Vibrations and waves: exercise sheet 7

Long chain with two atoms in the unit cell

Picture a long one-dimensional crystal with two atoms in the unit cell, A and B, of masses m_A and m_B. Call the repeat distance a. Imagine there is a spring force labelled J between both atoms and in both directions.

Write the equation for the energy of both atoms in unit cell labelled j, in terms of displacements u_j^A and u_j^B .

$$E_j^A = \frac{1}{2}J\left(u_j^A - u_j^B\right)^2 + \frac{1}{2}J\left(u_j^A - u_{j-1}^B\right)^2$$
$$E_j^B = \frac{1}{2}J\left(u_j^B - u_j^A\right)^2 + \frac{1}{2}J\left(u_j^B - u_{j+1}^A\right)^2$$

Using standard methods, convert the energy to forces.

$$F_j^A = -\frac{dE_j^A}{du_j^A} = -J\left(u_j^A - u_j^B\right) - J\left(u_j^A - u_{j-1}^B\right) = -J\left(2u_j^A - u_j^B - u_{j-1}^B\right)$$
$$F_j^B = -\frac{dE_j^B}{du_j^B} = -J\left(u_j^B - u_j^A\right) - J\left(u_j^B - u_{j+1}^A\right) = -J\left(2u_j^B - u_j^A - u_{j+1}^A\right)$$

Assume solutions of the form

$$u_j^A = A\exp\left(i(kx - \omega t)\right)$$
$$u_j^B = B\exp\left(i(kx - \omega t)\right)$$

And write the relevant equations of motion. Note that x for unit cell j can be written as j times the repeat distance a, and recall that the idea is to compute the force via the negative derivative of the potential energy, and then equate to acceleration. Divide through by mass. Substitute in the solution and divide through by common factors.

$$-J\left(2u_j^{\mathrm{A}}-u_j^{\mathrm{B}}-u_{j-1}^{\mathrm{B}}\right)=m_{\mathrm{A}}\ddot{u}_j^{\mathrm{A}}=-m_{\mathrm{A}}\omega^2u_j^{\mathrm{A}}$$
$$-J\left(2u_j^{\mathrm{B}}-u_j^{\mathrm{A}}-u_{j+1}^{\mathrm{A}}\right)=m_{\mathrm{B}}\ddot{u}_j^{\mathrm{B}}=-m_{\mathrm{B}}\omega^2u_j^{\mathrm{B}}$$
$$u_{j+1}^{\mathrm{A}}=\exp(+ika)u_j^{\mathrm{A}}$$
$$u_{j-1}^{\mathrm{B}}=\exp(-ika)u_j^{\mathrm{B}}$$
$$-J\left(2u_j^{\mathrm{A}}-u_j^{\mathrm{B}}-u_{j-1}^{\mathrm{B}}\right)=-J\left(2u_j^{\mathrm{A}}-u_j^{\mathrm{B}}\left(1+\exp(-ika)\right)\right)=-m_{\mathrm{A}}\omega^2u_j^{\mathrm{A}}$$
$$-J\left(2u_j^{\mathrm{B}}-u_j^{\mathrm{A}}-u_{j+1}^{\mathrm{A}}\right)=-J\left(2u_j^{\mathrm{B}}-u_j^{\mathrm{A}}\left(1+\exp(+ika)\right)\right)=-m_{\mathrm{B}}\omega^2u_j^{\mathrm{B}}$$
$$\frac{J}{m_{\mathrm{A}}}\left(2A-B\left(1+\exp(-ika)\right)\right)-\omega^2A=0$$
$$\frac{J}{m_{\mathrm{B}}}\left(2B-A\left(1+\exp(+ika)\right)\right)-\omega^2B=0$$
$$\Rightarrow\begin{pmatrix}\frac{2J}{m_{\mathrm{A}}}-\omega^2 & -\frac{J}{m_{\mathrm{A}}}\left(1+\exp(-ika)\right)\\ -\frac{J}{m_{\mathrm{B}}}\left(1+\exp(+ika)\right) & \frac{2J}{m_{\mathrm{B}}}-\omega^2\end{pmatrix}\cdot\begin{pmatrix}A\\ B\end{pmatrix}=0$$

You should end up with a matrix equation that looks something like:

$$\begin{pmatrix}\frac{2J}{m_{\mathrm{A}}}-\omega^2 & -\frac{J}{m_{\mathrm{A}}}\left(1+\exp(-ika)\right)\\ -\frac{J}{m_{\mathrm{B}}}\left(1+\exp(+ika)\right) & \frac{2J}{m_{\mathrm{B}}}-\omega^2\end{pmatrix}\cdot\begin{pmatrix}A\\ B\end{pmatrix}=0$$

First take the case k = 0. Show that the two solutions are

$$\omega^2=\begin{cases}0\\ 2J\left(\frac{1}{m_{\mathrm{A}}}+\frac{1}{m_{\mathrm{B}}}\right)\end{cases}$$

$$\begin{pmatrix} \dfrac{2J}{m_A}-\omega^2 & -\dfrac{2J}{m_A} \\ -\dfrac{2J}{m_B} & \dfrac{2J}{m_B}-\omega^2 \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

$$\begin{vmatrix} \dfrac{2J}{m_A}-\omega^2 & -\dfrac{2J}{m_A} \\ -\dfrac{2J}{m_B} & \dfrac{2J}{m_B}-\omega^2 \end{vmatrix} = 0 = \left(\frac{2J}{m_A}-\omega^2\right)\left(\frac{2J}{m_B}-\omega^2\right) - \frac{4J^2}{m_A m_B} = 0$$

$$= \frac{4J^2}{m_A m_B} - \left(\frac{2J}{m_A}+\frac{2J}{m_B}\right)\omega^2 + \omega^4 - \frac{4J^2}{m_A m_B}$$

$$= \omega^4 - \left(\frac{2J}{m_A}+\frac{2J}{m_B}\right)\omega^2 = 0$$

$$\Rightarrow \omega^2 = \begin{cases} 0 \\ 2J\left(\dfrac{1}{m_A}+\dfrac{1}{m_B}\right) \end{cases}$$

Show that for the first of these, $A = B$, and for the second, show that $Am_A = -Bm_B$.

$$\begin{pmatrix} \dfrac{2J}{m_A}-0 & -\dfrac{2J}{m_A} \\ -\dfrac{2J}{m_B} & \dfrac{2J}{m_B}-0 \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix} = 0 = \begin{pmatrix} \dfrac{2J}{m_A}A - \dfrac{2J}{m_A}B \\ \dfrac{2J}{m_B}B - \dfrac{2J}{m_B}A \end{pmatrix} \Rightarrow A = B$$

$$\begin{pmatrix} \dfrac{2J}{m_A}-2J\left(\dfrac{1}{m_A}+\dfrac{1}{m_B}\right) & -\dfrac{2J}{m_A} \\ -\dfrac{2J}{m_B} & \dfrac{2J}{m_B}-2J\left(\dfrac{1}{m_A}+\dfrac{1}{m_B}\right) \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix} = 0 = \begin{pmatrix} -\dfrac{2J}{m_B}A - \dfrac{2J}{m_A}B \\ -\dfrac{2J}{m_B}A - \dfrac{2J}{m_A}B \end{pmatrix} \Rightarrow Am_A = -Bm_B$$

Now try the case $k = \pi / a$, namely the wave length of the wave is twice the unit cell length. Show that the solutions are

$$\omega^2 = \begin{cases} \dfrac{2J}{m_A} \\ \dfrac{2J}{m_B} \end{cases}$$

$$\begin{pmatrix} \frac{2J}{m_A}-\omega^2 & -\frac{J}{m_A}(1-1) \\ -\frac{J}{m_B}(1-1) & \frac{2J}{m_B}-\omega^2 \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix} = 0 = \begin{pmatrix} \frac{2J}{m_A}-\omega^2 & 0 \\ 0 & \frac{2J}{m_B}-\omega^2 \end{pmatrix} \cdot \begin{pmatrix} A \\ B \end{pmatrix}$$

The result follows automatically.

Sketch the full graph. Identify what we called the acoustic and optic modes in the lecture.