Question:

Consider the normal modes of a linear chain, in which the masses are alternately M and m. Assuming that the force constants between nearest-neighbor atoms are equal, and the nearest-neighbor separation is $a/2$. M≠m and K=G

Find :

1- The dispersion relation $\omega(k) at\ k = 0\ and\ k = \frac{\pi}{a}$
2- The conditions for acoustic and optical modes.

Solution:

$M \neq m, \quad K = G$

$$M\frac{d^2u_s}{dt^2} = C_2(v_s - u_s) + C_1(v_{s-1} - u_s) = C_2v_s + C_1v_{s-1} - (C_1 + C_2)u_s$$

$$m\frac{d^2v_s}{dt^2} = C_2(u_s - v_s) + C_1(u_{s+1} - v_s) = C_2u_s + C_1u_{s+1} - (C_1 + C_2)v_s$$

Trying to solve the problem by the periodic solutions in the form of a traveling wave as follows:

$u_s = ue^{i(ksa-\omega t)}$ and $v_s = ve^{i(ksa-\omega t)}$

This leads us to the eigenvalue equation:

$$\begin{pmatrix} C_1 + C_2 - M\omega^2 & -(C_2 + C_1e^{-ika}) \\ -(C_2 + C_1e^{+ika}) & C_1 + C_2 - m\omega^2 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = 0$$

Then, the two solutions can be given as:

$$Mm\omega^4 - 2C(M + m)\omega^2 + 2C^2(1 - \cos ka) = 0$$

$$\omega^2 = \frac{2C(M + m) \pm \sqrt{4C^2(M + m)^2 - 8C^2Mm(1 - \cos ka)}}{Mm}$$

$$\omega^2 = \frac{2C(M + m) \pm \sqrt{4C^2(M + m)^2 - 16C^2Mm\sin\frac{ka}{2}}}{Mm}$$

At k= 0, let's assume

$$\omega^2 = \frac{2C(M+m) \pm \sqrt{4C^2(M+m)^2}}{Mm} = \frac{2C(M+m) \pm 2C(M+m)}{Mm}$$

$$\omega_-^2 = 0$$

$$\omega_+^2 = \frac{2C(M+m) + 2C(M+m)}{Mm} = \frac{4C(M+m)}{Mm}$$

$$\omega_+ = \sqrt{\frac{4C(M+m)}{Mm}}$$

At $= \frac{\pi}{a}$,

$$\omega^2 = \frac{2C(M+m) \pm \sqrt{4C^2(M+m)^2 - 16C^2Mm}}{Mm}$$

$$\omega^2 = \frac{2C(M+m) \pm \sqrt{4C^2(M-m)^2}}{Mm}$$

$$\omega^2 = \frac{2C(M+m) \pm 2C(M-m)}{Mm}$$

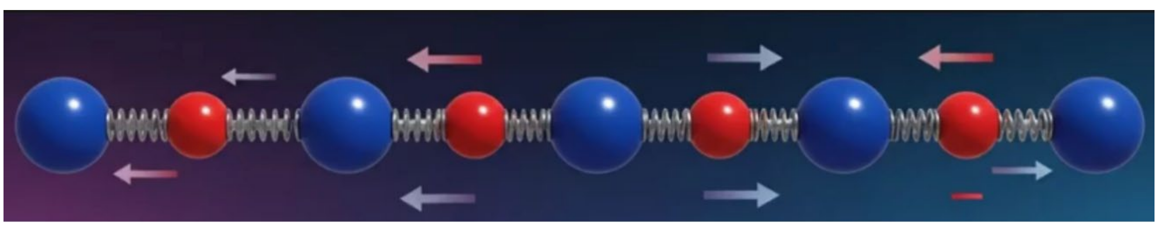
$$\omega_+^2 = \frac{2CM}{Mm}$$

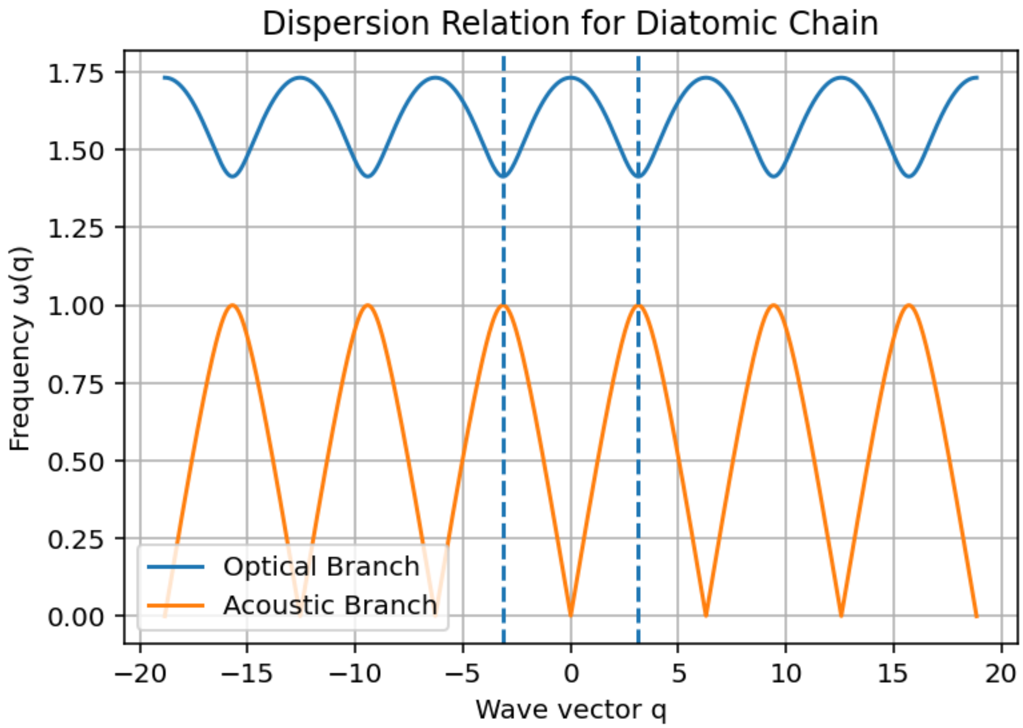
$$\omega_+^2 = \sqrt{\frac{2C}{m}}$$

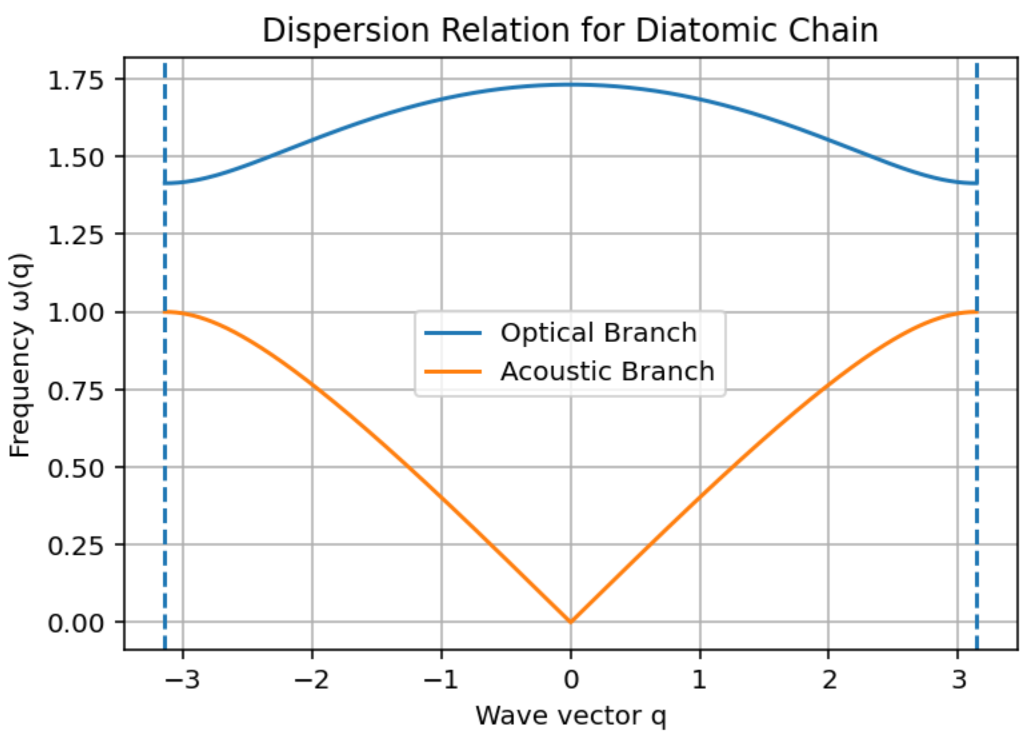
$$\omega_-^2 = \frac{2Cm}{Mm}$$

$$\omega_-^2 = \sqrt{\frac{2C}{M}}$$

For acoustic mode, $\omega \ \rightarrow 0$ $when\ k = 0$, so
ω_- $corresponds\ to\ the\ acoustic\ mode\ while\ \omega_+ represents\ the\ optical\ mode$




Dispersion Relation for Diatomic Chain
Frequency ω(q)
Wave vector q
Optical Branch
Acoustic Branch
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
−20
−15
−10
−5
0
5
10
15
20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