Lecture 2.2

Last time, we considered a 1D lattice of identical atoms, and we found the dispersion relation

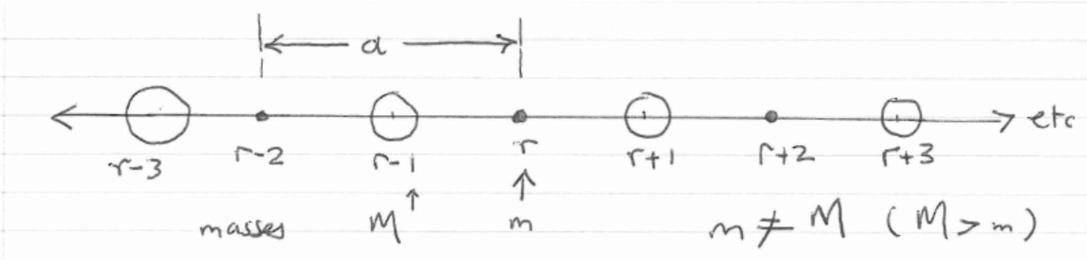
$$\omega = \pm\omega_m \sin\left(\frac{ka}{2}\right)$$

where k is the wavenumber, ω_m is a maximum frequency set by the spring constant and the mass of each atom, and a is the lattice spacing.

Now we consider a 1D lattice composed of low-mass m and large-mass $M > m$ atoms. This is *slightly* more complex, and shows rich behaviour: specifically, a *forbidden* range of frequencies.

Vibrational Modes of a Linear Lattice with a Diatomic Basis

Consider a linear chain where every other atom is a different mass. This is a 1D lattice with a 2 atom **basis**.



By analogy with Eq. 1, we have

$$u_r = A\exp\left[i\left(kra/2 - \omega t\right)\right] \quad (5)$$
$$v_{r+1} = B\exp\left[i\left(k(r+1)a/2 - \omega t\right)\right] \quad (6)$$
$$(7)$$

(Mathematica sheet working through these details is available on the course website.)

Again, use Hooke's law and nearest-neighbours to get equations which look similar to those for the monatomic lattice:

$$-m\omega^2 u_r = \quad m\frac{d^2u_r}{dt^2} = \mu\left[v_{r+1} + v_{r-1} - 2u_r\right]$$
$$-M\omega^2 v_{r+1} = \quad M\frac{d^2v_{r+1}}{dt^2} = \mu\left[u_{r+2} + u_r - 2v_{r+1}\right]$$

Substituting for u s and v s gives us

$$A\left[2\mu - m\omega^2\right] = \quad 2\mu B\cos\left(ka/2\right)$$
$$B\left[2\mu - M\omega^2\right] = \quad 2\mu A\cos\left(ka/2\right)$$

So

$$(2\mu - m\omega^2)(2\mu - M\omega^2) = 4\mu^2\cos^2\left(ka/2\right)$$

Expanding and grouping gives a quadratic in ω^2

$$mM\omega^4 - 2\mu(m+M)\omega^2 + 4\mu^2\sin^2\left(ka/2\right) = 0$$

(where we've used $1 - \cos^2\theta = \sin^2\theta$)

This gives

$$\omega^2 = \mu\left[\frac{1}{m} + \frac{1}{M}\right] \pm \mu\left[\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4}{mM}\sin^2\left(ka/2\right)\right]^{1/2}$$

or

$$\omega^2 = \mu\left[\frac{1}{m} + \frac{1}{M}\right] \pm \mu\left(\frac{1}{m} + \frac{1}{M}\right)\left[1 - \frac{4mM}{(m+M)^2}\sin^2\left(ka/2\right)\right]^{1/2}$$

This is the dispersion relation. (Reduces to monatomic case for $M \to m$ and halving the spacing $a \to a/2$.)

For each k we have **two** allowed values of ω. There are two branches of $\omega(k)$.

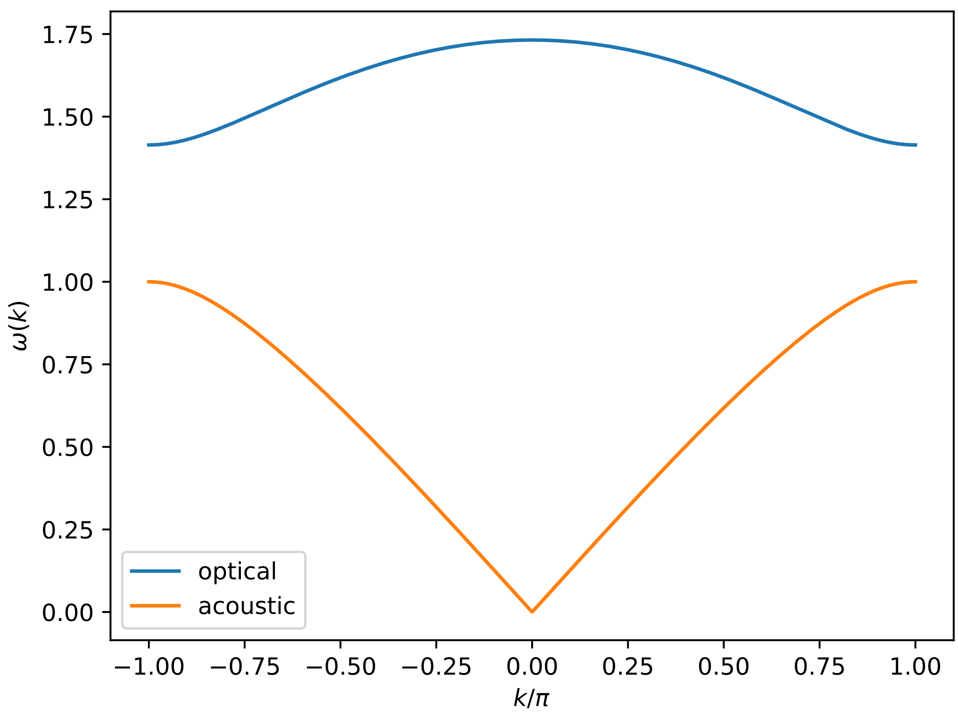
- One branch behaves like the monatomic solution:
  - the -ve root
  - usually referred to as the acoustic phonon branch

and

- One different branch
  - the +ve root
  - usually referred to as the optical phonon branch

Here's a plot with some typical numbers

```
import numpy as np
from numpy import sqrt, sin, pi
import matplotlib.pyplot as plt
omegapos = lambda k: sqrt(mu*(1/m+1/M)+mu*(1/m+1/M)*sqrt(1-4*m*M*sin(k*a/2)**2/(m+M)**2))
omeganeg = lambda k: sqrt(mu*(1/m+1/M)-mu*(1/m+1/M)*sqrt(1-4*m*M*sin(k*a/2)**2/(m+M)**2))
mu, m, M, a = 1., 1., 2., 1.
k = np.linspace(-pi,+pi,1000)
plt.plot(k/pi,omegapos(k), label='optical')
plt.plot(k/pi,omeganeg(k), label='acoustic')
plt.ylabel(r'$\omega(k)$')
plt.xlabel(r'$k/\pi$')
plt.legend()
plt.savefig('figs/1D-diatomic-dispersion.pdf')
plt.close('all')
```



Notes

Note 1: long wavelength limit

As before, for long-wavelengths or small wavenumbers, $\sin(ka/2) \approx ka/2$

So the term from Eq. becomes

$$\left[1 - \frac{4mM}{(m+M)^2}\sin^2(ka/2)\right]^{1/2} \approx \qquad \left[1 - \frac{4mM}{(m+M)^2}(ka/2)^2\right]^{1/2} \approx 1 - \frac{mM}{2(m+M)^2}(ka)^2$$

-ve root (acoustic phonons)

$$\omega^2 = \mu\left(\frac{1}{m} + \frac{1}{M}\right) - \mu\left(\frac{1}{m} + \frac{1}{M}\right)\left[1 - \frac{mM}{2(m+M)^2}(ka)^2\right]$$

$$\implies \omega^2 = \frac{\mu}{2}\left(\frac{1}{m} + \frac{1}{M}\right)\frac{mM}{(m+M)^2}(ka)^2$$

or

$$\omega = \sqrt{\frac{\mu}{2(m+M)}}ka \tag{8}$$

i.e. $\omega \propto k$, in accord with continuum prediction.

+ve root (optical phonons)

As $k \to 0$ we can neglect k^2 terms which appear in the square root, and we find

$$\omega^2 = 2\mu\left(\frac{1}{m} + \frac{1}{M}\right)$$

tends to a constant, so

$$\omega = \sqrt{2\mu\left(\frac{1}{m} + \frac{1}{M}\right)} = \omega_3 \tag{9}$$

Note 2: Behaviour at the 1st BZ boundary

Here, $k = \pm\pi/a$ so $\sin(ka/2) = 1$

Hence, from Eq. , the term becomes

$$\left[1 - \frac{4mM}{(m+M)^2}\sin^2(ka/2)\right]^{1/2} = \left[1 - \frac{4mM}{(m+M)^2}\right]^{1/2} = \frac{M-m}{M+M}$$

so we have

$$\omega^2 = \mu\left(\frac{1}{m} + \frac{1}{M}\right) \pm \mu\left(\frac{1}{m} + \frac{1}{M}\right)\left(\frac{M-m}{m+M}\right)$$

$$\omega^2 = \frac{\mu}{mM}\left[(M+m) \pm (M-m)\right] \tag{10}$$

-ve root (acoustic phonon)

$$\omega = \sqrt{\frac{2\mu}{M}} = \omega_1$$

+ve root (optical phonons)

$$\omega = \sqrt{\frac{2\mu}{m}} = \omega_2$$

Note 3: Acoustic branch corresponds roughly to monatomic lattice

Acoustic branch corresponds fairly well to monatomic lattice, now max angular frequency is

$$\omega_1 = \sqrt{\frac{2\mu}{M}}$$

and is independent of the mass of the lighter atoms. (Compare with the monatomic case: $\omega = \sqrt{\frac{4\mu}{m}}$.)

Can show that these lighter atoms are stationary at the BZ edge.

Note 4: Forbidden range

There is a frequency range $\omega_1 \ldots \omega_2$ for which no real value of k exists.

This is a **forbidden band**. Such bands are a recurring feature of waves in periodic media.

Note 5: Extra branch

The diatomic lattice introduces an extra range of allowed frequencies – the optical branch or mode

Note 6: Similar features in 3D

The situation with real, 3D lattice is more complex, but the same general features arise.