PHYS 143 Discussion Week 2 - Diatomic 1-D Crystal

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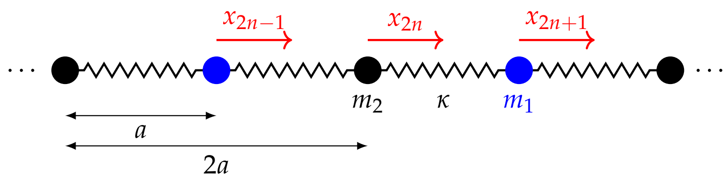
Problem Statement



Consider a 1-D chain of atoms, alternating between mass m_1 (odds) and mass $m_2 > m_1$ (evens), connected by springs of spring constant κ, with equilibrium spacing a (This is a toy-model for diatomic crystals, for example NaCl). Denote by x_i the displacement of mass i from equilibrium.

(a) Use Newton's law to write down the equation of motion for atom $i = 2n$ as a function of $x_{2n-1}, x_{2n}, x_{2n+1}$. Do the same for atom $i = 2n+1$. Then write down the entire system of equations of motion in matrix form:

$$\mathbb{M}\ddot{\mathbf{x}} = -\mathbb{K}\mathbf{x} \tag{0.1}$$

where $\mathbf{x} = (x_1(t), x_2(t), x_3(t), \ldots)^T$.

(b) Consider the travelling wave ansatz:

$$x_{2n}(t) = A_k \exp(i(2nka - \omega t)) \tag{0.2}$$

$$x_{2n+1}(t) = B_k \exp(i(2nka - \omega t)) \tag{0.3}$$

with $k = 2\pi/\kappa$ the wavevector(number). Substitute this into your result from (a) to obtain a system of equations for A_k, B_k.

(c) Use the result from (b) and solve for the normal mode frequencies $\omega_\pm$ of the system (as a function k), and sketch them for $-\frac{\pi}{2a} < k < \frac{\pi}{2a}$ (this is the so-called "First Bruillion Zone" - since the ωs are periodic, it suffices to look at their behaviour in this one region). The lower band of modes with frequency ω_- are called "acoustic" modes, while the upper bound of modes with frequency ω_+ are called "optical" modes. How large is the frequency gap between the two bands, and what is the interpretation of this gap?

(d) Let's try to get a bit more intuition for the acoustic mode dispersion - consider it in the limit where $ka \ll a$. You should recover the dispersion equation of the continuum wave equation. To make the connection more concrete, derive the wave equation from masses m connected by springs.

(e) Let's get more intuition for the normal mode motion in certain limits for the two bands. Calculate $\begin{pmatrix} A_k \\ B_k \end{pmatrix}$ for both the acoustic/optical modes for $ka = 0$ and comment on the result. Also, calculate $\begin{pmatrix} A_k \\ B_k \end{pmatrix}$ for both the acoustic/optical modes for $ka = \pm\frac{\pi}{2}$ and comment on the result.

Solution

(a) Using Hooke's Law, we can write down the equation of motion for the even/odd (light/heavy) atoms:

$$m_2\ddot{x}_{2n} = -\kappa(x_{2n} - x_{2n-1}) - k(x_{2n} - x_{2n+1}) \implies m_2\ddot{x}_{2n} = -\kappa\left(-x_{2n-1} - x_{2n+1} + 2x_{2n}\right) \tag{0.4}$$

$$m_1\ddot{x}_{2n+1} = -\kappa(x_{2n+1} - x_{2n}) - \kappa(x_{2n+1} - x_{2n+2}) \implies m_1\ddot{x}_{2n} = -\kappa\left(-x_{2n} - x_{2n+2} + 2x_{2n+1}\right) \tag{0.5}$$

In matrix form:

$$\begin{pmatrix} m_1 & & & \\ & m_2 & & \\ & & m_1 & \\ & & & \ddots \end{pmatrix} \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \vdots \end{pmatrix} = -\kappa \begin{pmatrix} 2 & -1 & 0 & 0 & \dots \\ -1 & 2 & -1 & 0 & \dots \\ 0 & -1 & 2 & -1 & \dots \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix} \tag{0.6}$$

(b) Plugging in the ansatz into the differential equations from (a):

$$\begin{aligned} &-\omega^2 m_2 A_k \exp(i(2nka - \omega t)) \\ &= -\kappa(-B_k \exp(i(2(n-1)ka - \omega t)) - B_k \exp(i(2nka - \omega t)) + 2A_k \exp(i(2nka - \omega t))) \end{aligned} \tag{0.7}$$

$$\begin{aligned} &-\omega^2 m_1 B_k \exp(i(2nka - \omega t)) \\ &= -\kappa(-A_k \exp(i(2nka - \omega t)) - A_k \exp(i(2(n+1)ka - \omega t)) + 2B_k \exp(i(2nka - \omega t))) \end{aligned} \tag{0.8}$$

Cancelling out the $\exp(i(2nka - \omega t))$ from both sides:

$$-\omega^2 m_2 A_k = -\kappa(-B_k \exp(-2ika) - B_k + 2A_k) \tag{0.9}$$

$$-\omega^2 m_1 B_k = -\kappa(-A_k - A_k \exp(2ika) + 2B_k) \tag{0.10}$$

We can write this in matrix form:

$$\begin{pmatrix} \omega^2 m_2 - 2\kappa & \kappa(1 + \exp(-2ika)) \\ \kappa(1 + \exp(2ika)) & \omega^2 m_1 - 2\kappa \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{0.11}$$

(c) We can set the determinant of the above matrix to zero to find the normal mode frequencies:

$$\det \begin{pmatrix} \omega^2 m_2 - 2\kappa & \kappa(1 + \exp(-2ika)) \\ \kappa(1 + \exp(2ika)) & \omega^2 m_1 - 2\kappa \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{0.12}$$

Which yields:

$$\begin{aligned} m_1 m_2 \omega^4 - 2\kappa(m_1 + m_2)\omega^2 + 4\kappa^2 - \kappa^2(1 + \exp(-2ika))(1 + \exp(2ika)) = 0 \\ \implies m_1 m_2 \omega^4 - 2\kappa(m_1 + m_2)\omega^2 + 2\kappa^2(1 - \cos(2ka)) = 0 \end{aligned} \tag{0.13}$$

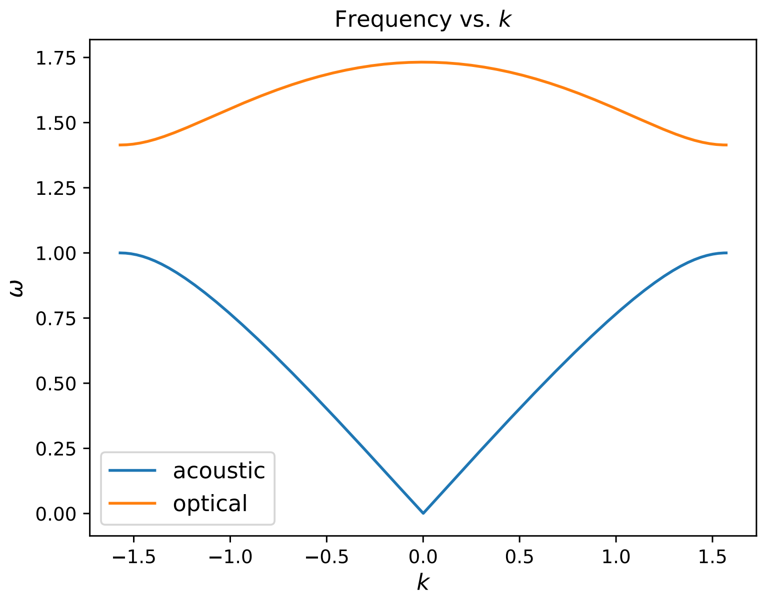
Which is a quadratic equation in ω^2:

$$\begin{aligned} \omega_\pm^2 &= \frac{2\kappa(m_1 + m_2) \pm \sqrt{4\kappa^2(m_1 + m_2)^2 - 4m_1 m_2(2\kappa^2(1 - \cos(2ka)))}}{2m_1 m_2} \\ &= \frac{\kappa}{m_1 m_2}\left((m_1 + m_2) \pm \sqrt{(m_1 + m_2)^2 - 2m_1 m_2(1 - (1 - 2\sin^2(ka)))}\right) \\ &= \frac{\kappa}{m_1 m_2}\left((m_1 + m_2) \pm \sqrt{(m_1 + m_2)^2 - 4m_1 m_2 \sin^2(ka)}\right) \\ &= \frac{\kappa(m_1 + m_2)}{m_1 m_2}\left(1 \pm \sqrt{1 - \frac{4m_1 m_2}{(m_1 + m_2)^2}\sin^2(ka)}\right) \end{aligned} \tag{0.14}$$

Frequencies are positive and so taking the positive square root:

$$\omega_{\pm} = \sqrt{\frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 \pm \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2(ka)}\right)} \tag{0.15}$$

Sketching (taking $m_2 = a = \kappa = 1, m_1 = 2$) for $k \in [-\frac{\pi}{a}, \frac{\pi}{a})$:



The difference in frequency between the two bands we can evaluate at $k = \frac{\pi}{2a}$:

$$\begin{aligned}\Delta\omega = \omega_+ - \omega_- &= \sqrt{\frac{\kappa(m_+1+m_2)}{m_1m_2}}\left[\sqrt{1+\sqrt{1-\frac{4m_1m_2}{(m_1+m_2)^2}}} - \sqrt{1-\sqrt{1-\frac{4m_1m_2}{(m_1+m_2)^2}}}\right] \\ &= \sqrt{2\kappa}\left|\frac{1}{\sqrt{m_1}} - \frac{1}{\sqrt{m_2}}\right|\end{aligned} \tag{0.16}$$

the interpretation of the gap is that there are no sound waves in the material which can take frequency values in the gap.

Comment: Much like photons are “quanta” of the electromagnetic field, phonons are “quanta” of vibrations/sound (with the field the elastic medium). Therein, the energies of the photons are given by $E = \hbar\omega$ where ω are the frequencies you found above. This tells us that phonon energies appear in bands, with a gap.

(d) Looking at the acoustic band dispersion:

$$\omega_{-} = \sqrt{\frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 - \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2(ka)}\right)} \tag{0.17}$$

For $ka \ll 1$ this becomes:

$$\begin{aligned}
\omega_- &\approx \sqrt{\frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1-\sqrt{1-\frac{4m_1m_2}{(m_1+m_2)^2}(ka)^2}\right)} \\
&\approx \sqrt{\frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1-\left(1-\frac{1}{2}\frac{4m_1m_2}{(m_1+m_2)^2}(ka)^2\right)\right)} \\
&= \sqrt{\frac{2\kappa a^2}{m_1+m_2}}k
\end{aligned} \tag{0.18}$$

This looks like the wave equation dispersion:

$$\omega = ck \tag{0.19}$$

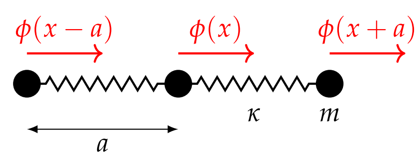
with wave speed:

$$c^2 = \frac{2\kappa a^2}{m_1+m_2} \tag{0.20}$$

For N masses, we have total mass $\frac{m_1+m_2}{2}N$, total spring constant $K = \frac{\kappa}{N}$, and total length $L = aN$, so:

$$c^2 = \frac{KL^2}{M} \tag{0.21}$$

To make the connection more concrete - we consider the same setup, just with all masses the same m:



$\phi(x)$ measures the distance from equilibrium of a mass situated at position x. The force on mass m at $x+a$ is (as we derived before):

$$F_{\text{Hooke}} = F_{x+a} + F_{x-a} = \kappa[\phi(x+a,t) - 2\phi(x,t) + \phi(x-a,t)] \tag{0.22}$$

and Newton's Law says:

$$F_{\text{Newton}} = m\frac{\partial^2}{\partial t^2}\phi(x,t) \tag{0.23}$$

So:

$$\frac{\partial^2}{\partial t^2}\phi(x,t) = \frac{\kappa}{m}[\phi(x+a,t) - 2\phi(x,t) + \phi(x-a,t)] \tag{0.24}$$

If we have N weights with total length $L = Na$, total mass $M = Nm$, and total spring constant $K = \frac{\kappa}{N}$ (spring constants add as $\frac{1}{k_{\text{eq}}} = \sum_i \frac{1}{k_i}$), we can write:

$$\frac{\partial^2}{\partial t^2}\phi(x,t) = \frac{KL^2}{M}\frac{[\phi(x+a,t) - 2\phi(x,t) + \phi(x-a,t)]}{a^2} \tag{0.25}$$

Taking $N \to \infty, a \to 0$ we can recognize the RHS as a second derivative in space and so:

$$\frac{\partial^2\phi}{\partial t^2} = \frac{KL^2}{M}\frac{\partial^2\phi}{\partial x^2} \tag{0.26}$$

which is the wave equation with:

$$c^2 = \frac{KL^2}{M}. \tag{0.27}$$

So we get the same result as the $ka \ll 1$ limit of the discrete model!

(e) Back to the discrete model. Lets study the eigenvectors for $ka = 0$. For the acoustic mode, we have:

$$\omega_-^2 = \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 - \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2(0)}\right) = 0 \tag{0.28}$$

and so:

$$\begin{pmatrix} -2\kappa & 2\kappa \\ 2\kappa & -2\kappa \end{pmatrix}\begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{0.29}$$

which tells us that:

$$\begin{pmatrix} A_k \\ B_k \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{0.30}$$

and so $\frac{A_k}{B_k} \approx 1$ for $ka \ll 1$, i.e. the masses oscillate in phase for acoustic modes for $ka \ll 1$ (again as we would expect for sound waves).

For the optical modes, we have:

$$\omega_+^2 = \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 + \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2(0)}\right) = \frac{2\kappa(m_1+m_2)}{m_1 m_2} \tag{0.31}$$

so:

$$\begin{pmatrix} \frac{2\kappa(m_1+m_2)}{m_1m_2}m_2 - 2\kappa & 2\kappa \\ 2\kappa & \frac{2\kappa(m_1+m_2)}{m_1m_2}m_1 - 2\kappa \end{pmatrix}\begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{0.32}$$

from which we get:

$$\begin{pmatrix} A_k \\ B_k \end{pmatrix} = \begin{pmatrix} m_1 \\ -m_2 \end{pmatrix} \tag{0.33}$$

So for $ka \ll 1$, $\frac{A_k}{B_k} \approx -\frac{m_1}{m_2}$ and the atoms oscillate out of phase. This is where this mode gets the name "acoustic". When charged ions move out of phase in a crystal, this creates a time-varying dipole moment, so the vibrations of the lattice can emit or absorb radiation - hence optical!

Let's also study the dynamics when $ka = \pm\frac{\pi}{2}$ at the Bruillion zone boundary. There the frequencies look like:

$$\begin{aligned}
\omega_\pm^2 &= \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 \pm \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2(\frac{\pi}{2})}\right) \\
&= \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 \pm \frac{1}{m_1+m_2}\sqrt{(m_1+m_2)^2 - 4m_1m_2}\right) \\
&= \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 \pm \frac{1}{m_1+m_2}\sqrt{(m_1-m_2)^2}\right) \\
&= \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(1 \pm \frac{m_1-m_2}{m_1+m_2}\right) \\
&= \frac{\kappa(m_1+m_2)}{m_1 m_2}\left(\frac{m_1+m_2}{m_1+m_2} \pm \frac{m_1-m_2}{m_1+m_2}\right) \\
&= \frac{\kappa}{m_1 m_2}(m_1+m_2 \pm (m_1-m_2))
\end{aligned} \tag{0.34}$$

so:

$$\omega_+ = \frac{2\kappa}{m_2}, \quad \omega_- = \frac{2\kappa}{m_1} \tag{0.35}$$

For the acoustic mode:

$$\begin{pmatrix} \frac{2\kappa}{m_2}m_2 - 2\kappa & \kappa(1+\exp(-i\pi)) \\ \kappa(1+\exp(i\pi)) & \frac{2\kappa}{m_2}m_1 - 2\kappa \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 2\kappa(\frac{m_2}{m_1} - 1) \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{0.36}$$

so $A_k = 1, B_k = 0$ and so the even atoms oscillate while the odd ones stay fixed.
Then for the optical mode:

$$\begin{pmatrix} \frac{2\kappa}{m_1}m_2 - 2\kappa & \kappa(1+\exp(-i\pi)) \\ \kappa(1+\exp(i\pi)) & \frac{2\kappa}{m_1}m_1 - 2\kappa \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = \begin{pmatrix} 2\kappa(\frac{m_1}{m_2} - 1) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{0.37}$$

so $A_k = 0, B_k = 1$ and so the even atoms stay fixed while the odd ones stay fixed.

A nice visual + interactive graph for this problem can be found here.