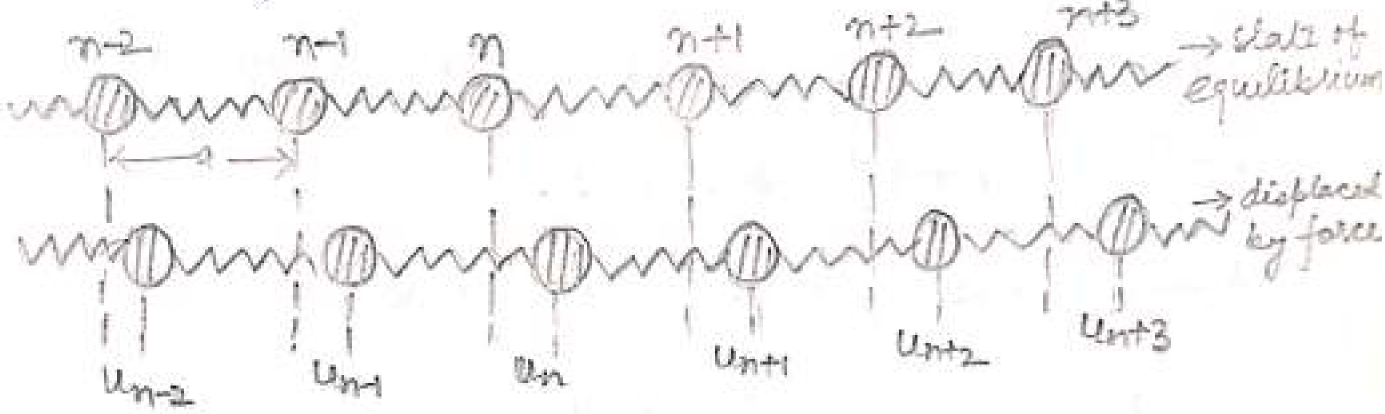
Chapter - 2

Elementary Lattice Dynamics

Vibrations of 1-D monoatomic lattice :→
(To study the elastic vibrations of a crystal)



Consider linear chain of atoms of equal masses, which are equally spaced by distance 'a', with the help of a massless spring undergoing elastic vibrations.

Let at any instant of time 't', the displacement of n^{th}, $(n-1)^{th}$, $(n-2)^{th}$ atoms from their mean positions by u_n, u_{n-1}, u_{n-2} respectively.

Let the spring constant be β.

Force exerted by a spring on an atom

$$F = \beta u$$

Above equation indicates that the elastic response (displacement) of atoms of crystal is a linear function of the forces.

The net force on the n^{th} atom is due to the forces due to atom at $(n-1)^{th}$ & $(n+1)^{th}$ positions.

Now, force on n^{th} due to $(n+1)^{th}$

$$F_n^{(n+1)} = \beta\,(u_{n+1} - u_n)$$

Force on n^{th} atom due to $(n-1)^{th}$

$$F_n^{(n-1)} = \beta\,(u_n - u_{n-1})$$

The net force on the n^{th} atom is

$$F = \beta\,(u_{n+1} - u_n) - \beta\,(u_n - u_{n-1})$$

$$F = \beta\,(u_{n+1} + u_{n-1} - 2u_n)$$

Using Newton's IInd law, equation of motion of an n^{th} atom can be written as

$$m\frac{d^2u_n}{dt^2} = \beta\,(u_{n+1} + u_{n-1} - 2u_n) \quad \text{— ①}$$

where $\frac{d^2u_n}{dt^2}$ represents the acceleration of the n^{th} atom.

eq (1) is a differential equation & has travelling wave solutions of the form

$u_n = u_0 \exp i(\omega t - Kx)$ $\left\{ \begin{array}{l} x = na \text{ for} \\ n^{th} \text{ atom} \end{array} \right.$

$u_n = u_0 \exp i(\omega t - Kna)$

$K = 2\pi/\lambda$, wave vector or propagation vector & $x = na$ & ω is angular frequency of the wave.

$u_{n+1} = u_0 \exp\{ i(\omega t - K(n+1)a)\}$

$u_{n+1} = u_0 \exp\{ i(\omega t - Kna - Ka)\}$

$u_{n-1} = u_0 \exp\{ i(\omega t - K(n-1)a)\}$

$u_{n-1} = u_0 \exp\{ i(\omega t - Kna + Ka)\}$

Putting $\frac{d^2 u_n}{dt^2} = -\omega^2 u_0 \exp\{ i(\omega t - kna)\}$

Putting in eq (1)

$$-m\omega^2 \cancel{u_0} \exp\{\cancel{i(\omega t - kna)}\} = \beta(e^{-ika} + e^{ika} - 2) \cancel{u_0 \exp\{ i(\omega t - kna)\}}$$

$$-m\omega^2 = \beta\{ e^{ika} - 2 + e^{-ika}\}$$

$$-m\omega^2 = \beta\{ e^{ika/2} - e^{-ika/2}\}^2$$

$\left\{ \begin{array}{l} \text{using } \sin x = \dfrac{e^{ix} - e^{-ix}}{2i} \\ \sin^2 x = -\frac{1}{4}(e^{ix/2} - e^{-ix/2})^2 \end{array} \right\}$

$$-m\omega^2 = -4\beta \sin^2\left(\frac{ka}{2}\right)$$

$$\boxed{w = \pm \sqrt{\frac{4\beta}{m}} \sin\left(\frac{ka}{2}\right)} \quad \text{—— (2)}$$

If c = longitudinal stiffness and

ρ = mass / length of the line

then,
$$\beta = c/a$$

$$\rho = m/a \Rightarrow m = \rho a$$

<u>Note:</u> A line of length a contains a massless spring and an atom of mass m.

$$w = \pm 2 \sqrt{\frac{c}{a \cdot \rho a}} \sin\left(\frac{ka}{2}\right)$$

$$w = \pm \frac{2}{a} \sqrt{\frac{c}{\rho}} \sin\left(\frac{ka}{2}\right)$$

$$\boxed{w = \pm \frac{2}{a} v_s \sin\left(\frac{ka}{2}\right)} \quad \text{—— (3)}$$

where, $v_s = \sqrt{\frac{c}{\rho}}$ = velocity of sound waves in solids.

Now, from equation (3)

$$W = \sqrt{\frac{4\beta}{m}} \left| \sin \frac{Ka}{2} \right|$$ { since freq cannot be −ve, ∴ taking only +ve

1) At low frequencies

ie for $K \longrightarrow 0$

$$\lim_{K \to 0} \sin \frac{Ka}{2} \sim \frac{Ka}{2}$$

{ $K = \frac{2\pi}{\lambda}$
$K \longrightarrow 0$
$\lambda \longrightarrow \infty$
$\nu \longrightarrow 0$ }

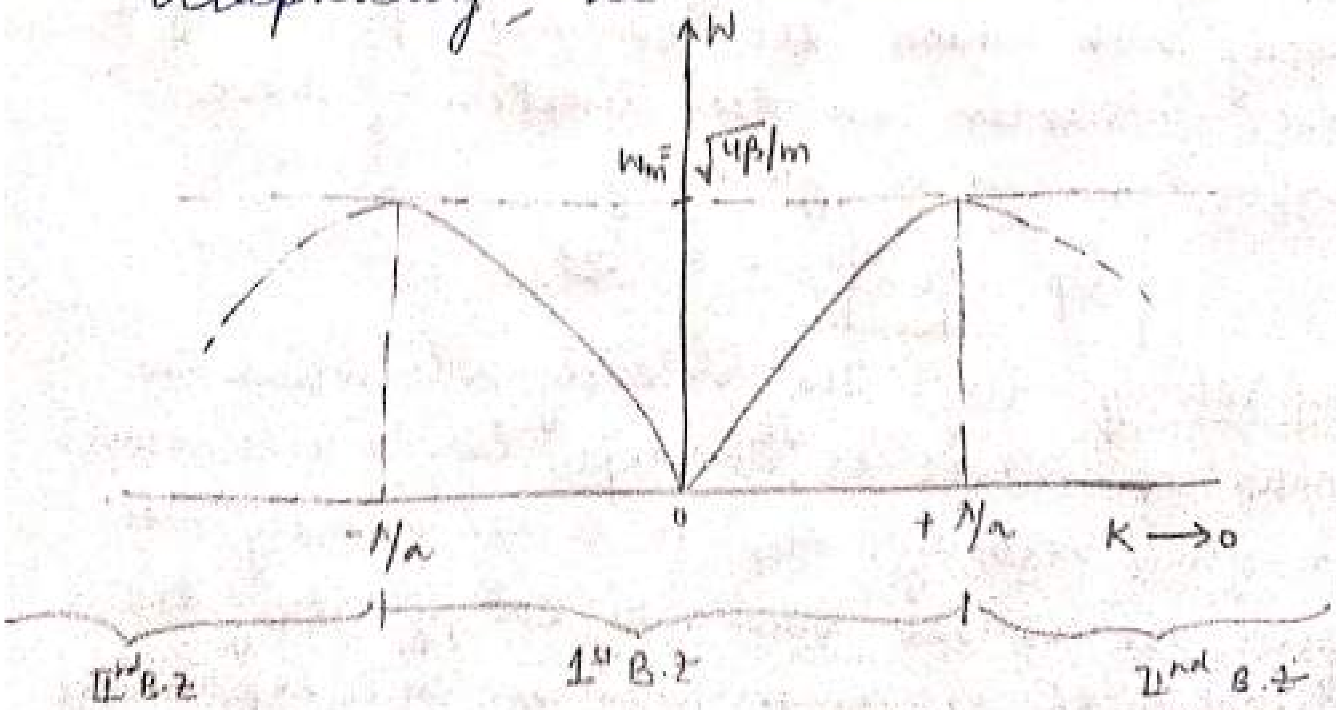
$$\boxed{W = \sqrt{\frac{4\beta}{m}} \cdot \frac{Ka}{2}}$$ {using eq ② } ⟶ ④

$$W = \left(\sqrt{\frac{4\beta}{m}} \cdot \frac{a}{2} \right) \cdot K$$ ⟶ Constt.

⇒ W is directly proportional to K

∴ $W \propto K$, ie W varies with K linearly.

Graphically, we can show it as



⑥

The max. value of W is when

$\Rightarrow \sin\left(\frac{Ka}{2}\right) = 1$

$$\Rightarrow \boxed{W = \sqrt{\frac{4\beta}{m}} = W_{max} = W_m = \frac{2}{a} v_s} \quad \text{--- (5)}$$

and the value of K at which

$W = W_{max}$ is

$$\sin\left(\frac{Ka}{2}\right) = \sin\left(\frac{\pi}{2}\right)$$

$$\Rightarrow \frac{Ka}{2} = \frac{\pi}{2} \Rightarrow \boxed{K = \pi/a}$$

The region $-\pi/a < K < \pi/a \Rightarrow$ 1st Brillouin Zone

" " $\pi/a < K < 2\pi/a$ & $-\frac{2\pi}{a} < K < -\pi/a \Rightarrow$ 2nd B.Z

Introducing here, a very important concepts:

Phase velocity :- (v_p) The velocity with which a wave travels is known phase velocity or the velocity with which, the constant phase of a wave advances in the direction of wave propagation. It is given by

$$\boxed{v_p = \frac{W}{K}} \quad \text{--- (6)}$$

Group Velocity :- (v_g) The velocity with which the group of waves or its envelope travels is known as group velocity. Also, it is the velocity with which the waves transmits energy along the direction of wave propagation. It is expressed as

$$\boxed{v_g = \frac{dw}{dK} = \frac{\Delta w}{\Delta K}} \quad — ⑦$$

Hence, At low frequencies ie $K \to 0$

$$\lim_{K\to 0} \sin\frac{Ka}{2} \text{ is } \frac{Ka}{2}$$

Using eq ③

$$w = \frac{2}{\cancel{a}} v_s \cdot \frac{K\cancel{a}}{\cancel{2}} = v_s \cdot K$$

Now, Phase velocity $v_p = \frac{w}{K} = v_s$

Group velocity $v_g = \frac{dw}{dK} = v_s$

$\Rightarrow$ Phase velocity is equal to group velocity

$$\boxed{v_p = v_g}$$

Note :- when $v_p = v_g \Rightarrow$ Medium is Non dispersive.

when $v_p \neq v_g \Rightarrow$ Medium is dispersive.

2) At higher frequencies :

$$w = \sqrt{\frac{4\beta}{m}} \left|\sin\left(\frac{Ka}{2}\right)\right|$$

or

$$= \frac{2}{a} v_s \left|\sin\left(\frac{Ka}{2}\right)\right|$$

$$v_p = \frac{w}{K}$$

$$\boxed{v_p = \frac{2 v_s}{Ka} \sin\left(\frac{Ka}{2}\right)} \quad — ⑧$$

$$v_g = \frac{dw}{dK}$$

$$v_g = \frac{\cancel{2}}{\cancel{a}} v_s \cos\left(\frac{Ka}{2}\right) \frac{\cancel{a}}{\cancel{2}} = v_s \cos\left(\frac{Ka}{2}\right)$$

8

$$\boxed{v_g = v_s \cos\left(\frac{Ka}{2}\right)} \quad \text{— (9)} \quad \Rightarrow v_p \neq v_g$$

Both v_p & v_g are functions of frequency. This is referred to as phenomenon of dispersion & the medium is known as <u>dispersive medium</u>.

3) At frequency (W_{max}), $W = \sqrt{\frac{4\beta}{m}} = \frac{2v_s}{a}$, which represents the maximum angular frequency of vibrations

$$K = \frac{\pi}{a} \Rightarrow \frac{2\pi}{\lambda} = \pi/a$$

$$\Rightarrow \boxed{\lambda = 2a} \quad \text{— (10)}$$

$$v_p = \frac{W}{K} = \frac{2}{a}\frac{v_s}{K} = \frac{2}{a}\frac{v_s}{\pi}a \qquad \{K = \pi/a$$

$$\boxed{v_p = \frac{2v_s}{\pi}} \quad \text{— (11)}$$

$$\boxed{v_g = \frac{dW}{dK} = 0}$$

$\Rightarrow$ There is no transfer of signal or energy corresponding to this frequency limit and hence the wave behaves like a standing wave. (not travelling wave).

From, Bragg law

$$2d\sin\theta = n\lambda$$

for 1st order ($n=1$), for normal incidence ($\theta = 90°$, glancing angle of incidence) $\sin 90 = 1$

$$2d = \lambda$$

This is similar to equation (10), which is equivalent to the condition for bragg's reflection

$\Rightarrow$ The only vibration of frequency $w < \sqrt{\frac{4\beta}{m}}$ $\left(\text{or } \frac{2v_s}{a}\right)$ can propagate through the lattice. Hence, the lattice behaves as low pass filter which transmits only if the frequency lies between 0 & $\frac{2v_s}{a}$.

Now
$a = 10^{-10}$ m & $v_s = 10^{4}$ m/s.

$\therefore$ The maximum frequency can be transmitted is $\simeq 10^{14}$/sec.

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