. 4.1. vibration modes of leaner monatomic lattice

The vibration of leaner lattice consist of monatomic leaner series , is one of the simples type of vibration modes. The aim of studying this mod is to find the dispersion relation between the angular frequency (ω) (of the vibrated atom) and the wave vector (k) of the wave which is formed from the vibration.

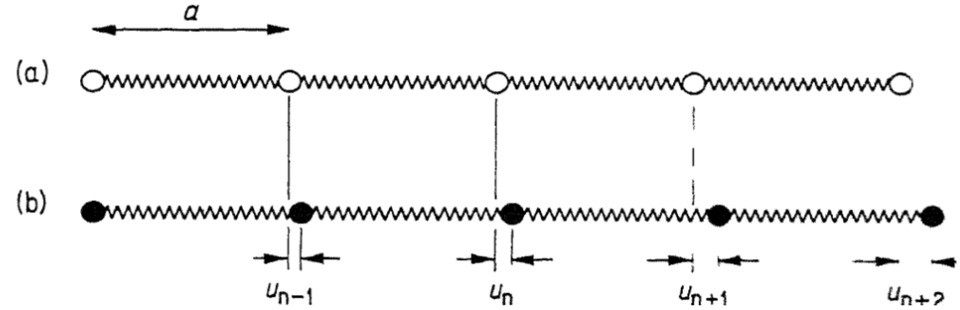

Fig.1. (a) monatomic leaner series in its equilibrium positions. (b) atomic displacement from its equilibrium positions.

Where (a) is the lattice constant and (U) is the atomic displacement from its equilibrium positions. After solving the equation of motion we get

$$\omega = \pm 2\left(\frac{\mu}{m}\right)^{1/2} \sin\left(\frac{ka}{2}\right) \quad \text{.................................(1)}$$

Equation (2) is called the dispersion relation between the angular frequency (ω) (of the vibrated atom) and the wave vector (k) of the wave which is formed from the vibration.

The positive or negative signal (+),(-) describe the transfer direction, and the motion is periodic with the time see fig.(2).

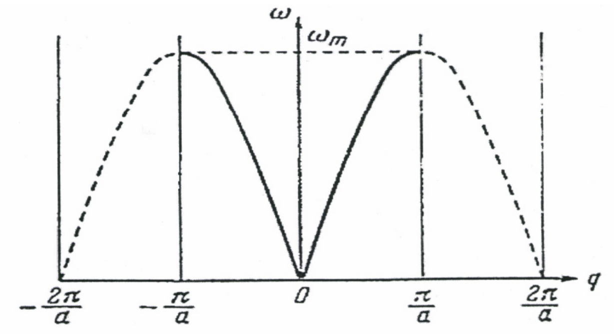

Fig.-2 : Vibrations of a linear monatomic chain (spectrum).

4.1.1The general Properties conclude from the dispersion relation and Fig.(2)

1- There is a maximum value of the angular frequency ($\omega = \omega_{max}$) at ($k = \frac{\pi}{a}$) or its odd

multiples, and this results mean that there is an upper limit or cutoff frequency of elastic waves (sound waves) in the solid materials;

$$\omega = 2\left(\frac{\mu}{m}\right)^{1/2} \sin\left(\frac{ka}{2}\right) = 2\left(\frac{\mu}{m}\right)^{1/2} \sin\left(\frac{\pi}{2}\right) = 2\left(\frac{\mu}{m}\right)^{1/2}$$

$$\omega = \omega_{\max} = 2\left(\frac{\mu}{m}\right)^{1/2}$$

The $\omega_{\max}$ value depends on the force constant and the atomic mass as in above equation of $\omega_{\max}$. So we can write equation (2) as

$$\boxed{\omega = \omega_{\max} \sin\left(\frac{ka}{2}\right)} \quad \text{..........................(2)}$$

2- For each wave vector k there is angular frequency ω and all probability of vibration is limited by k values in the range $(-\frac{\pi}{a} \le k \le \frac{\pi}{a})$. This range is called the first Brillouin zone for leaner lattice. The next range which follow the first Brillouin zone with half periodic ($\pm\frac{\pi}{2}$) to each sides is called the second Brillouin zone, $[(\frac{\pi}{a} \le k \le \frac{2\pi}{a}), (-\frac{\pi}{a} \le k \le -\frac{2\pi}{a})$.

3- For the waves which have large wavelength λ (when the wave vector k is small), the frequencies of this waves transfer through lattice, while the other frequencies will soon vanishes, therefore the lattice work as mechanical filter to remove or release the low frequencies. As the wave vector (k) is very small and from equations (1) and (2) we find;

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

$$\omega = 2\left(\frac{\mu}{m}\right)^{1/2} \sin\frac{ka}{2} = \left(\frac{\mu}{m}\right)^{1/2} ak = \frac{\omega_{\max}}{2} ak$$

$$2\pi v = \left(\frac{\mu}{m}\right)^{1/2} ak = \left(\frac{\mu}{m}\right)^{1/2} a\frac{2\pi}{\lambda}$$

$$\lambda v = \left(\frac{\mu}{m}\right)^{1/2} a \Rightarrow V_0 = \left(\frac{\mu}{m}\right)^{1/2} a = \frac{\omega_{\max} a}{2}$$

$$\omega = V_0 k = \left(\frac{\mu}{m}\right)^{1/2} ak = \frac{\omega_{\max} a}{2} k$$

4- For the waves with small wavelengths (when k is large), then the wavelengths is very small ($\lambda << a$) that is mean the wave vector is large and the wave propagation velocity is not constant but its decreases with the increasing of the wave vector, when $k = \frac{\pi}{a}$ then the wavelength is equal to:

$k = \frac{\pi}{a} = \frac{2\pi}{\lambda} \Rightarrow\Rightarrow\Rightarrow \qquad \lambda = 2a$

As a result the restoring force and frequancy in this case is in higher possible value, but when $\lambda >> 2a$ we can note that the atomic lattice move in one direction and in the same phase as shown in Fig.(3). In this case the effective restoring on the atoms is very small which act on the angular frequency ω. When the wavelength is go to the infinity i.e.: the lattice moves as one elastic body which lead to vanishing the restoring force and this answer when $\omega = 0$ at $k = 0$

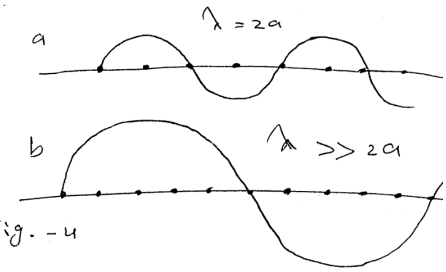

Fig. - 4

4.2-Phase velocity and group velocity in the lattice

(a) Phase velocity V_{ph} is the velocity of intrinsic wave propagate with certain frequency ω and wave vector k and is given by

$V_{ph} = \frac{\omega}{k}$ **, From equation(10),**

$$V_{ph} = \frac{\omega}{k} = \frac{2}{k}\left(\frac{\mu}{m}\right)^{1/2} \sin\left(\frac{ka}{2}\right) = \frac{2V_0}{ka} \sin\frac{ka}{2} \qquad \text{…(3)}$$

$$where \qquad V_0 = \left(\frac{\mu}{m}\right)^{1/2} a$$

(b) group velocity V_g is the propagation velocity of unlimited number of frequencies and is given by

$V_g = \frac{\partial \omega}{\partial k}$, **From equation (10),** $V_g = \frac{\partial \omega}{\partial k} = 2\left(\frac{\mu}{m}\right)\frac{a}{2}\cos\left(\frac{ka}{2}\right) = V_0 \cos\left(\frac{ka}{2}\right)$ **……….(4)**

For the waves which have large wavelength λ (when the wave vector k is very small)

$$V_{ph} = \frac{\omega}{k} = \left(\frac{\mu}{m}\right)^{1/2} a = V_0 \,, \quad V_g = \frac{\partial \omega}{\partial k} = \left(\frac{\mu}{m}\right)^{1/2} a = V_0$$

So at $\lambda >> a$, where (when the wave vector k is very small)

$$V_{ph} = V_g = V_0$$

At $k = \frac{\pi}{a} \Rightarrow\Rightarrow\Rightarrow \qquad \lambda = 2a\,, \; V_{ph} = \frac{2V_0}{\pi}, \qquad V_g = 0$