Sound waves – several atoms per unit cell

From the total potential energy $U_{\text{tot}} = \frac{1}{2}\sum_{\mathbf{ij}\,ab} \vec{u}_{\mathbf{i}}^{a} C_{\mathbf{ij}}^{ab} \vec{u}_{\mathbf{j}}^{b}$ we obtain the equation of motion $m_a \ddot{\vec{u}}_{\mathbf{i}}^{a} = -\sum_{\mathbf{j}\,b} C_{\mathbf{ij}}^{ab} \vec{u}_{\mathbf{j}}^{b}$

The plane wave $\vec{u}_{\mathbf{i}}^{a}(t) = \vec{\tilde{u}}_{\mathbf{k}}^{a} e^{i(\mathbf{k}\cdot\mathbf{i}-\omega t)}$ is a solution of the above equation of motion if ω and $\vec{\tilde{u}}_{\mathbf{k}}^{a}$ satisfy

$$\sum_b \tilde{C}_{\mathbf{k}}^{ab} \vec{\tilde{u}}_{\mathbf{k}}^{b} = \omega^2 m_a \vec{\tilde{u}}_{\mathbf{k}}^{a}$$

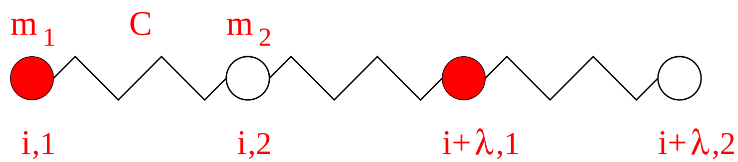
$$\text{or} \quad \sum_b \left(\frac{1}{\sqrt{m_a}} \tilde{C}_{\mathbf{k}}^{ab} \frac{1}{\sqrt{m_b}} \right) \left(\sqrt{m_b}\, \vec{\tilde{u}}_{\mathbf{k}} \right) = \omega^2 \left(\sqrt{m_a}\, \vec{\tilde{u}}_{\mathbf{k}}^{a} \right)$$

where the matrix $\tilde{C}_{\mathbf{k}}^{ab}$ is given by

$$\tilde{C}_{\mathbf{k}}^{ab} = \sum_{\mathbf{j}} C_{\mathbf{ij}}^{ab} e^{-i(\mathbf{i}-\mathbf{j})\cdot\mathbf{k}}$$

The eigenvalues of $\left(\frac{1}{\sqrt{m_a}} \tilde{C}_{\mathbf{k}}^{ab} \frac{1}{\sqrt{m_b}} \right)$ determines ω^2.

A 1D model



Calculate 2×2 **matrices** $\left(C_{ij}^{ab}\right)$

$$U_{\text{tot}} = \frac{1}{2}\sum_{ij,ab} u_i^a C_{ij}^{ab} u_j^b = \frac{1}{2}\sum_{i,ab} u_i^a C_{ii}^{ab} u_i^b + \sum_{i<j,ab} u_i^a C_{ij}^{ab} u_j^b$$

- Spring $(i,1;i,2)$:

$$\frac{1}{2}C(u_i^1 - u_i^2)^2$$

- Spring $(i,2;i+\lambda,1)$:

$$\frac{1}{2}C(u_i^2 - u_{i+\lambda}^1)^2 = \frac{C}{2}(u_i^2)^2 + \frac{C}{2}(u_{i+\lambda}^1)^2 - C_1 u_i^2 u_{i+\lambda}^2$$

Collect terms:

- $\left(C^{ab}_{ii}\right)$: $\frac{1}{2}C(u^1_i - u^2_i)^2 + \frac{C}{2}(u^2_i)^2 + \frac{C}{2}(u^1_i)^2 = \frac{1}{2}\begin{pmatrix} u^1_i & u^2_i \end{pmatrix}\left(C^{ab}_{ii}\right)\begin{pmatrix} u^1_i \\ u^2_i \end{pmatrix}$

$$\left(C^{ab}_{ii}\right) = C\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

- $\left(C^{ab}_{i,i+\lambda}\right)$: $-Cu^2_i u^1_{i+\lambda} = \begin{pmatrix} u^1_i & u^2_i \end{pmatrix}\left(C^{ab}_{i,i+\lambda}\right)\begin{pmatrix} u^1_i \\ u^2_i \end{pmatrix}$

$$\left(C^{ab}_{i,i+\lambda}\right) = -C\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

- $\left(C^{ab}_{i,i-\lambda}\right)$: $C^{ab}_{ij} = C^{ab}_{i+\lambda,j+\lambda}, \quad C^{ba}_{ji} = C^{ab}_{ij} \longrightarrow$

$$\left(C^{ab}_{i,i-\lambda}\right) = -C\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Calculate 2×2 **matrix** $\tilde{C}_k^{ab} = \sum_j C_{ij}^{ab} e^{-\mathbf{i}(i-j)k}$:

$$\tilde{C}_k^{ab} = C_{ii}^{ab} + C_{i,i+\lambda}^{ab} e^{ik\lambda} + C_{i,i-\lambda}^{ab} e^{-ik\lambda}$$

$$\left(\tilde{C}_k^{ab}\right) = C \begin{pmatrix} 2 & -1 - e^{\mathrm{i}k\lambda} \\ -1 - e^{-\mathrm{i}k\lambda} & 2 \end{pmatrix}$$

2×2 **matrix**

$$\left(\frac{1}{\sqrt{m_a}} \tilde{C}_k^{ab} \frac{1}{\sqrt{m_b}}\right) = C \begin{pmatrix} \frac{2}{m_1} & \frac{-1-e^{\mathrm{i}k\lambda}}{\sqrt{m_1 m_2}} \\ \frac{-1-e^{-\mathrm{i}k\lambda}}{\sqrt{m_1 m_2}} & \frac{2}{m_1} \end{pmatrix} =$$

$$C\left[\frac{1}{m_1} + \frac{1}{m_2} + \left(\frac{1}{m_1} - \frac{1}{m_2}\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{1+\cos k\lambda}{\sqrt{m_1 m_2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{\sin k\lambda}{\sqrt{m_1 m_2}} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}\right.$$

The eigenvalues of the above matrix gives ω^2:

$$\omega^2 = C\left[\frac{1}{m_1} + \frac{1}{m_2} \pm \sqrt{\left(\frac{1}{m_1}\right)^2 + \left(\frac{1}{m_2}\right)^2 + \frac{2\cos k\lambda}{m_1 m_2}}\ \right]$$