The one dimensional diatomic lattice :-

Consider, the one dimensional diatomic lattice,

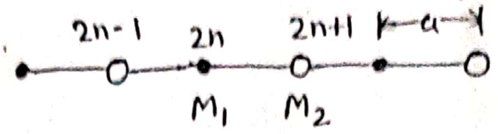


Fig. 1

Fig shows a diatomic lattice in which the unit cell is composed of two atoms of masses M_1 and M_2, and 'a' is the distance between two neighboring atoms.
For ex- NaCl

The motion of this lattice can be treated as same as the motion of the monoatomic lattice. Since, there are two different types of atoms. we have two equations of motion.

$$\left.\begin{aligned} M_1 \frac{d^2 u_{2n+1}}{dt^2} &= -\alpha\left(2u_{2n+1} - u_{2n} - u_{2n+2}\right), \\ M_2 \frac{d^2 u_{2n+2}}{dt^2} &= -\alpha\left(2u_{2n+2} - u_{2n+1} - u_{2n+3}\right) \end{aligned}\right\} \quad (1)$$

Where, n is an integral index, All atoms with mass M_1 are labeled as even and those with mass M_2 as odd. The two eqs. in (1) are coupled. By writing a similar set for each cell in the crystal, we have a total of 2N coupled differential equations. ~~that~~ (N is the no. of unit cells in the lattice). We get a solution in the form of a travelling wave, in matrix form.

$$\begin{bmatrix} u_{2n+1} \\ u_{2n+2} \end{bmatrix} = \begin{bmatrix} A_1 e^{iqx_{2n+1}} \\ A_2 e^{iqx_{2n+2}} \end{bmatrix} e^{-i\omega t} \quad (2)$$

$X_n = na$

Second relation

$$-\omega^2 M_2 A_2 e^{iq(2n+2)a} = -\alpha\left[2A_2 e^{iq(2n+2)a} - A_1 e^{iq(2n+1)a} - A_1 e^{iq(2n+3)a}\right]$$

If we cancel common factor e^{iq2na} from both sides, we have.

$$-\omega^2 M_2 A_2 e^{i2qa} = -\alpha\left[2A_2 e^{i2qa} - A_1 e^{iqa} - A_1 e^{i3qa}\right]$$

If we cancel common factor e^{i2qa} from both sides, we have

$$-\omega^2 M_2 A_2 = -\alpha\left[2A_2 - A_1 e^{-iqa} - A_1 e^{iqa}\right]$$

$$(2\alpha - \omega^2 M_2)A_2 - \alpha(e^{-iqa} - e^{iqa})A_1 = 0$$

Using Euler relation $e^{iy} - e^{-iy} = 2\cos y$, we have

$$(2\alpha - \omega^2 M_2)A_2 - 2\alpha\cos(qa)A_1 = 0$$

$$-\{2\alpha\cos(qa)\}A_1 + \{2\pi - \omega^2 M_2\}A_2 = 0 \quad (3)$$

Similarly from first relation

$$-\omega^2 M_1 A_1 e^{iq(2n+1)a} = -\alpha\left[2A_1 e^{iq(2n+1)a} - A_2 e^{iq2na} - A_2 e^{iq(2n+2)a}\right]$$

Comparing coefficient of $e^{iq(2n+1)a}$

$$-\omega^2 M_1 A_1 = -\alpha\left[2A_1 - A_2 e^{-iqa} - A_2 e^{iqa}\right]$$

$$(2\alpha - \omega^2 M_1)A_1 - 2\alpha\cos(qa)A_2 = 0 \quad (4)$$

Note that all the atoms of Mass M_1 have the same amplitude A_1, and all those of mass M_2 have amplitude A_2. Substituting (2) into (1) and ~~make some straight~~ simplifying, we find

$$\begin{bmatrix} 2\alpha - M_1\omega^2 & -2\alpha\cos(qa) \\ -2\alpha\cos(qa) & 2\alpha - M_2\omega^2 \end{bmatrix}\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0 \qquad (5)$$

(*) - - - (*)

Eq^n (5) is a matrix eq^n equivalent to a set of two simultaneous eq^{ns} in the unknown A_1 and A_2. Since the eq^{ns} are homogeneous, a nontrivial solution exists only if the ~~displacemen~~ determinant of the matrix in eq^n (5) vanishes. This leads to the secular eq^n,

$$\begin{vmatrix} 2\alpha - M_1\omega^2 & -2\alpha\cos(qa) \\ -2\alpha\cos(qa) & 2\alpha - M_2\omega^2 \end{vmatrix} = 0 \qquad (6)$$

This is a quadratic eq^n in ω^2 and can be solved into two roots:

$$\omega^2 = \alpha\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \alpha\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2(qa)}{M_1 M_2}} \qquad (7)$$

$$\because \ (2\alpha - M_1\omega^2)(2\alpha - M_2\omega^2) - 4\alpha^2\cos^2(qa) = 0$$

$$4\alpha^2 - 2\alpha M_2\omega^2 - 2\alpha M_1\omega^2 + M_1 M_2\omega^4 - 4\alpha^2\cos^2(qa) = 0$$

$$M_1 M_2\omega^4 - 2\alpha(M_1 + M_2)\omega^2 - 4\alpha\left[1 + \cos^2(qa)\right] = 0$$

$$\omega^4 - 2\alpha\frac{(M_1 + M_2)}{M_1 + M_2}\omega^2 - \frac{4\alpha^2}{M_1 M_2}\sin^2(qa) = 0$$

Corresponding to the two signs in (7) there are thus two dispersion relations, and consequently two dispersion curves, or branches, associated with the diatomic lattice.

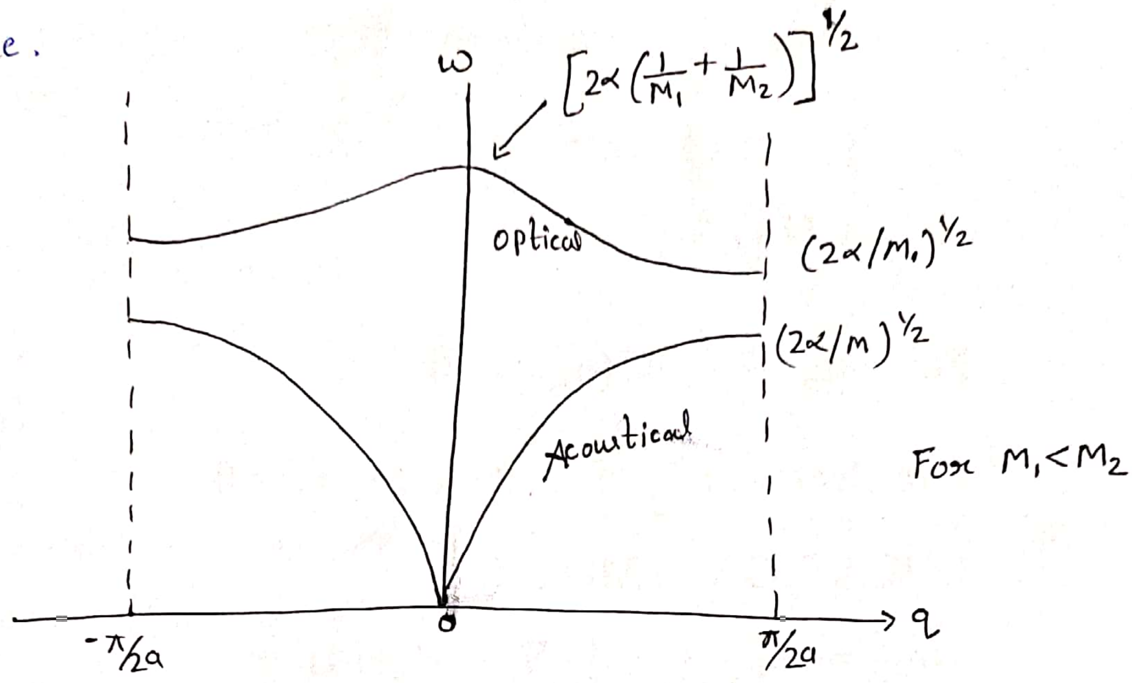


Fig. 2

In fig. 2., the lower curve corresponding to the minus sign in eqn (7) is the acoustical branch, while the upper curve is the optical branch.

The acoustic branch begins at the point $q=0$, $\omega=0$. As q increases, the curve rises, linearly at first (which explains ~~an~~ why this branch is called acoustic), but then rate of rise decreases. Eventually the curve saturates at the value $q=\pi/2a$, as can be seen from (7), at a freq. $(2\alpha/M_2)^{1/2}$. It is assumed that $M_1 < M_2$. As for the optical branch, it begins at $q=0$ with a finite frequency

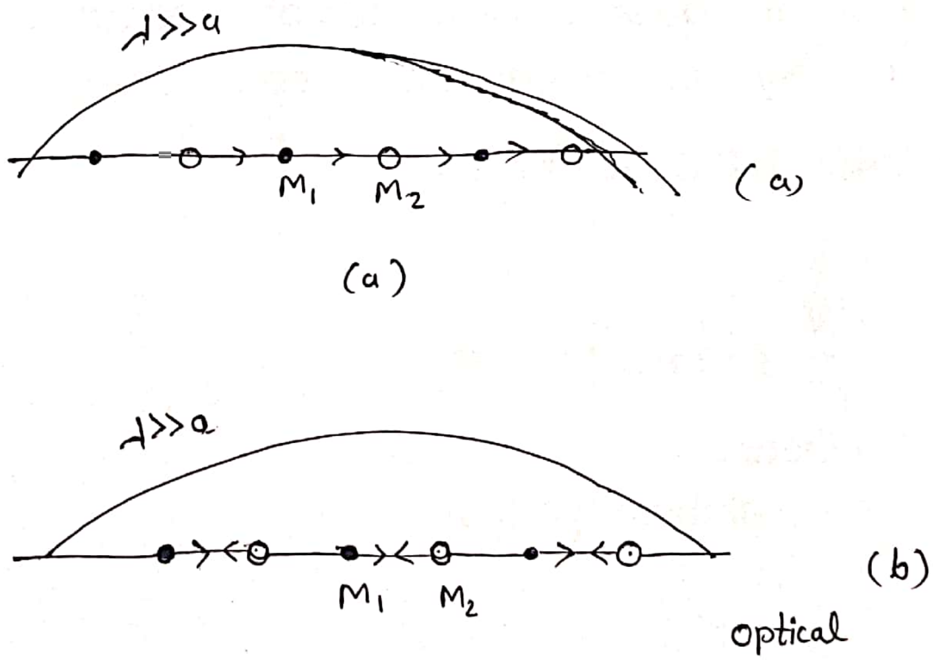
$$\omega = \left[2\alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\right]^{1/2} \quad (8)$$

and then decreases slowly, saturating at $q=\pi/2a$ with a frequency $(2\alpha/M_1)^{1/2}$. The frequency of this branch does not vary appreciably over the entire q-range, and it is often taken to be approximately a constant.

The frequency range between the top of acoustical branch and the bottom of the optical branch is forbidden, and the lattice cannot transmit such a wave; waves in this region is strongly attenuated (frequency gap). Therefore the diatomic lattice acts as a BAND PASS MECHANICAL FILTER.

These two branches are dynamical distinct by comparing them at the value $q \simeq 0$. We may use (5) to find the ratio of the amplitude A_2/A_1. Inserting $\omega = 0$, for the acoustic branch, ~~one finds~~ the eq^n is satisfied only if

$$A_1 = A_2 \qquad \text{——— (9)}$$



(a)

Fig 3

Thus, for this branch the two atoms in the cell, or molecules, have the same amplitude and are also in phase. In other words, the molecule (and the whole lattice) oscillates as a rigid body, with the centre of mass moving back and forth as shown in 3(a). As q increases, the two atoms in the molecule no longer satisfy (7) exactly, but they still move approximately in phase with each other.

On the other hand, if we substitute

$$\omega = \left[2\alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\right]^{1/2}$$

for the optical branch, we find that

$$M_1 A_1 + M_2 A_2 = 0 \qquad (10)$$

This means that the optical oscillation takes place in such a way that the center of mass of the cell remains fixed. The two atoms move π out of phase with each other, and the ratio of their amplitudes $(A_2/A_1) = -(M_1/M_2)$. This type of oscillation around the center of mass is well known in the study of molecular vibrations. As 'q' increases beyond zero, the frequency of the diatomic vibration decreases, but the decrease is not large because the atoms continue to oscillate approximately π out of phase with each other throughout the entire q-range.