Sound waves in lattice

From the total potential energy

$$U_{\text{tot}} = \frac{1}{2} \sum_{\mathbf{ij}} \vec{u}_{\mathbf{i}} C_{\mathbf{ij}} \vec{u}_{\mathbf{j}}$$

we obtain the equation of motion

$$m \ddot{\vec{u}}_{\mathbf{i}} = - \sum_{\mathbf{j}} C_{\mathbf{ij}} \vec{u}_{\mathbf{j}}$$

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

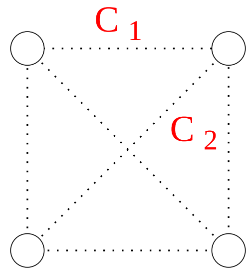
$$\tilde{C}_{\mathbf{k}} \ \vec{\tilde{u}}_{\mathbf{k}} = m\omega^2 \ \vec{\tilde{u}}_{\mathbf{k}}$$

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

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

The eigenvalues of $\tilde{C}_{\mathbf{k}}$ determines $m\omega^2$.

Spring-bead model of a square lattice



Calculate 2×2 **matrices** $C_{\mathbf{ij}}$

$$U_{\text{tot}} = \frac{1}{2}\sum_{\mathbf{ij}} \vec{u}_{\mathbf{i}} C_{\mathbf{ij}} \vec{u}_{\mathbf{j}} = \frac{1}{2}\sum_{\mathbf{i}} \vec{u}_{\mathbf{i}} C_{\mathbf{ii}} \vec{u}_{\mathbf{i}} + \sum_{\mathbf{i}<\mathbf{j}} \vec{u}_{\mathbf{i}} C_{\mathbf{ij}} \vec{u}_{\mathbf{j}}$$

- Link $(\mathbf{i}, \mathbf{i}+\mathbf{x})$:

$$\frac{1}{2}C_1[(\vec{u}_{\mathbf{i}} - \vec{u}_{\mathbf{i}+\mathbf{x}}) \cdot \mathbf{x}]^2 = \frac{1}{2}C_1(u^x_{\mathbf{i}} - u^x_{\mathbf{i}+\mathbf{x}})^2 = \frac{C_1}{2}(u^x_{\mathbf{i}})^2 + \frac{C_1}{2}(u^x_{\mathbf{i}+\mathbf{x}})^2 - C_1 u^x_{\mathbf{i}} u^x_{\mathbf{i}+\mathbf{x}}$$

- Link $(\mathbf{i}, \mathbf{i}+\mathbf{y})$:

$$\frac{1}{2}C_1[(\vec{u}_{\mathbf{i}} - \vec{u}_{\mathbf{i}+\mathbf{y}}) \cdot \mathbf{y}]^2 = \frac{C_1}{2}(u^y_{\mathbf{i}})^2 + \frac{C_1}{2}(u^y_{\mathbf{i}+\mathbf{y}})^2 - C_1 u^y_{\mathbf{i}} u^y_{\mathbf{i}+\mathbf{y}}$$

- Link $(\mathbf{i}, \mathbf{i}+\mathbf{x}+\mathbf{y})$:

$$\frac{1}{2}C_2[(\vec{u}_{\mathbf{i}} - \vec{u}_{\mathbf{i+x+y}}) \cdot \frac{\mathbf{x}+\mathbf{y}}{\sqrt{2}}]^2 = \frac{C_2}{4}(u^x_{\mathbf{i}} + u^y_{\mathbf{i}} - u^x_{\mathbf{i+x+y}} - u^y_{\mathbf{i+x+y}})^2$$
$$= \frac{C_2}{4}(u^x_{\mathbf{i}} + u^y_{\mathbf{i}})^2 + \frac{C_2}{4}(u^x_{\mathbf{i+x+y}} + u^y_{\mathbf{i+x+y}})^2$$
$$- \frac{C_2}{2}(u^x_{\mathbf{i}} + u^y_{\mathbf{i}})(u^x_{\mathbf{i+x+y}} + u^y_{\mathbf{i+x+y}})$$

- Link $(\mathbf{i}, \mathbf{i}+\mathbf{x}-\mathbf{y})$:

$$\frac{1}{2}C_2[(\vec{u}_{\mathbf{i}} - \vec{u}_{\mathbf{i+x-y}}) \cdot \frac{\mathbf{x}-\mathbf{y}}{\sqrt{2}}]^2 = \frac{C_2}{4}(u^x_{\mathbf{i}} - u^y_{\mathbf{i}} - u^x_{\mathbf{i+x-y}} + u^y_{\mathbf{i+x-y}})^2$$
$$= \frac{C_2}{4}(u^x_{\mathbf{i}} - u^y_{\mathbf{i}})^2 + \frac{C_2}{4}(u^x_{\mathbf{i+x-y}} - u^y_{\mathbf{i+x-y}})^2$$
$$- \frac{C_2}{2}(u^x_{\mathbf{i}} - u^y_{\mathbf{i}})(u^x_{\mathbf{i+x-y}} - u^y_{\mathbf{i+x-y}})$$

Collect terms:

- $C_{\mathbf{ii}}$:

$$
\begin{aligned}
&\frac{C_1}{2}(u_{\mathbf{i}}^x)^2|_{(\mathbf{i},\mathbf{i}+\mathbf{x})} + \frac{C_1}{2}(u_{\mathbf{i}}^x)^2|_{(\mathbf{i},\mathbf{i}-\mathbf{x})} + \frac{C_1}{2}(u_{\mathbf{i}}^y)^2|_{(\mathbf{i},\mathbf{i}+\mathbf{y})} + \frac{C_1}{2}(u_{\mathbf{i}}^y)^2|_{(\mathbf{i},\mathbf{i}-\mathbf{y})}\\
&+\frac{C_2}{4}(u_{\mathbf{i}}^x + u_{\mathbf{i}}^y)^2|_{(\mathbf{i},\mathbf{i}+\mathbf{x}+\mathbf{y})} + \frac{C_2}{4}(u_{\mathbf{i}}^x + u_{\mathbf{i}}^y)^2|_{(\mathbf{i},\mathbf{i}-\mathbf{x}-\mathbf{y})}\\
&+\frac{C_2}{4}(u_{\mathbf{i}}^x - u_{\mathbf{i}}^y)^2|_{(\mathbf{i},\mathbf{i}+\mathbf{x}-\mathbf{y})} + \frac{C_2}{4}(u_{\mathbf{i}}^x - u_{\mathbf{i}}^y)^2|_{(\mathbf{i},\mathbf{i}-\mathbf{x}+\mathbf{y})}\\
&=(C_1 + C_2)[(u_{\mathbf{i}}^x)^2 + (u_{\mathbf{i}}^y)^2] = \frac{1}{2}\begin{pmatrix} u_{\mathbf{i}}^x & u_{\mathbf{i}}^y \end{pmatrix} C_{\mathbf{ii}} \begin{pmatrix} u_{\mathbf{i}}^x \\ u_{\mathbf{i}}^y \end{pmatrix}
\end{aligned}
$$

$$
C_{\mathbf{ii}} = 2(C_1 + C_2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
$$

- $C_{\mathbf{i},\mathbf{i}+\mathbf{x}}$: $-C_1 u^x_{\mathbf{i}} u^x_{\mathbf{i}+\mathbf{x}} = \begin{pmatrix} u^x_{\mathbf{i}} & u^y_{\mathbf{i}} \end{pmatrix} C_{\mathbf{i},\mathbf{i}+\mathbf{x}} \begin{pmatrix} u^x_{\mathbf{i}+\mathbf{x}} \\ u^y_{\mathbf{i}+\mathbf{x}} \end{pmatrix} \longrightarrow C_{\mathbf{i},\mathbf{i}+\mathbf{x}} = -C_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

- $C_{\mathbf{i},\mathbf{i}+\mathbf{y}}$: $-C_1 u^y_{\mathbf{i}} u^y_{\mathbf{i}+\mathbf{y}} = \begin{pmatrix} u^x_{\mathbf{i}} & u^y_{\mathbf{i}} \end{pmatrix} C_{\mathbf{i},\mathbf{i}+\mathbf{y}} \begin{pmatrix} u^x_{\mathbf{i}+\mathbf{y}} \\ u^y_{\mathbf{i}+\mathbf{y}} \end{pmatrix} \longrightarrow C_{\mathbf{i},\mathbf{i}+\mathbf{y}} = -C_1 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

- $C_{\mathbf{i},\mathbf{i}+\mathbf{x}+\mathbf{y}}$:

$$-\frac{C_2}{2}(u^x_{\mathbf{i}} + u^y_{\mathbf{i}})(u^x_{\mathbf{i}+\mathbf{x}+\mathbf{y}} + u^y_{\mathbf{i}+\mathbf{x}+\mathbf{y}}) = \begin{pmatrix} u^x_{\mathbf{i}} & u^y_{\mathbf{i}} \end{pmatrix} C_{\mathbf{i},\mathbf{i}+\mathbf{x}+\mathbf{y}} \begin{pmatrix} u^x_{\mathbf{i}+\mathbf{x}+\mathbf{y}} \\ u^y_{\mathbf{i}+\mathbf{x}+\mathbf{y}} \end{pmatrix}$$

$$C_{\mathbf{i},\mathbf{i}+\mathbf{x}+\mathbf{y}} = -\frac{C_2}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

- $C_{\mathbf{i},\mathbf{i}+\mathbf{x}-\mathbf{y}}$:

$$-\frac{C_2}{2}(u^x_{\mathbf{i}} - u^y_{\mathbf{i}})(u^x_{\mathbf{i}+\mathbf{x}-\mathbf{y}} - u^y_{\mathbf{i}+\mathbf{x}-\mathbf{y}}) = \begin{pmatrix} u^x_{\mathbf{i}} & u^y_{\mathbf{i}} \end{pmatrix} C_{\mathbf{i},\mathbf{i}+\mathbf{x}-\mathbf{y}} \begin{pmatrix} u^x_{\mathbf{i}+\mathbf{x}-\mathbf{y}} \\ u^y_{\mathbf{i}+\mathbf{x}-\mathbf{y}} \end{pmatrix}$$

$$C_{\mathbf{i},\mathbf{i}+\mathbf{x}-\mathbf{y}} = -\frac{C_2}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} C_{\mathbf{i,i-x+y}} & C_{\mathbf{i,i+y}} & C_{\mathbf{i,i+x+y}} \\ C_{\mathbf{i,i-x}} & C_{\mathbf{i,i}} & C_{\mathbf{i,i+x}} \\ C_{\mathbf{i,i-x-y}} & C_{\mathbf{i,i-y}} & C_{\mathbf{i,i+x-y}} \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{C_2}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} & -C_1\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & -\frac{C_2}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ -C_1\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & 2(C_1 + C_2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & -C_1\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ -\frac{C_2}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} & -C_1\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & -\frac{C_2}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \end{pmatrix}$$

$C_{\mathbf{ij}}$ Satisfies

$$\sum_{\mathbf{j}} C_{\mathbf{ij}} = 0$$

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

$$
\begin{aligned}
\tilde{C}_{\mathbf{k}} &= C_{\mathbf{ii}} + C_{\mathbf{i},\mathbf{i}+\mathbf{x}} e^{ik_x} + C_{\mathbf{i},\mathbf{i}-\mathbf{x}} e^{-ik_x} + \cdots \\
&= C_{\mathbf{ii}} + 2C_{\mathbf{i},\mathbf{i}+\mathbf{x}} \cos k_x + 2C_{\mathbf{i},\mathbf{i}+\mathbf{y}} \cos k_y + 2C_{\mathbf{i},\mathbf{i}+\mathbf{x}+\mathbf{y}} \cos(k_x + k_y) \\
&\qquad + 2C_{\mathbf{i},\mathbf{i}+\mathbf{x}-\mathbf{y}} \cos(k_x - k_y) \\
&= \begin{pmatrix} a & c \\ c & b \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
a &= 2C_1(1 - \cos k_x) + C_2[2 - \cos(k_x + k_y) - \cos(k_x - k_y)] \\
b &= 2C_1(1 - \cos k_y) + C_2[2 - \cos(k_x + k_y) - \cos(k_x - k_y)] \\
c &= C_2[-\cos(k_x + k_y) + \cos(k_x - k_y)]
\end{aligned}
$$

- Eigenvalues of $\tilde{C}_{\mathbf{k}}$ give rise to $m\omega^2$

$$
\omega = \frac{1}{\sqrt{m}} \sqrt{\frac{a+b}{2} \pm \sqrt{\left(\frac{a-b}{2}\right)^2 + c^2}}
$$