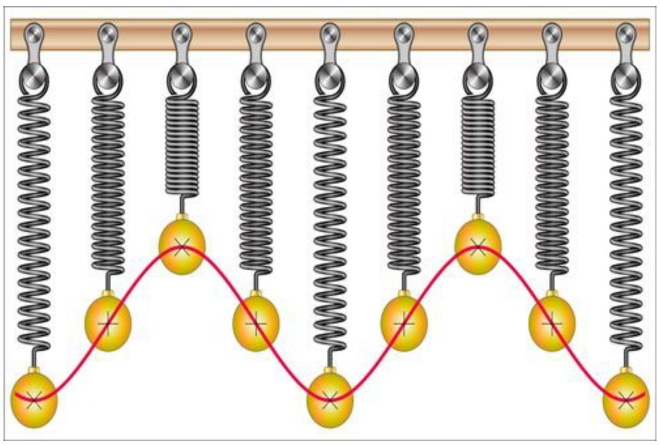
Chapter #4:
Vibrations in a Crystal

Lecture 1: Fundamentals of Lattice Vibrations in Crystals

4-1 Introduction



I. What is the vibration of a particle? And what is its frequency?
II. What is lattice vibration? And what causes this vibration in solids?
III. How is the atomic displacement resulting from lattice vibration described mathematically?
IV. What is a transverse lattice-vibration wave?
V. What is a longitudinal lattice-vibration wave?

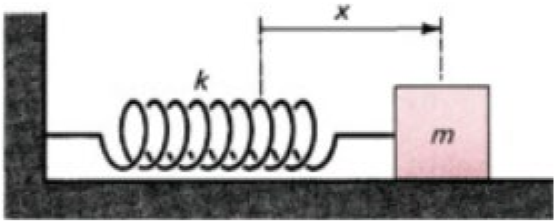
Recall from Chapter 3 that atoms in a crystal are held together by interatomic forces, which can be described by a potential energy function. At the equilibrium separation, the potential energy is minimum, and this defines the stable structure of the crystal.

Now, if atoms are slightly displaced from this equilibrium position, restoring forces arise due to the shape of the potential energy curve. These restoring forces lead to oscillations of atoms about their equilibrium positions.

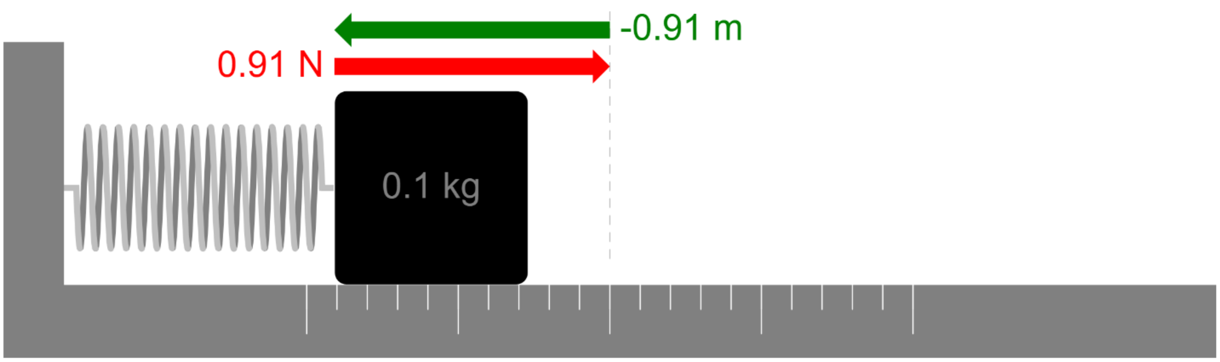
Therefore, lattice vibrations are a natural consequence of the interatomic bonding discussed in Chapter 3.

I. Particle Vibration

In the adjacent figure, when we try to pull the body of mass m away from its equilibrium position and then release it, the particle will oscillate back and forth about the equilibrium position. Also, the particle cannot escape from the equilibrium position.



The back-and-forth motion of the particle around the equilibrium position is called **"vibration."**



As we have learned, the frequency of this vibration can be found using:

$$\omega = \frac{2\pi}{T}$$

Where T is the period time.

And $\omega = \sqrt{\frac{k}{m}}$

Where:

- m: mass of the particle
- k: spring constant

➢ Lattice vibrations are the foundation of phonons, heat capacity, and thermal conductivity.

From Newton's law: $F = ma$

From Hooke's law: $-k(x - x_0) = m\ddot{x}$

We will try to find the solution to this equation as follows:

If we choose:

$x(t) = A\cos(\omega t + \varphi)$ and equilibrium position is at x_0=0:

Solve: $-k(x - x_0) = m\frac{d^2x}{dt^2}$

$-kA\cos(\omega t + \varphi) = -mA\omega^2\cos(\omega t + \varphi)$

$\omega^2 = \frac{k}{m}$ (Relationship for oscillatory motion).

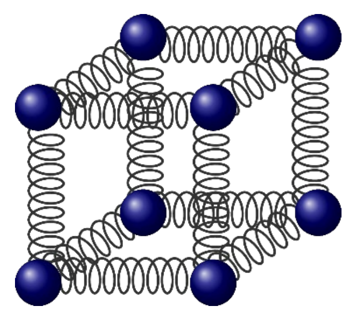
Think about it:

- Heavier mass → slower motion
- Stronger spring → faster motion"

🗣"If the potential well is deeper, do you expect atoms to vibrate faster or slower?"

👉 Deeper well → larger k → higher frequency

II. Lattice Vibration in Solids



As we learned in Chapter 1, solids consist of an ordered arrangement of atoms.
We can view this arrangement from two perspectives:

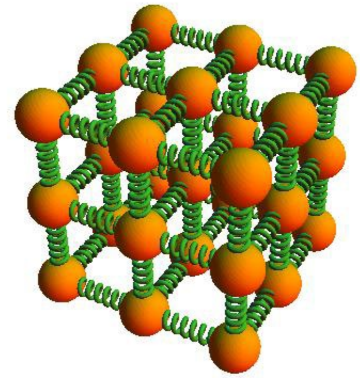
1. **No interaction between atoms**
   Meaning the motion of any atom does not affect other atoms.
   Thus, each atom moves freely (like a gas), and there is **no lattice vibration**.
   (This case is not of interest here.)
2. **There is interaction between atoms**
   The motion of any atom affects other atoms.

Therefore, the motion of one atom affects the motion of the entire lattice.

The collective motion of atoms inside solids is called:
“Lattice vibration.”

The cause of lattice vibration is the **interaction between atoms**.

The lattice vibrates in collective modes called **normal modes**.



These normal modes take the form of waves propagating through the crystal, which is why the atomic displacement can be written as a wave function.

What are the normal modes?

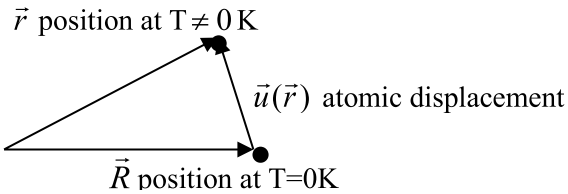
When many atoms are connected (like your lattice of springs), they **do not vibrate randomly**.

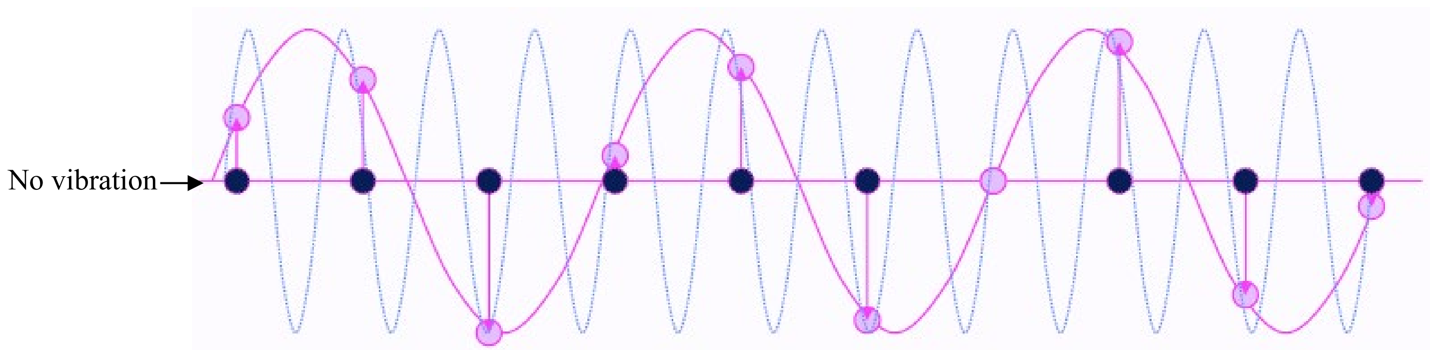
Instead, they vibrate in **organized patterns** where:

- All atoms move with the **same frequency**.
- Each atom has a **fixed phase relation** with others.

👉 These special vibration patterns are called **Normal Modes.**

III. Atomic Displacement





Atomic displacement:

- Position at T=0 : no vibration
- Position at T>0K : atoms vibrate

The displacement is given by:

$$u = u_0 e^{i(qx - \omega t)}$$

Where:

- u_0: amplitude
- q: wave vector (direction of wave propagation)
- ω: angular frequency

In three dimensions:

$$\vec{u}_q(\vec{r}, t) = u_0 e^{i(\vec{q}.\vec{r} - \omega t)} \hat{r}$$

We replace the displacement position with the lattice vector R, so the equation becomes:

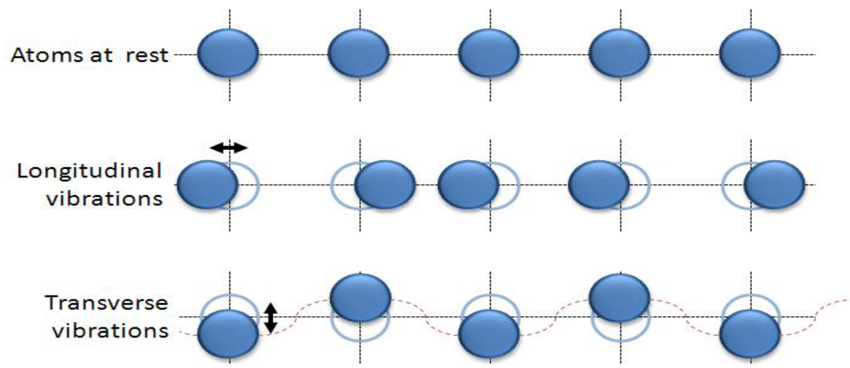
$$\vec{u}_q\left(\vec{R}_l^0\right) = u_0 e^{i\left(\vec{q}.\vec{R}_l^0 - \omega t\right)} \hat{r}$$

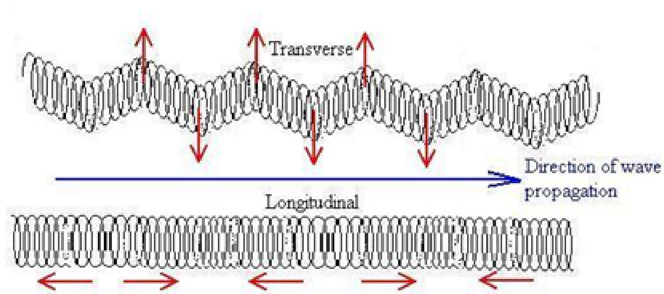
We use $\overrightarrow{R_l}$ because atoms occupy discrete lattice points.

- R_l^0 : represents the atomic equilibrium position
- l is simply a label that tells us which lattice point we are talking about.

IV. Types of Lattice Vibrations

By comparing the direction of displacement and propagation:



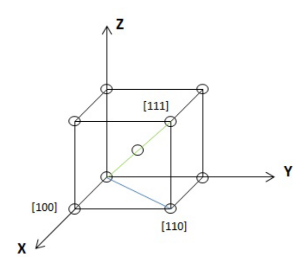


1. If the displacement is **perpendicular** to the propagation direction ($\vec{u} \perp \vec{q}$)
   The vibration is called a **transverse vibration**
   (similar to electromagnetic waves).
2. If the displacement $\vec{u}$ is **parallel** to the propagation direction $\vec{q}$
   The vibration is called **longitudinal vibration**
   (similar to sound waves).

Exercise (1)

Suppose a vibration in a cubic lattice solid propagates along the [111] direction, and atoms vibrate in the (111) plane. Determine whether the vibration is **longitudinal or transverse**.

Hint: You can use the figure that shows the [111] direction.



Exercise (2)

Using $\vec{u}_q\left(\vec{R}_l^0\right) = u_0 e^{i\left(\vec{q}.\vec{R}_l^0 - \omega t\right)}$.

Prove that:

$$\vec{u}_{\vec{q}}(R_l^0) = \vec{u}_{\vec{q}+\vec{G}}(R_l^0).$$

Hint: $e^{i\vec{G}.\vec{R_l}} = 1$, Where $\vec{G}$ is a reciprocal lattice vector.

Exercise (3) (student presentation)

Discuss the physical origin of lattice vibrations and analyze their impact on the thermal properties of solids. Support your answer with examples.