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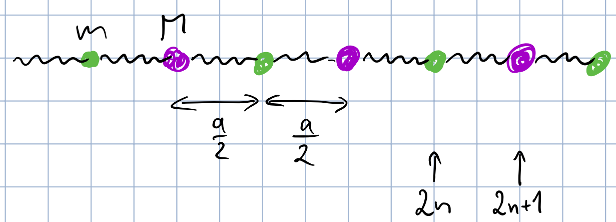


a – lattice constant

ϕ_i – displacement of the i-th atom

Equations of motion:

$$\begin{cases} m\ddot{\phi}_{2n} = \kappa\left(\phi_{2n+1} - \phi_{2n} - \phi_{2n} + \phi_{2n-1}\right) \\ M\ddot{\phi}_{2n+1} = \kappa\left(\phi_{2n+2} - \phi_{2n+1} - \phi_{2n+1} + \phi_{2n}\right) \end{cases}$$

Seek for the normal modes:

$$\begin{cases} \phi_{2n} = A e^{i\left(q 2n \frac{a}{2} - \omega_q t\right)} \\ \phi_{2n+1} = B e^{i\left[q(2n+1)\frac{a}{2} - \omega_q t\right]} \end{cases} \rightarrow \begin{cases} -m\omega_q^2 A = \kappa\left(Be^{iq\frac{a}{2}} - 2A + Be^{-iq\frac{a}{2}}\right) \\ -M\omega_q^2 B = \kappa\left(Ae^{iq\frac{a}{2}} - 2B + Ae^{-iq\frac{a}{2}}\right) \end{cases}$$

$$\underbrace{\begin{pmatrix} -m\omega_q^2 + 2\kappa & -2\kappa\cos\frac{qa}{2} \\ -2\kappa\cos\frac{qa}{2} & -M\omega_q^2 + 2\kappa \end{pmatrix}}_{\mathbb{M}} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

Existence of nontrivial solutions requires that $\det\mathbb{M} = 0$.

$$\det\mathbb{M} = 0 \rightarrow \left(-M\omega_q^2 + 2\kappa\right)\left(-m\omega_q^2 + 2\kappa\right) - 4\kappa^2\cos^2\frac{qa}{2} = 0$$

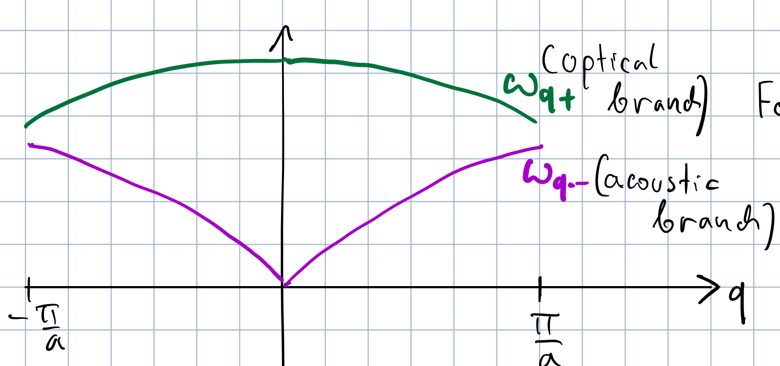
$$Mm\left(\omega_q^2\right)^2 - 2\kappa(M+m)\,\omega_q^2 + 4\kappa^2\left(1 - \cos^2\frac{qa}{2}\right) = 0$$

$$\Delta = 4\kappa^2(M+m)^2 - 16Mm\kappa^2\left(1 - \cos^2\frac{qa}{2}\right) = 4\kappa^2(M-m)^2 + 16Mm\kappa^2\cos^2\frac{qa}{2} > 0$$

$$\omega_q^2 = \frac{1}{2Mm}\left(2\kappa(M+m) \pm \sqrt{4\kappa^2(M-m)^2 + 16\kappa^2 Mm\cos^2\frac{qa}{2}}\right)$$

$$\omega_q^2 = \frac{\kappa}{Mm}\left[(M+m) \pm \sqrt{(M-m)^2 + 4Mm\cos^2\frac{qa}{2}}\right]$$

We obtain two families of solutions for $\omega_q \rightarrow \omega_{q+}, \omega_{q-}$



For $q \rightarrow 0$: $\omega_{q\pm}^2 \simeq \frac{\kappa}{Mm}\left[M+m \pm \sqrt{(M-m)^2 + 4Mm\left(1-\left(\frac{qa}{2}\right)^2\right)}\right]$

$$= \frac{\kappa}{Mm}\left[(M+m) \pm \sqrt{(M+m)^2 - Mmq^2a^2}\right]$$

$$\omega_{q\pm}^2 \simeq \frac{\kappa}{Mm}(M+m)\left[1 \pm \sqrt{1 - \frac{Mm}{(M+m)^2}q^2a^2}\right] \simeq$$

$$\simeq \frac{\kappa}{Mm}(M+m)\left[1 \pm 1 \mp \frac{Mm}{2(M+m)^2} q^2 a^2\right]$$

$$\omega_{q+} \overset{q\approx 0}{\simeq} \sqrt{\frac{2\kappa(M+m)}{Mm}} = \text{const}$$

$$\omega_{q-} \overset{q\approx 0}{\simeq} \underbrace{\sqrt{\frac{\kappa}{2(M+m)}}\, a}_{v_s} q = \text{const}\cdot q$$

b) $\omega_q \in \left[0, \sqrt{\frac{2\kappa(M+m)}{Mm}}\,\right]$

c) For $m=M$ we have $\omega_q^2 = \frac{\kappa}{m^2}\left[2m \pm \sqrt{4m^2\cos^2\frac{qa}{2}}\right]$

$$\omega_q^2 = 2\frac{\kappa}{m}\left(1 \pm \left|\cos\frac{qa}{2}\right|\right) \qquad q \in \left]-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

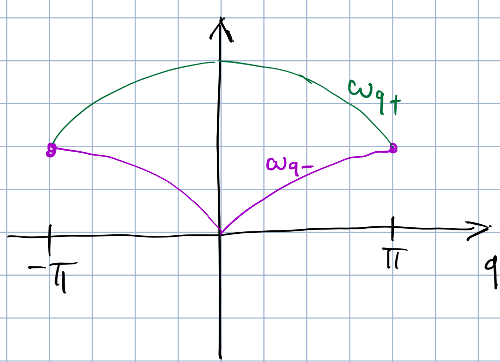
$$\rightarrow \omega_q^2 = \frac{2\kappa}{m}\left(1 \pm \cos\frac{qa}{2}\right)$$

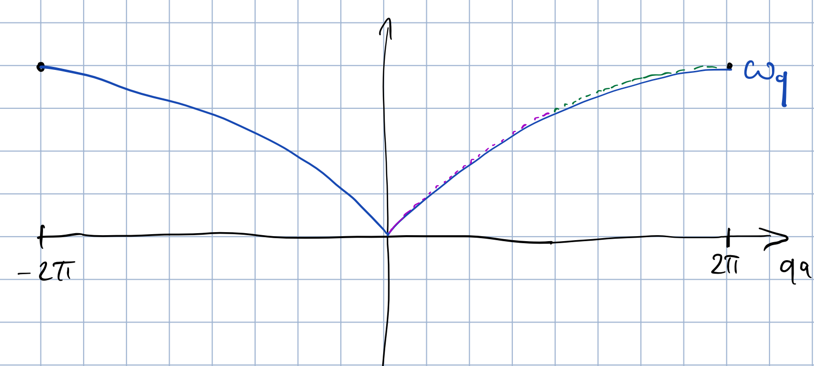
$$\omega_q^2 = \frac{2\kappa}{m}\left(1 \pm \left(\cos^2\frac{qa}{4} - \sin^2\frac{qa}{4}\right)\right)$$

Recall that (see the lecture) we should recover $\omega_q^2 = 4\frac{\kappa}{m}\sin^2\frac{qa}{4}$ with $q \in \left]-\frac{\pi}{\frac{1}{2}a}, \frac{\pi}{\frac{1}{2}a}\right]$

- $\omega_{q-}^2 = \frac{2\kappa}{m}\left(1-\cos^2\frac{qa}{4} + \sin^2\frac{qa}{4}\right) = 4\frac{\kappa}{m}\sin^2\frac{qa}{4}$
- $\omega_{q+}^2 = \frac{2\kappa}{m}\left(1+\cos^2\frac{qa}{4} - \sin^2\frac{qa}{2}\right) = \frac{4\kappa}{m}\cos^2\frac{qa}{4}$

Compare:

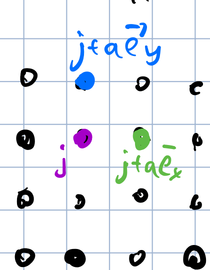




For $|qa| < \pi$ ω_{q-} coincides with ω_q. For $|qa| \in [\pi, 2\pi]$ we obtain a unique correspondence between ω_q and ω_{q+}.

(2)

$$\hat{H} = \sum_j \frac{\vec{p}_j^{\,2}}{2m} + \sum_{j,\vec{\alpha}} \frac{m\omega_0^2}{2}\left(\phi_j - \phi_{j+\vec{\alpha}}\right)^2$$



We will use the diagonalization procedure by Fourier transform.