Day 3: Wednesday – 50 minutes

Many coupled masses (a total of *N*)

Reading: Main Ch. 12 (especially 12.2).

Lessons from lab 1:
1. Experimentally determined dispersion relation for 5-oscillator chain.
2. Linear at low frequency
3. Maximum frequency
4. Information repeated for higher wave vectors – no new physics

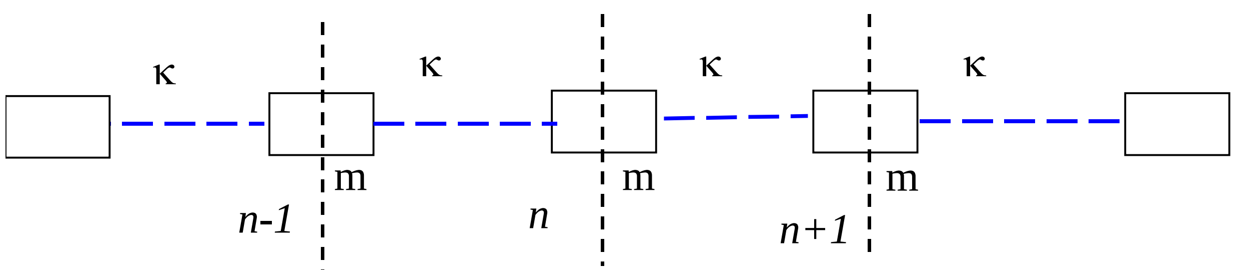
We continue with many masses coupled *to their nearest neighbors* by Hooke's Law springs and find the possible longitudinal motion of such a system. (Coupling with other springs to next neighbors is a homework example). This system is a model for other types of coupled oscillations (transverse motion of these masses, coupled LC circuits, pendulums ….)

Newton's law – how things move:

$$\vec{F} = \frac{d\vec{p}}{dt} = m\frac{d^2\vec{r}}{dt^2} \qquad \text{(for point masses)}$$

So if we know what $\vec{F}$ is, we know about trajectory!

Hooke's Law: $F = -\kappa\psi$ (one dimension) where ψ is the displacement from equilibrium. Constrain to longitudinal direction. Only one mass and one spring per cell – relax this later.



Force on mass *n*: $F_n = -\kappa(\psi_n - \psi_{n-1}) - \kappa(\psi_n - \psi_{n+1})$

Check each term for sign of force relative to displacement!

Newton: $F_n = m_n\ddot{\psi}$, so plug in forces for equal masses:

$$m\ddot{\psi}_{n-1} = -\kappa(\psi_{n-1} - \psi_{n-2}) - \kappa(\psi_{n-1} - \psi_n)$$
$$m\ddot{\psi}_n = -\kappa(\psi_n - \psi_{n-1}) - \kappa(\psi_n - \psi_{n+1})$$
$$m\ddot{\psi}_{n+1} = -\kappa(\psi_{n+1} - \psi_n) - \kappa(\psi_{n+1} - \psi_{n+2})$$

Normal modes:

1. All particles oscillate with same frequency – normal mode $\psi_n = A_n e^{i\omega t}$. Coefficients are complex. Note frequency has no subscript to tell you about particle – all particles have same frequency.
2. Furthermore, as we saw in lab, the amplitudes of the particles' oscillations form the envelope of a sinusoid in the normal modes, so we'll further assume: $\psi_n = Ae^{i(nka-\delta)}e^{i\omega t}$ where *na* counts the particle's position along the chain, and $k = \frac{2\pi}{\lambda}$ (wave vector in 3d) where λ is the wavelength of the envelope that describes the initial position of the masses in that mode.

So, put normal mode solution into Newton:

$$-m\omega^2 Ae^{inka-i\delta}e^{i\omega t} = -\kappa\left(Ae^{inka-i\delta}e^{i\omega t} - Ae^{i(n-1)ka-i\delta}e^{i\omega t}\right) - \kappa\left(Ae^{inka-i\delta}e^{i\omega t} - Ae^{i(n+1)ka-i\delta}e^{i\omega t}\right)$$

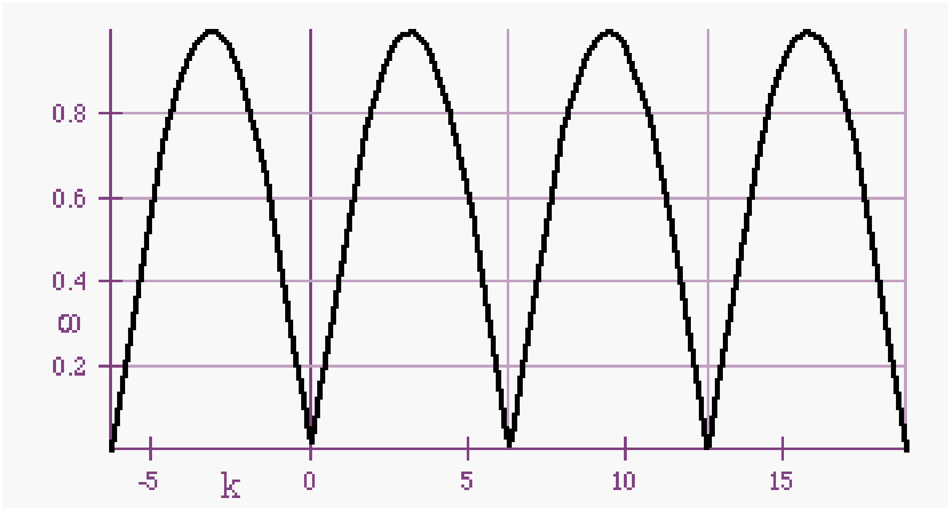
$$\frac{m\omega^2}{\kappa}e^{inka} = -e^{i(n-1)ka} + 2e^{inka} - e^{i(n+1)ka}$$

$$\omega^2 = \frac{2\kappa}{m}\left(1 - \frac{e^{ika} + e^{-ika}}{2}\right) = \frac{2\kappa}{m}(1 - \cos ka)$$

$$\omega^2 = \frac{4\kappa}{m}\sin^2\frac{ka}{2}$$

$$\omega(k) = 2\sqrt{\frac{\kappa}{m}}\sin\frac{ka}{2}$$

This is the DISPERSION RELATION (ω as a function of k). It is plotted below for $\omega_{\max} = 2\sqrt{\frac{\kappa}{m}} = 1$ and $a = 1$.



1. Note the repetition of information after $k = \frac{\pi}{a}$. 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.

2. There is a maximum frequency

3. We haven't specified frequencies yet, but we do know how they're related to initial displacements of particles.

4. Should check 2 – particle limit.

5. For small values of *ka* we have $\omega = 2\sqrt{\frac{\kappa}{m}}\frac{a}{2}k \cong v_s k$ -- linear dispersion (sound velocity)

Boundary conditions determine *k* and frequency:

To find particular values of ω and *k*, we need to specify boundary conditions, and the total number of masses *N* comes into play.

For the monatomic chain, we have found that the dispersion relation is

$\omega = \omega_{max} \sin\left(\frac{ka}{2}\right)$ with, as yet, no restriction on either ω or *k*. Now, let's consider the effect of the boundary (end of the chain). We will consider two kinds of boundary conditions: **fixed** boundary conditions and **periodic** boundary conditions.

Fixed boundary conditions:

Recall $\psi_n = Ae^{i(nka-\delta)}e^{i\omega t}$.

If we fix the ends of the chain at all times (*i.e.* require the 0th and (N+1)th masses to be fixed), we will then have standing waves. This means

$$\psi_n = \mathrm{Re}\left(A_0 e^{i(nka)}e^{i\omega t}\right) = \mathrm{Re}\left(Ae^{i(nka-\delta)}e^{i\omega t}\right) = 0$$

$A_0 = \mathrm{Re}\left(Ae^{i(k.0.a-\delta)}\right) = A\cos(-\delta) = 0$ which implies $\delta = \frac{\pi}{2}$ and

$A_n = \mathrm{Re}\left(Ae^{i(kna-\pi/2)}\right) = A\cos(kna - \pi/2) = A\sin kna$. These are the eigenmodes.

Furthermore

$$A_{N+1} = A\sin[k(N+1)a] = 0 \quad \Longrightarrow \quad k(N+1)a = q\pi$$

$$k_q = \frac{q\pi}{(N+1)a}$$

with q having values 1,2 … N (N distinct modes). Notice that if $q < 0$, we get no new information, since sin(x) = -sin(-x) and the entire displacement is the same except for a phase which can be absorbed into the time dependence.

Now that we have k, we can find the related frequencies, and our problem is solved. Each "allowed" value of k will correspond to a particular frequency as determined by the dispersion relation, $\omega(k)$.

Brillouin zone boundary: Setting $q = N + 1$ gives $k = \pi/a$. This k vector defines the Brillouin zone boundary.

Periodic boundary conditions are different. Here we have no requirement on the amplitude, but rather on the displacement as a whole. We require only that the motion of the 0th mass be the same as the motion of the (N+1)th, or generally that the motion of the *n*th mass be the same as the motion of the (*N*+*n*)th:

$$\begin{aligned}&\psi_n = \psi_{n+N+1}\\ &\Rightarrow \mathrm{Re}\left(Ae^{i(kna-\delta)}\right) = \mathrm{Re}\left(Ae^{i(k(n+N+1)a-\delta)}\right)\\ &\Rightarrow kna-\delta = k(n+N+1)a-\delta \pm 2\pi q\end{aligned}$$

which simplifies to $k_q = \pm\frac{2\pi q}{(N+1)a}$. (with no requirement on δ).

1. We see that the *k* spacing has doubled ($q = (N+1)/2$ gives the BZB)! Have we lost half the modes? No! In this case the different signs of *q* ARE distinct. Positive and negative *q* values correspond to oppositely propagating traveling waves. Thus $q = 0, \pm 1, \ldots \pm(N+1)/2$ give physically distinct modes (now it's clear why the minus sign above was dropped). This running wave set of states is simply a different basis set from the standing wave set.
2. Note that one generally sees periodic boundary conditions written as $\psi_n = \psi_{n+N}$ and not $\psi_n = \psi_{n+N+1}$ as written above. Why? In our problem of *N* atoms with fixed boundary conditions, we really introduced a fictitious 0th and (*N*+1)th atom and made them stationary. So we really had *N*+1 unit cells in our problem. With the periodic boundary conditions, we let the 0th and *N*th atom (which are really the same atom) participate in the motion, so again we really had *N*+1 unit cells.

Now the problem is complete. We know which *k* values are allowed (from applying the boundary conditions), and we know the corresponding frequency (from the dispersion relation). We also know the eigenvectors (the relative displacements of the masses in a particular mode) because we know ω and *k*.