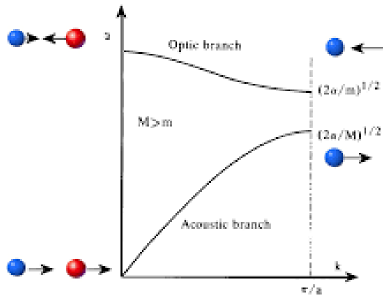
Class notes on:

Monoatomic and diatomic lattice vibration



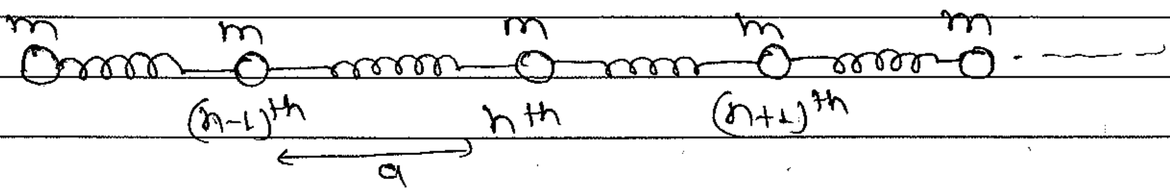
★ Lattice Vibration :-

lattice may be regarded as a Chain of atom which are connected through elastic spring such that vibration of one atom is transferd to the another atom. This atoms vibrate in their normal mode.

Motion of atom under mechanical force give ~~to~~ Acoustical branch and motion of atoms under electromagnetic force give to optical branch.

(1) Vibration of 1-dimentional monoatomic lattice.

No. of atom per primitive unit cell = 1



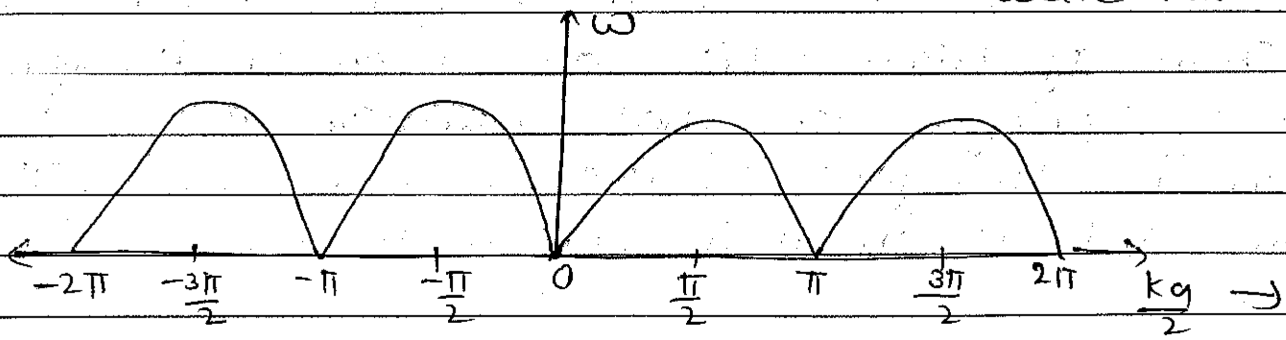
Energy quanta of lattice vibration is known as phonon. Phonon is a boson particle.

Let us consider the displacement of $(n-1)^{th}$, n^{th}, and $(n+1)^{th}$ ~~at~~ atom are u_{n-1}, u_n, u_{n+1}

and this atoms are vibrate harmonically and there is no thermal expansion of the crystal. Then frequency of vibration is given by

$$\boxed{\omega = \sqrt{\frac{4c}{m}}\ \sin\frac{ka}{2}}$$

c = spring constant
k = wave number



(i) If $k \to 0$ (λ is large)

$$\sin\frac{ka}{2} \simeq \frac{ka}{2}$$

$$\omega = \sqrt{\frac{4c}{m}}\ \frac{ka}{2}$$

Phase velocity $V_p = \frac{\omega}{k} = \frac{a}{2}\sqrt{\frac{4c}{m}}$

Group velocity $V_g = \frac{d\omega}{dk} = \frac{a}{2}\sqrt{\frac{4c}{m}}$

$\boxed{V_p = V_g}$ (non-disspressive medium)

So both phase velocity and group velocity are equal ~~in~~ and independent of wave vector

So medium behave like as a non-disperssive medium.

(ii) If ~~ω~~ k is large

$$\omega = \sqrt{\frac{4c}{m}} \sin \frac{ka}{2}$$

$$V_p = \frac{\omega}{K} = \frac{1}{K}\sqrt{\frac{4c}{m}} \sin \frac{Ka}{2}$$

$$V_g = \frac{d\omega}{dk} = \frac{a}{2}\sqrt{\frac{4c}{m}} \cos \frac{ka}{2}$$

$$\boxed{V_p \neq V_g}$$

The group velocity of any particle at brillaun zone boundary is equal to zero. So first brilliaun zone is define as-

$$V_g = 0 \Rightarrow \cos \frac{ka}{2} = 0$$

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

$$-\frac{\pi}{a} < K < \frac{\pi}{a}$$

and ~~at~~ short wavelength the phase velocity is not equal to group velocity. So medium is behave like as a disperssive medium.

$$\omega = \sqrt{\frac{4c}{m}} \sin \frac{ka}{2}$$

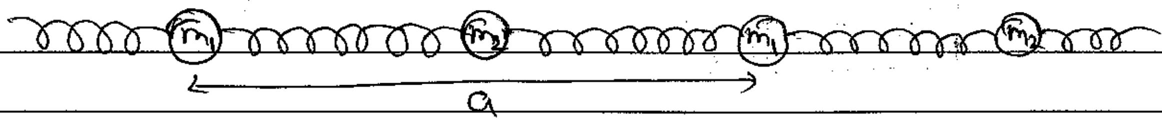
$\because \left(\sin \frac{ka}{2}\right)_{max.} = 1$

$$\boxed{\omega_{max.} = \sqrt{\frac{4c}{m}}}$$

So 1-D mono atomic lattice pass the wave which have frequency 0 to $\omega_{max.}$ So it is also known as low pass filter

☆ One ~~dimention~~ dimensional diatomic lattice :-

No. of atom per unit cell is two.



let $\boxed{m_1 < m_2}$

frequency of vibration-

$$\omega^2 = c\left[\frac{1}{m_1} + \frac{1}{m_2}\right] \pm c\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka/2}{m_1 m_2}}$$

(i) If we take (+) sign optical Branch.

(ii) If we take (−) sign Acoustical Branch

(i) For optical branch :-

$$\omega_+^2 = c\left[\frac{1}{m_1} + \frac{1}{m_2}\right] + c\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka/2}{m_1 m_2}}$$

→ If $K \to 0$; $\sin^2 \frac{ka}{2} \simeq 0$

$$\omega_+^2 = 2C\left[\frac{1}{m_1} + \frac{1}{m_2}\right] \Rightarrow \boxed{\omega_+ = \sqrt{\frac{2C(m_1+m_2)}{m_1 m_2}}}$$

→ At $K \to \pi/a$; $\sin^2 \pi/2 = 1$

$$\omega_+^2 = C\left[\frac{1}{m_1} + \frac{1}{m_2}\right] + C\sqrt{\frac{1}{m_1^2} + \frac{1}{m_2^2} + \frac{2}{m_1 m_2} - \frac{4}{m_1 m_2}}$$

$$\omega_+^2 = C\left[\frac{1}{m_1} + \frac{1}{m_2}\right] + C\left[\frac{1}{m_1} - \frac{1}{m_2}\right] \quad (m_1 < m_2)$$

$$\omega_+^2 = \frac{2C}{m_1} \Rightarrow \boxed{\omega_+ = \sqrt{\frac{2C}{m_1}}}$$

☆ If $K=0$ then frequency become 0 then it is known as Acoustical branch. and If $\omega \neq 0$ then it is known as optical branch.

(ii) For acoustical Branch :-

$$\omega_-^2 = C\left[\frac{1}{m_1} + \frac{1}{m_2}\right] - C\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka/2}{m_1 m_2}}$$

(i) If $K \to 0$; $\sin \frac{ka}{2} \simeq \frac{ka}{2}$

$$\omega_-^2 = C\left[\frac{1}{m_1} + \frac{1}{m_2}\right] - C\left[\frac{1}{m_1} + \frac{1}{m_2}\right]\left[1 - \frac{k^2 a^2 m_1^2 m_2^2}{m_1 m_2 (m_1+m_2)^2}\right]^{1/2}$$

$$= C\left[\frac{1}{m_1}+\frac{1}{m_2}\right] - C\left[\frac{1}{m_1}+\frac{1}{m_2}\right]\left[1 - \frac{k^2a^2m_1m_2}{2(m_1+m_2)^2}\right]$$

$$\omega_-^2 = C\left(\frac{m_1+m_2}{m_1m_2}\right)\frac{k^2a^2m_1m_2}{2(m_1+m_2)^2}$$

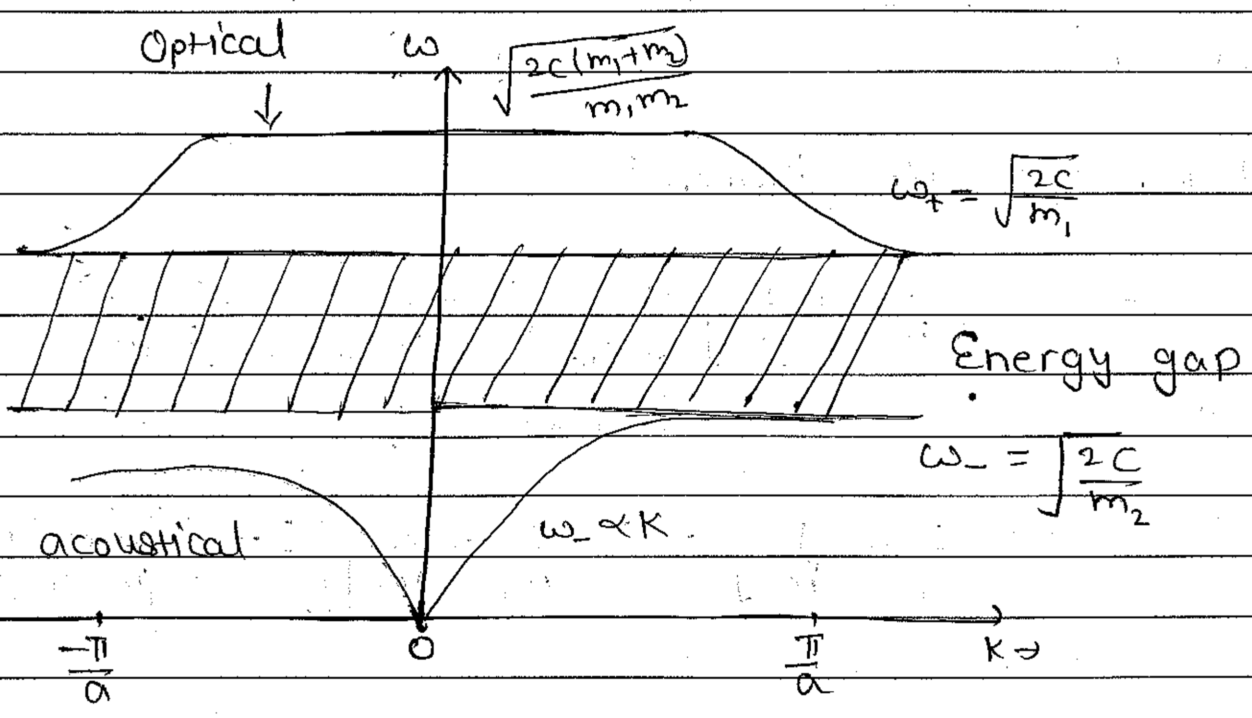
$$\omega_- = ka\sqrt{\frac{C}{2(m_1+m_2)}}$$

$\boxed{\omega_- \propto k}$ (non- despersive)

→ At $k \rightarrow \frac{\pi}{a}$

$$\omega_-^2 = C\left[\frac{1}{m_1}+\frac{1}{m_2}\right] - C\left[\frac{1}{m_1}-\frac{1}{m_2}\right]$$

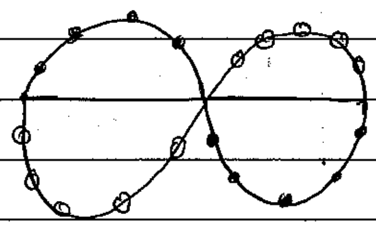
$$\omega_-^2 = \frac{2C}{m_2} \Rightarrow \boxed{\omega_- = \sqrt{\frac{2C}{m_2}}}$$



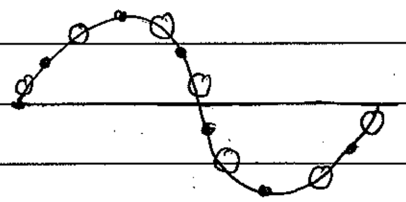
AT zone boundary in case of acoustical branch the lighter atom will be at rest. and in case of optical branch the havier atom will be at rest.

The optical frequency and acoustical frequency are seperated by a rigon which is known as forbidden energy gap. so it is also known as band stock filter. The frequency gap is propotional to m_2/m_1

★ In the optical branch the centre of mass of two atom remain fix but in the acoustical branch the centre of mass move with the atom.



Optical



Acoustical branch

★ No. of Branches:-

No. of atoms per primitive unit cell = P

	Acoustical Branch	Optical Branch
1 − D	1	P − 1
2 − D	2	2P − 2
3 − D	3	3P − 3

Q. Find the no. of acoustical and optical branch for diamond.

Sol.:- $P = 2$ & 3D structure

Acoustical Branch $= 3$

Optical branch $= 3 \times 2 - 3 = 3$

total $= 3 + 3 = 6$