Topic 8: Many coupled oscillators representing a crystal

Recap

1. We looked at a model with *N* balls on a linear string with fixed ends – redraw
2. We assumed normal mode solutions based on sine waves that form harmonics, and obtained an equation for the frequencies of each mode.
3. We noted that for *N* balls we would have *N* normal modes.
4. We remarked that the model would represent a continuum if the balls represented atoms.

Today we are going to extend this to the case where our set of springs has no connected ends and thus represents a crystalline solid.

Wave equation

We now look at one atom in a string.

Use the previous formula

$$\begin{aligned} F_j &= m\frac{\partial^2 u_j}{\partial t^2} = -k\left(u_j - u_{j-1}\right) - k\left(u_j - u_{j+1}\right) \\ &= k\left(-\Delta u\big|_{j,j-1} + \Delta u\big|_{j+1,j}\right) = k\,\partial^2 u_j \end{aligned}$$

We denote the separation as ℓ,

each atom has mass m,

So we can write the above equation as

$$\begin{aligned} &m\frac{\partial^2 u_j}{\partial t^2} = k\,\partial^2 u_j \\ &\frac{\partial^2 u_j}{\partial t^2} = \frac{k}{m}\partial^2 u_j = \frac{k\ell^2}{m}\frac{\partial^2 u_j}{\ell^2} = \frac{k\ell^2}{m}\frac{\partial^2 u_j}{\partial x^2} \\ &\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2} \end{aligned}$$

The pre-factor is the square of the velocity of the wave, which we will explore next time.

Note that m/ℓ corresponds (in a one-dimensional sense) to the density.

The term $k\ell$ has units of force, and corresponds to the stiffness K.

Thus we can write the wave equation in a way that gives us the velocity of a wave:

$$\frac{\partial^2 u}{\partial t^2} = \frac{k\ell^2}{m}\frac{\partial^2 u}{\partial x^2} = \frac{K}{\rho}\frac{\partial^2 u}{\partial x^2}$$

$$c = \sqrt{\frac{K}{\rho}}$$

Note that there are many ways to derive this equation.

The power of this equation will comes from the solution in terms of travelling waves. We propose the following solution

$$u(x,t) = u_0 \exp\big(i(kx - \omega t)\big)$$

$$\frac{\partial u}{\partial t} = -i\omega u_0 \exp\big(i(kx - \omega t)\big)$$

$$\frac{\partial^2 u}{\partial t^2} = -\omega^2 u_0 \exp\big(i(kx - \omega t)\big)$$

$$\frac{\partial u}{\partial x} = iku_0 \exp\big(i(kx - \omega t)\big)$$

$$\frac{\partial^2 u}{\partial x^2} = -k^2 u_0 \exp\big(i(kx - \omega t)\big)$$

$$\frac{1}{\omega^2}\frac{\partial^2 u}{\partial t^2} = \frac{1}{k^2}\frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\omega^2}{k^2}\frac{\partial^2 u}{\partial x^2} = c^2\frac{\partial^2 u}{\partial x^2}$$

What does this equation mean?

1. We note that we can add one period = $2\pi/\omega$ and get the same, so in time we have periodicity. This is exactly what we have come across before.
2. For the spatial part, we can add $2\pi/k$ to the position and again get exactly the same. This means that k = $2\pi/\lambda$ where is the λ wavelength.
3. On this basis, $\omega/k = f\lambda$ represents the velocity of the wave, c

The travelling wave solution now allows the maxima of the wave to travel forward in space, whereas up to now the maximum have been fixed in space.

Writing $\omega = ck$, the wave equation can be written as

$$u(x,t) = u_0 \exp\big(ik(x - ct)\big)$$

So consider the peak when $x - ct = \lambda$, the exponential has value 1. Moving forward in time will mean that x increases, namely the wave move forwards. We have $\Delta x = c\Delta t$, ie c = $\Delta x/\Delta t$, namely a velocity. This is called the *phase velocity*.

Group velocity

We now consider the case where the speed of the wave depends on its wavelength; we call this dispersion.

Let's consider two waves

$$u_1 = A\exp\big(i(k_1x-\omega_1t)\big) \quad ; \quad u_2 = A\exp\big(i(k_2x-\omega_2t)\big)$$

$$\begin{aligned}\exp ia+\exp ib &= \exp(ia/2)\big(\exp(ia/2)+\exp(ib-ia/2)\big)\\ &= \exp\big(i(a+b)/2\big)\big(\exp\big(i(a-b)/2\big)+\exp\big(i(b-a)/2\big)\big)\\ &= 2\exp\big(i(a+b)/2\big)\cos\big((a-b)/2\big)\\ u_1+u_2 &= 2A\exp\big(i\big((k_1+k_2)x-(\omega_1+\omega_2)t\big)/2\big)\cos\big(\big((k_1-k_2)x-(\omega_1-\omega_2)t\big)/2\big)\end{aligned}$$

What we have here is beating again, with the cosine term being the envelope. So we consider the velocity of the envelop:

$$c=\frac{\omega_1-\omega_2}{k_1-k_2}$$

In the limit where the waves are very close in frequency and wave vector, we could write

$$c=\frac{\Delta\omega}{\Delta k}\to\frac{\partial\omega}{\partial k}=c_{\mathrm{g}}$$

which is called the *group velocity*. This is the velocity at which the envelope travels, whether for two waves or more for a localised distribution.

Wave vector

We need to think about the idea of the wave vector. This is an important concept.

It is not just a case of defining a new variable for the sake of it, but it makes sense to use this variable.

Consider the case from last time, where our base wavelength was very long, and then shrunk. So we had waves of wavelength, in order, λ, $\lambda/2$, $\lambda/3$, $\lambda/4$,...

This is a strange way of incrementing, but in terms of k, we would have the set

$$\frac{2\pi}{\lambda},2\frac{2\pi}{\lambda},3\frac{2\pi}{\lambda},4\frac{2\pi}{\lambda},\cdots$$

where we go from small to large in a linear way. The problem with using wavelength is that we go from very large – even near infinity – to small, which is not a useful way of doing things.

So wave vector defines the wavelength. In three dimensions it also defines the direction of the wave. The wave equation in three dimensions can be written as

$$u(\mathbf{r},t)=u_0\exp\big(i(\mathbf{k}\cdot\mathbf{r}-\omega t)\big)$$

Here the three-dimensional wave vector is a vector pointing in the direction in which the wave is travelling, and with modulus

$$|\mathbf{k}| = 2\pi / \lambda$$

Because of the dot product, all positions on a line passing through **r** and perpendicular to **k** will have the same dot product value, and hence will move the same way.

*Draw picture showing **k**, **r** and line perpendicular to **k**.*

This defines a plane wave.

For now we will only consider the one-dimensional case, but in Condensed Matter we need to consider always the three dimensional case, to describe vibrations of the crystal lattice and the behaviour of the electrons.

Example of wave-particle duality

Consider a particle of mass m. It's momentum and kinetic energy are

$$p = mv \quad ; \quad E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

From wave-particle duality we can write the momentum as

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar k$$

It follows that the energy can be written as

$$E = \frac{\hbar^2 k^2}{2m} \equiv hf = \hbar\omega$$

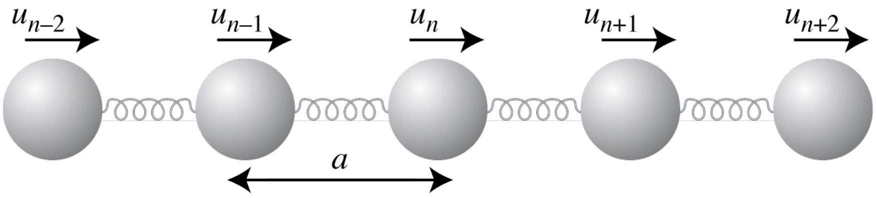
In this case the phase velocity is not very interesting. The group velocity though is obtained as

$$\frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{1}{\hbar}\frac{\hbar^2 k}{m} = \frac{p}{m} = v$$

So in wave particle duality, the group velocity gives the velocity of the particle. Group velocity is often associated with the velocity of the energy flow, which is going to be the velocity of the particle.

One dimensional crystal

So now we consider a one-dimensional crystal consisting of one atom in the unit cell, and bonds represented by springs. Allow displacements in the longitudinal direction.



We do a trick here. We don't want any boundaries to have to consider. So we consider our chain of atoms as joined at the two ends. So any wave will just move around the chain. This is called "periodic boundary condition" and is a common trick in studying crystals.

So we study the waves in the same way as before, as for the static chain.

Consider one atom and its two neighbours. It's energy due to displacements is

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

The force experience by the atom is

$$F = -\frac{\mathrm{d}E}{\mathrm{d}u_j} = -J\left(u_j - u_{j-1}\right) - J\left(u_j - u_{j+1}\right) = -J\left(2u_j - u_{j-1} - u_{j+1}\right)$$

In the fixed end model, we assumed sinusoidal standing waves, ie they didn't go anywhere. Now we use the travelling wave solution. We write

$$\begin{aligned}
u_j &= u_0 \exp\left(i\left(kja - \omega t\right)\right) \\
u_{j-1} &= u_0 \exp\left(i\left(k(j-1)a - \omega t\right)\right) \\
u_{j+1} &= u_0 \exp\left(i\left(k(j+1)a - \omega t\right)\right) \\
2u_j - u_{j-1} - u_{j+1} &= u_0 \exp\left(i\left(kja - \omega t\right)\right)\left(2 - \exp(-ika) - \exp(ika)\right) \\
&= 2u_0 \exp\left(i\left(kja - \omega t\right)\right)\left(1 - \cos ka\right) \\
&= 4u_0 \exp\left(i\left(kja - \omega t\right)\right)\sin^2 ka/2
\end{aligned}$$

Now we equate the force to mass x acceleration:

$$\begin{aligned}
&-4Ju_0 \exp\left(i\left(kja - \omega t\right)\right)\sin^2 ka/2 = m\ddot{u}_j = -m\omega^2 u_0 \exp\left(i\left(kja - \omega t\right)\right) \\
&4J\sin^2 ka/2 = m\omega^2 \\
&\omega = \sqrt{\frac{4J}{m}}\left|\sin(ka/2)\right|
\end{aligned}$$

Plot this graph, showing zero solutions at multiples of 2π/a.

Note

1. This is called a dispersion curve
2. In the limit that k → 0 we have a linear relationship:

$$\omega = \sqrt{\frac{4J}{m}}\left|\sin(ka/2)\right| \simeq \sqrt{\frac{4J}{m}}ka/2 = a\sqrt{\frac{J}{m}}k$$

$$c = a\sqrt{\frac{J}{m}}$$

Thus we link the velocity of sound to the bond interaction.

For this reason, this is called an acoustic mode. The phase velocity = the group velocity = speed of sound

3. In the limit k → π/a, the slope goes to zero. This means that the group velocity is zero, which defines a *standing wave*. Note that all the oscillations that we have discussed before are standing waves. Draw the picture of alternate atoms moving in opposite directions. This is what happens when the wavelength of the sound wave is reduced from the size of the crystal down to twice the atomic spacing.
4. Note that we started from a repeat structure and generate in the space of *k* another repeat pattern. This is called the reciprocal lattice, because it has units of 1/length. This argument can be generalised to three dimensions.
5. So what happens when k = 2π/a. Draw the picture of a single wavelength, and note that the atoms don't move, or else all move the same way but stay at rest.
6. Note that if we go to even shorter wavelengths, we need to think about what happens to the way the wave affects the atom. Draw in a short wavelength and note that the atom only moves when the wave is at the position of the atom.

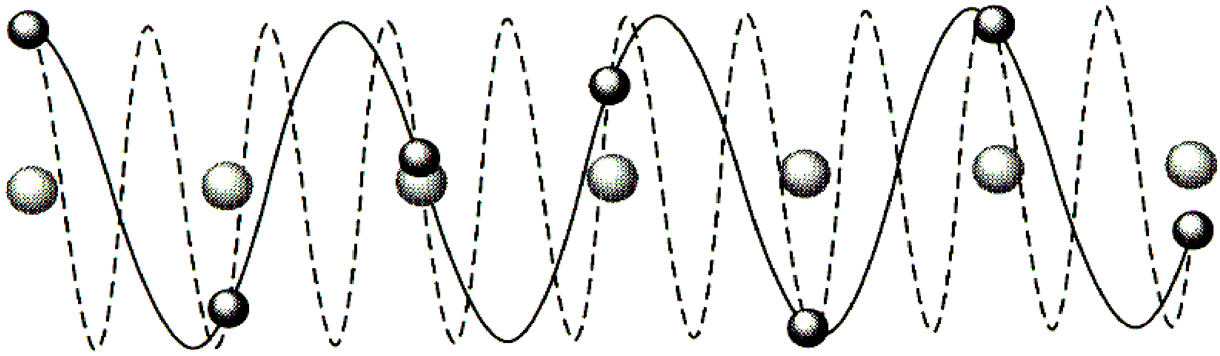
Idea of the role of reciprocal lattice vectors

So lets explore this further by considering two wave vectors:

$$k \quad ; \quad k' = k + \frac{2\pi}{a}$$

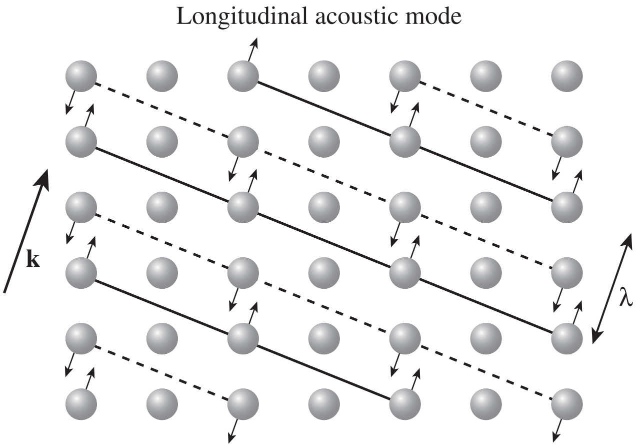
$$\Rightarrow \quad \begin{array}{c} \exp(ikja) \\ \exp(ik'ja) = \exp(ikja)\exp\big(i(2\pi/a)ja\big) = \exp(ikja) \end{array}$$

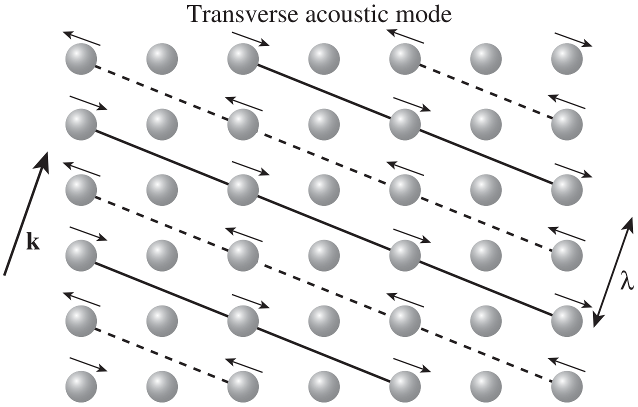
So we see that the addition of any factor of 2π/a is the same as if you didn't add it, when it comes to the atoms.



Extension to three dimensions

Show a picture of what happens in a two-dimensional plane





Highlight wave vector

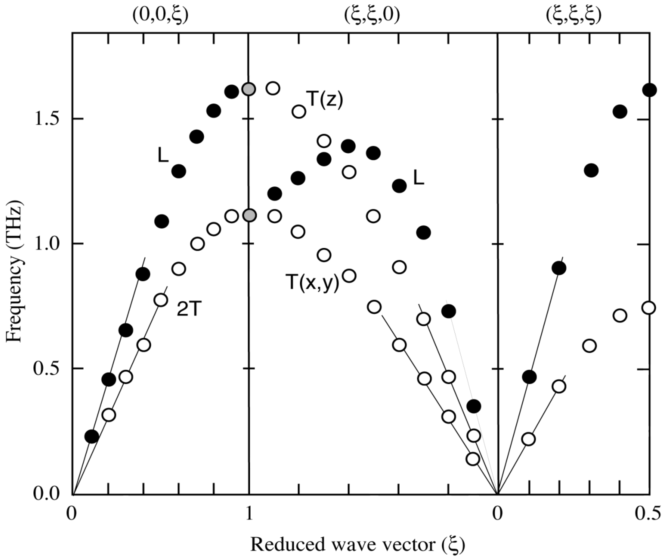
Highlight longitudinal and transverse modes. Note that always transverse modes have lower frequency.

Comment on the way to measure these by neutron scattering

1. Direct a beam of neutrons onto the sample, where the neutrons have kinetic energies that are similar to the energies of vibrations, and wavelengths similar to the interatomic spacing. You can do this because neutrons have a similar mass to the atom. Note that the energies are not high – typically of order of room temperature.

2. Measure the scattering as functions of the change in wave vector of the neutron – note that this is three dimensional so there will be a change in direction of the neutron – and change in energy.
3. Relate change in wave vector to the wave vector of a wave. Relate change in energy to a quantum of energy of the vibration.
4. We have a resonant behaviour as for before – when the energy change matches the energy of a quantum of vibration, we get absorption of energy, and we see scattering at that energy change.

Show a diagram of measured dispersion curves for argon.



Considering all modes

Note that all modes operate at the same time, and the waves do not interact. Because the waves have frequencies that are not linearly related, and we never go back to our starting point.

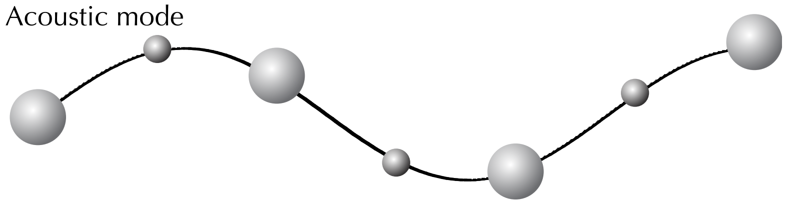
What determines the amplitude. Note that the amplitude of a wave will be excited by temperature, and will depend on restoring force. Hence expect the amplitude of any mode will be proportional to T/ω^2.

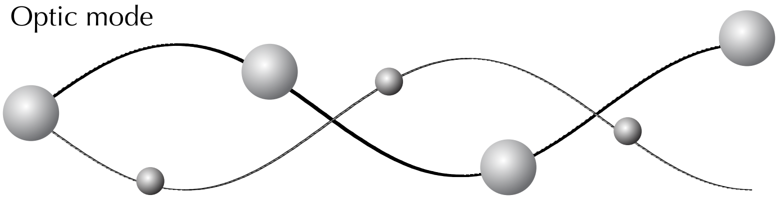
Show movie of argon.

More complex crystals

So now we have something like our coupled oscillators!

Show a diatomic chain. Show for zero wave vector the displacements of modes. Show diagram of optic and acoustic modes:





Note

1. In-phase motions are acoustic modes, with frequency going to zero at zero wave vector
2. Out-of-phase motions are higher frequency, and are called optic modes
3. Sketch dispersion curve
4. Show movies of NaCl

Summary

1. We have explored the vibrations of a crystal in terms of travelling wave normal modes.
2. We have derived an equation for the dispersion curve of the case of one atom in the unit cell
3. We have explored some aspects of this solution.