**Diatomic chain:**

Hooke's Law: \( F = -\kappa \psi \) (one dimension) where \( \psi \) is the displacement from equilibrium. Constrain to longitudinal direction. Two masses and two springs per cell. The dark masses are larger \((M)\), the light ones small \((m)\). For simplicity, only one type of spring. Distance from cell to cell is \( a \), therefore interatomic distance is \( a/2 \). Many texts use \( a \) for interatomic distance, \( 2a \) for cell size.

Equilibrium position is \( x_n^0 = \frac{na}{2} \)

Actual position is \( x_n = \frac{na}{2} + \psi_n \)

Force on mass \( n \):

\[
F_n = -\kappa(\psi_n - \psi_{n-1}) - \kappa(\psi_n - \psi_{n+1})
\]

Newton: \( F_n = M\ddot{x}_n \), so plug in forces for equal masses:

\[
M\ddot{x}_n = \kappa(\psi_{n+1} - 2\psi_n + \psi_{n-1})
\]

But different for \( n-1 \) mass:

\[
F_{n-1} = -\kappa(\psi_{n-1} - \psi_{n-2}) - \kappa(\psi_{n-1} - \psi_{n})
\]

Newton: \( F_n = m\ddot{x}_{n-1} \), so plug in forces for equal masses:

\[
m\ddot{x}_{n-1} = \kappa(\psi_{n-2} - 2\psi_{n-1} + \psi_n)
\]
Normal modes:
1. All particles oscillate with same frequency – normal mode – but the small and large masses can have different amplitudes:
   \[ \psi_n = Ae^{i(kna/2 - \omega t)} \text{ for } M \text{ masses.} \]
   \[ \psi_n = \alpha Ae^{i(kna/2 - \omega t)} \text{ for } m \text{ masses.} \]
   \( \alpha \) determines amplitude and phase of \( m \) oscillations relative to \( M \) oscillations.
   Note frequency has no subscript to tell you about particle – all particles have same frequency in given mode.
   \( k = \frac{2\pi}{\lambda} \)

So, put normal mode solution into Newton:
Cancel time dependence, \( A \)

\[ -M\omega^2 e^{i\kappa a/2} = -\kappa (e^{i\kappa a/2} - \alpha e^{i(n-1)a/2}) - \kappa (e^{i\kappa a/2} - \alpha e^{i(n+1)a/2}) \]
\[ -\alpha m\omega^2 e^{i(n-1)a/2} = -\kappa (\alpha e^{i(n-1)a/2} - e^{i(n-2)a/2}) - \kappa (\alpha e^{i(n-1)a/2} - e^{i\kappa a/2}) \]

\[ -M\omega^2 = \kappa(\alpha e^{i\kappa a/2} + \alpha e^{-i\kappa a/2} - 2) \]
\[ -\alpha m\omega^2 = \kappa(e^{i\kappa a/2} + e^{-i\kappa a/2} - 2\alpha) \]

Simplify more
\[ -M\omega^2 = 2\alpha\kappa \cos(ka/2) - 2\kappa \]
\[ -\alpha m\omega^2 = 2\kappa \cos(ka/2) - 2\alpha\kappa \]

Now obtain 2 different expressions for \( \alpha \):
\[ \alpha = \frac{2\kappa - M\omega^2}{2\kappa \cos(ka/2)} \]
\[ \alpha = \frac{2\kappa \cos(ka/2)}{2\kappa - m\omega^2} \]

Equate them to get the DISPERSION RELATION \( \omega(k) \)
\[ \frac{2\kappa \cos(ka/2)}{2\kappa - m\omega^2} = \frac{2\kappa - M\omega^2}{2\kappa \cos(ka/2)} \]
\[ \Rightarrow 4\kappa^2 \cos^2(ka/2) = (2\kappa - m\omega^2)(2\kappa - M\omega^2) \]
\[ \omega^2 = \kappa \left( \frac{1}{M} + \frac{1}{m} \right) \pm \kappa \left[ \left( \frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \sin^2(ka/2) \right]^{1/2} \]
Worth repeating with an index \( q \) on the frequency and the wave vector, to label the mode, not the particles

\[
\omega_q^2 = \kappa \left( \frac{1}{M} + \frac{1}{m} \right) \pm \kappa \left[ \left( \frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \sin^2 \left( \frac{k_q a}{2} \right) \right]^{1/2}
\]

There are two branches to the dispersion curve, so each mode \( q \) has two frequencies (need new index!)
Lower branch (in-phase motion of \( M, m \)) is called ACoustIC branch.
Higher branch (out-of-phase motion of \( M, m \)) is called OPTIC branch.

Note the repetition of information after \( k = \frac{\pi}{a} \) (just as before – \( a \) is cell spacing)
This is called the Brillouin zone boundary and corresponds to a wavelength of \( \lambda = 2a \). Smaller wavelengths are physically meaningless as we found in lab.

Plot for \( m = 1, M = 2, a = \pi, \kappa = 0.5 \).

1. There is a maximum frequency for acoustic branch, and max and min for optic.
2. Linear dispersion relation for low frequencies in acoustic branch.
3. We haven’t specified frequencies yet, but we do know how they’re related to initial displacements of particles.
4. Should check limit as $m \to M$.

Can also go back and get $\alpha$ (one for acoustic and one for optical) now that we know frequencies:

\[ \alpha_a = \frac{2K \cos\left(\frac{ka}{2}\right)}{2K - \omega^2 m} \quad \alpha_o = \frac{2K \cos\left(\frac{k a}{2}\right)}{2K - \gamma^2 m} \]

Check limit as $m \to M$. 
\[ m = 1 \quad M = 1.1 \quad K = 0.5 \quad a = \pi \]
PH427/527 - Periodic Systems

For the diatomic chain, find the wave vectors, vibration frequencies, and values of the constant $\alpha$ at the following special points:

Group 1: Long wavelength optical vibration
Group 2: Brillouin zone optical vibration
Group 3: Brillouin zone acoustic vibration

Interpret your results in a way that illustrates the physical behavior of the system.
Articulate what distinguishes an acoustic from an optical vibration.

If you finish early, move on to another task, swapping roles of taskmaster, cynic, & recorder.