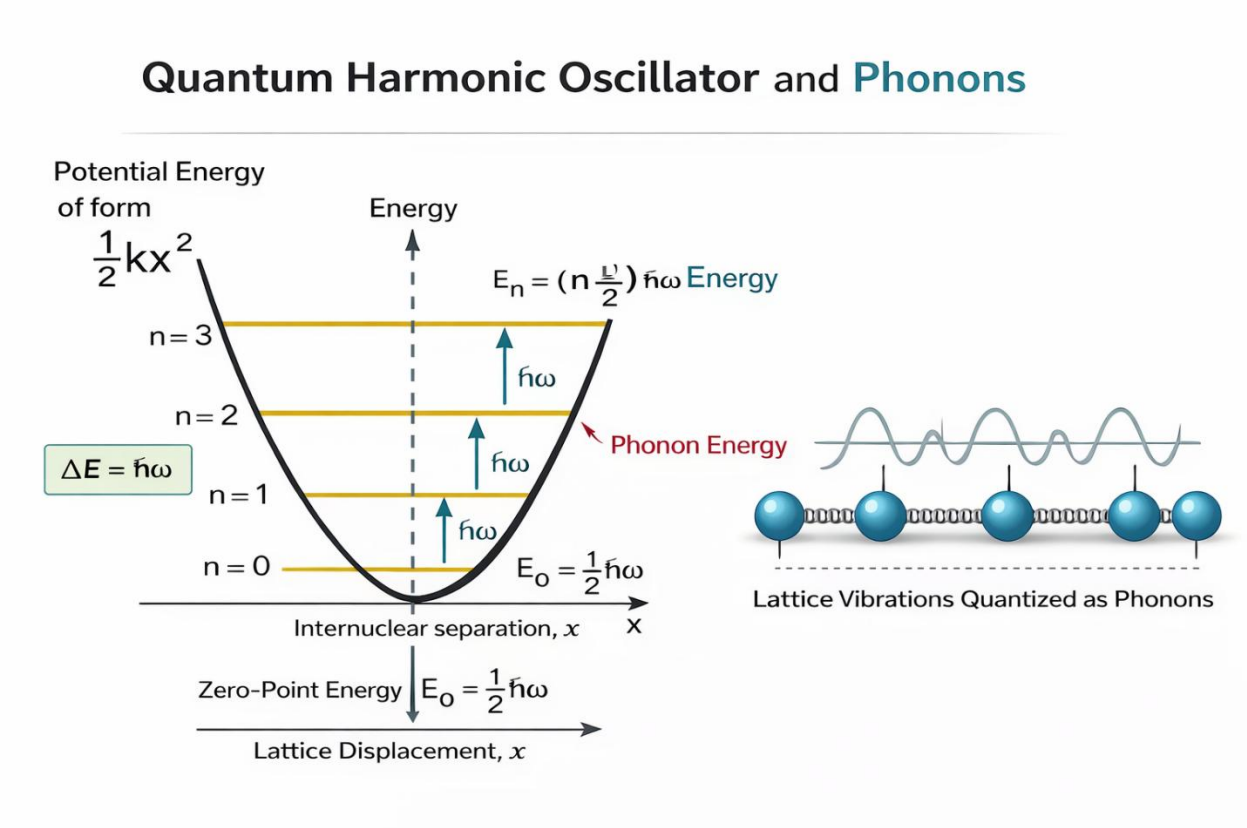
$$E_0 = \frac{1}{2}\hbar\omega$$

👉 This means:

The oscillator still has motion even in the ground state (n=0)

(This is called *zero-point energy*).

This reflects the quantum-mechanical zero-point fluctuations of the oscillator, even at absolute zero temperature.



📊 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,…
- 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.

$$\Delta E = E_{n+1} - E_n = \hbar\omega$$

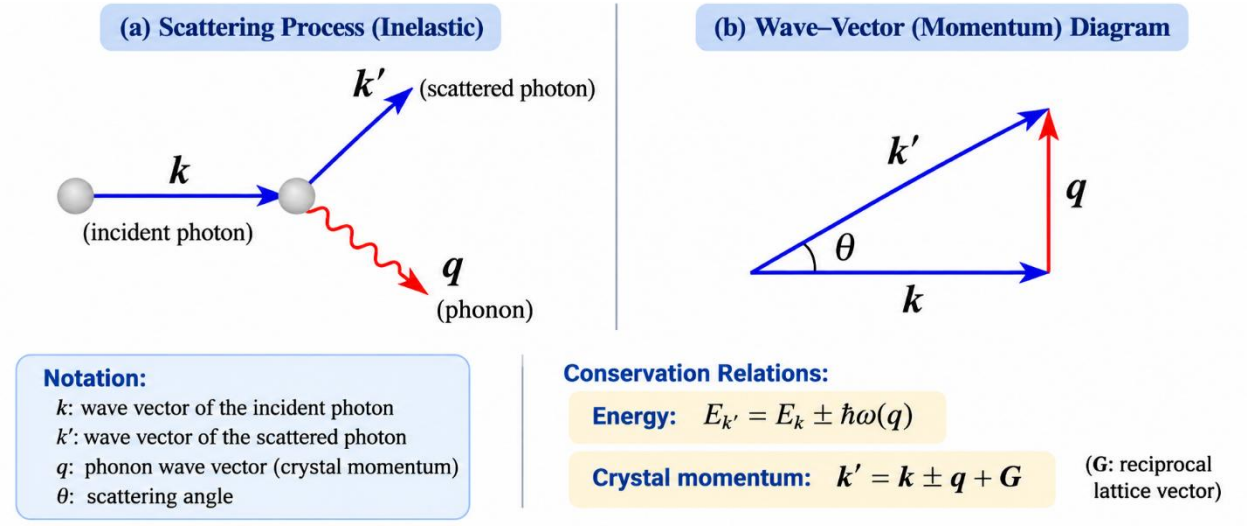
- ω here is the same frequency from the dispersion relation ω(q) discussed in the last three lectures.

▨ 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:

$$\vec{K}` = \vec{K} + \vec{G} \qquad (2)$$

◇ 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)

➢ The photon changes its direction.
➢ Its energy remains unchanged.
➢ No phonon is created or annihilated in this ideal elastic-scattering process.

Inelastic Scattering

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

$$\vec{K}` \pm q = \vec{K} + \vec{G} \qquad (3)$$

More precisely,

When a phonon is involved:

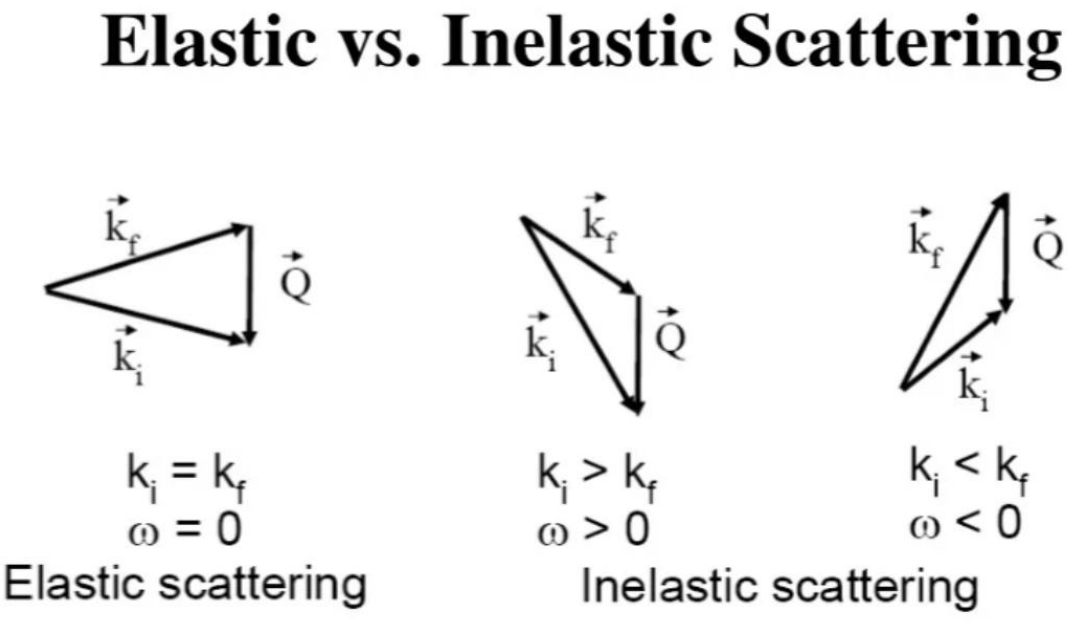
- Energy changes:

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

- Momentum (more precisely, crystal momentum) changes:

$$k_f = k_i \pm q$$

  - ◇ Where:
    - $\vec{q}$: 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.**



Phonons play an important role in determining the thermal properties of solids. They contribute to the heat capacity and thermal conductivity of crystals. Their interactions with electrons and other phonons also influence several physical properties of materials.

Option:

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

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