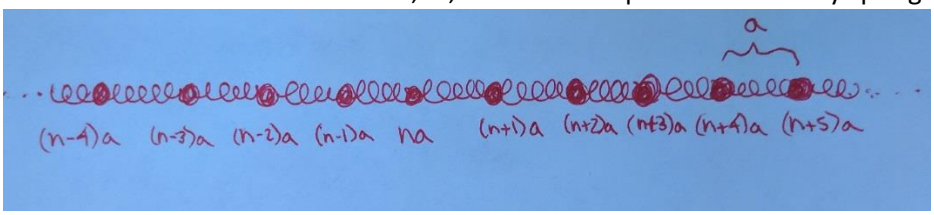
Lecture 11:

- **Representative from CalTeach/MAST**
- **Review: 1D lattice**
- **Higher dimension lattices: transverse waves**
- **Counting number of dispersions**
- **Quantization of elastic waves**

Review

1D lattice:

Consider a line of identical masses, m, a distance a apart connected by springs.



The position of each mass is labeled as in the image below, with some central mass chosen to have the position label na (n is an integer).

When a mass is displaced from its equilibrium position, we call this **displacement** $u(va)$, where v is an integer. For the n-th atom, this small but arbitrary displacement has the label u(na)

When all of the atoms are subjected to small but arbitrary dispacements, the total potential energy is given by:

$$U_{tot} = \frac{1}{2} C \sum_n [u(na) - u([n+1]a)]^2$$

Here, the term in parenthesis after the sum measures how far a given **spring** has been stretch and compressed. It is for this reason that we only count the neighbor to the right of each atom. Now, write equation of motion **for atom located at position na**

$$ma = F$$

$$m\frac{\partial^2 u(na)}{\partial t^2} = -\frac{\partial U_{tot}}{\partial u(na)}$$

Plugging this into the equation of motion above (most terms drop out because u(na) only appears twice in the sum:

$$m\frac{\partial^2 u(na)}{\partial t^2} = -C[2u(na) - u([n-1]a) - u([n+1]a)]$$

We are seeking wave-like solutions, which have the form:

$$u(na, t) \propto e^{i(kna - \omega t)}$$

Substitute the solution $u(na,t) \propto e^{i(kna-\omega t)}$ into the equation of motion and drop common exponential terms that remain:

$$m\omega^2 = C[2 - 2coska]$$

Solve for dispersion relation ($\omega\ vs\ k$)

$$\omega = \sqrt{\frac{2C(1-coska)}{m}}$$

Use the trig identity $\sin^2\frac{\theta}{2} = \frac{1-cos\theta}{2}$

$$\omega = 2\sqrt{\frac{C}{m}}\left|sin\frac{ka}{2}\right|$$

The absolute value appears around the sine to ensure that ω is positive

This solution describe a propagating wave with

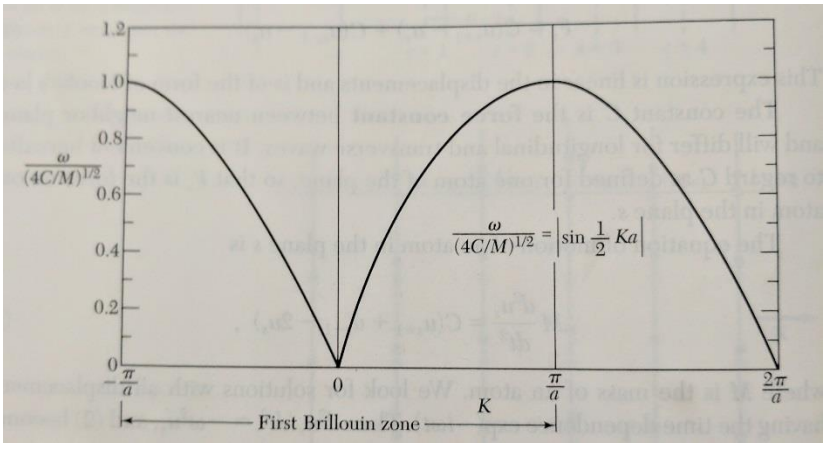
Phase velocity: $v_p = \omega/k$

Group velocity: $v_g = \frac{\partial\omega}{\partial k}$

For the dispersion relation for this propagating wave, we consider small k where $sin\theta \sim \theta$

$$v_{g,small\ k} = a\sqrt{\frac{C}{m}}$$

A plot of the dispersion relation is shown below:

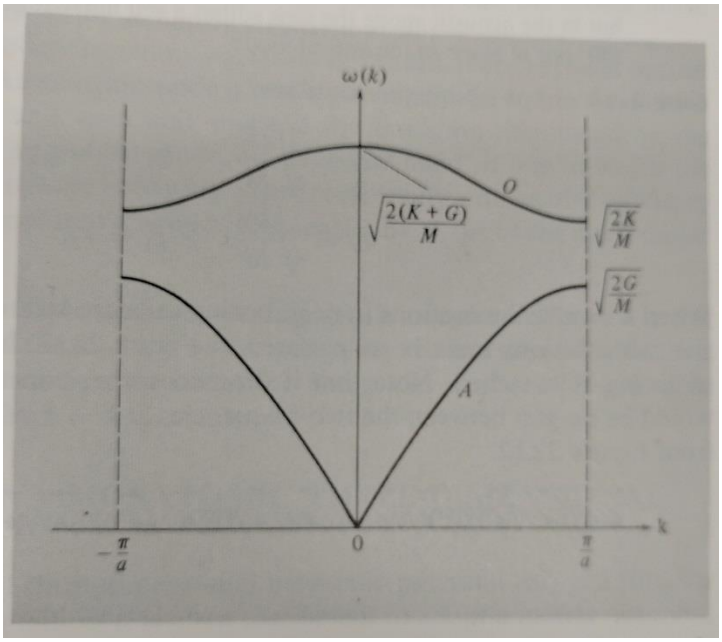


Since the frequency goes as the absolute value of the sine of momentum (k), the dispersion relation is a function which repeats infinitely. However, beyond the **first brillouin zone**, the information is redundant.

When we consider a one dimensional lattice with two types of atoms, and either set the masses to be different or the spring constants to be different (or both) we derive two types of solutions:

$$\omega^2 = \frac{(C_1 + C_2)}{m} \pm \frac{1}{m}\sqrt{C_1^2 + 2C_1C_2 coska + C_2^2}$$

This has two distinct branches: an acoustic (A) similar to the one we had before and a new one called an optical branch (O)



Higher dimensions: transverse waves

To extract transverse waves, we need to consider a system with more than one dimensions.

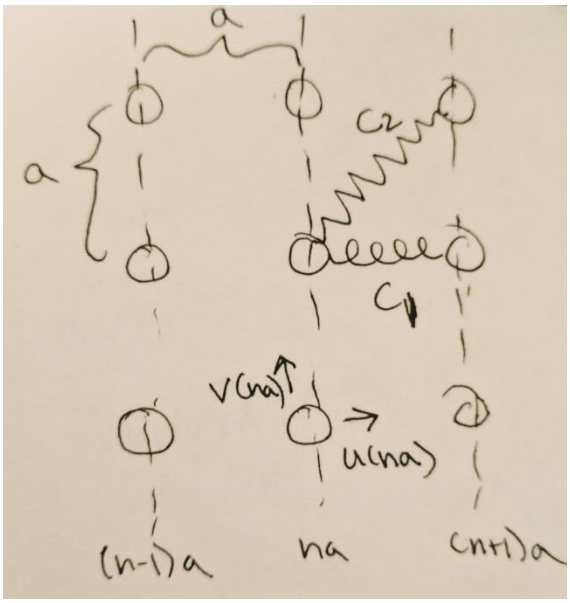
Consider a square lattice (2D) with identical atoms spaced a apart in all directions. Every atom has 8 nearest neighbors instead of 2. Because some of those neighbors are further apart than others, we use two spring constants.

C_1: for atoms separated by a

C_2: for atoms separated by $a\sqrt{2}$

Displacements in the x-direction are indicated by u, and displacements in the y-direction are indicated by v.

We label columns of atoms with the position indices (n-1)a,na,(n+1)a, (n+2)a….and we make our problem simpler by only considering modes in which all the atoms in a column move together as a unit. Of course, the atoms in a 2D lattice are not necessarily constrained in this way, but we are solving a simpler problem to enhance tractability. Notice that if we displace plane (n+1)a to the right, spring C_2 contributes a spring constant $C_2/\sqrt{2}$ in the x direction, and the atom in the center of the drawing will feel that force from **two** C_2 springs on its right, but only one C_1 spring. Similarly, if we translate plane (n+1)a **up**, the total upward force on the central atom will be proportional to $2C_2/\sqrt{2}$



We derive equations of motion as before, so I won't go into too much detail.

$$m\partial^2 u(na)/\partial t^2 = -C_1[2u(na) - u([n-1]a) - u([n+1]a)] - \frac{2C_2}{\sqrt{2}}[2u(na) - u([n-1]a) - u([n+1]a)]$$

$$m\partial^2 v(na)/\partial t^2 = -\frac{2C_2}{\sqrt{2}}[2v(na) - v([n-1]a) - v([n+1]a)]$$

First, consider a transverse wave: displacements in the y direction, but propagation in the x direction (we have implicitly plugged in na for x in the exponent).

$$v = v_0 e^{i(kna-\omega t)}$$

Plug this into the equation for v above

$$m\omega^2 = 2C_2/\sqrt{2}[2 - 2coska]$$

Use half-angle trig identities as before

$$\omega = 2\left|sin\frac{ka}{2}\right|\sqrt{\frac{2C_2}{m\sqrt{2}}}$$

In the limit of very small k, $v_{g,transverse} = \frac{\partial\omega}{\partial k} = a\sqrt{\frac{2C_2}{m\sqrt{2}}}$

Now we consider a longitudinal wave:

$$u = u_0 e^{i(kna-\omega t)}$$

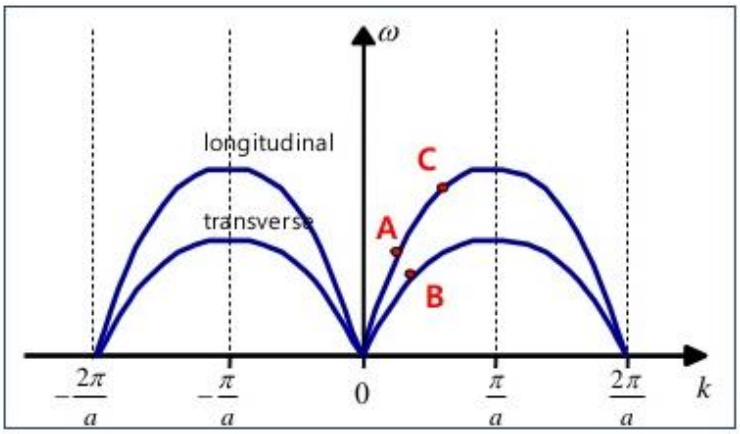
Plug this in to the first formula above

$$m\omega^2 = C_1[2 - 2coska] + 2C_2/\sqrt{2}[2 - 2coska]$$

$$\omega = 2\left|sin\frac{ka}{2}\right|\sqrt{\frac{C_1}{m}+\frac{2C_2}{m\sqrt{2}}}$$

In the limit of very small k, $v_{g,longitudinal} = \frac{\partial\omega}{\partial k} = a\sqrt{\frac{C_1}{m}+\frac{2C_2}{m\sqrt{2}}} > v_{g,transverse}$

Thus, we end up with **two** acoustic branches with different propagation velocities



(ignore A, B, C letters)

Question: why does the longitudinal branch have a faster group velocity?

The model of the 2D lattice will also have optical branches branches, which will not be derived here.

Counting how many branches we have

The examples we have seen in class so far:

Model	# Acoustic branches	# optical branches
1D, 1 atom per basis	1	0
1D, 2 atoms per basis	1	1
2D, 1 atom per basis	2 (1 Long., 1 Trans.)	?
3D, 1 atom per basis	3 (1 Long., 2 Trans.—based on propagating waves in continuous media in last chapter)	?

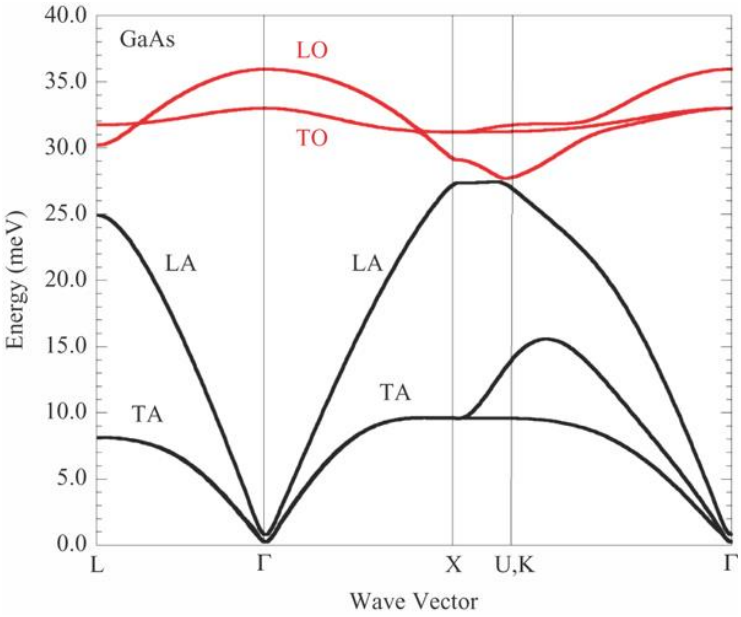
It turns out that for p atoms in the basis and D dimensions in the system there are **pD normal modes** in total (intuition: each atom can independently move in D dimensions; so in 3D, each atom can independently move in x, y, and z direction)

We see in the table above that D of the modes are in the **acoustic** branch

Thus, **D(p-1)** are in the **optical** branch. This means that a material with a monatomic basis will not have any optical phonons.

The image below shows atomic vibration dispersions in GaAs, a 3D material with 2 atoms in the primitive basis. The letters on the horizontal axis denote different propagation directions ([100]=$\Gamma \rightarrow X$,[110]=$\Gamma \rightarrow K$,[111]=$\Gamma \rightarrow L$). Γ is at k=0. We expect 3 acoustic dispersions and 3 optical ones. Notice

that in some propagation directions, the transverse branches are degenerate and it only looks like there are 2 total, but in less symmetric ones (e.g. [110]) they are not and you clearly see the expected result of 3 optical and 3 acoustic branches.



Quantization of elastic waves

So far, we have not explicitly called on the quantum nature of atoms in a solid.

It turns out that the energy of crystal lattice vibrations is **quantized**, meaning the ω variable we have been using does not exhibit continuum values, but rather, exhibits discrete values.

A quantum of crystal lattice vibration is called a **phonon.** Generally, the suffix –on in physics connotes something that behaves as a discrete particle. So just like light can behave like both a particle and a wave in different circumstances, so can waves originating from atomic vibrations in solids.

Going back to the definition of a quantum harmonic oscillator, the energy of an elastic mode of angular frequency ω is:

$$E = \left(n + \frac{1}{2}\right)\hbar\omega$$

$\frac{1}{2}\hbar\omega$ is the zero point energy of the mode, and when $n > 0$ it means that the mode is occupied by n phonons

Quantization of phonon amplitude

Consider a wave solution in 1 dimension of the form $u = u_0 cos\ Kx cos\ \omega t$, where u_0 is the amplitude

The energy of a mode in a harmonic oscillator is, on average, distributed half between kinetic energy and half between potential energy.

The **kinetic energy** per unit volume is given by $\frac{1}{2}\rho v^2 = \frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2 = \frac{1}{2}\rho u_0^2\omega^2 \cos^2 Kx \sin^2 \omega t$ where ρ is the mass density.

In a crystal of volume V, this comes out to $\frac{1}{4}\rho u_0^2\omega^2 \sin^2 \omega t$
where the extra factor of ½ comes from the avg value of Cos^2 in a spatial integration interval.

The average value of $\sin^2 \omega t$ over time is similarly ½, so the time and spatially averaged kinetic energy is given by:

$\frac{1}{8}\rho V\omega^2 u_0^2 = \frac{1}{2}\left(n + \frac{1}{2}\right)\hbar\omega$ where the extra factor of ½ on the right side comes because on average half of the energy of a harmonic oscillator is kinetic energy

This gives:

$$u_0 = 4\left(n + \frac{1}{2}\right)\hbar/\rho V\omega$$

This shows that the amplitude of a lattice wave does not take on continuous values, but rather, is allowed discrete quantized values based on the integer n

Quantization of momentum

Quantization of momentum can be derived by adding boundary conditions to our 'guess' of a solution, $u = u_0 e^{i(kna-\omega t)}$, specifically, periodic boundary conditions. We assume that there are N atoms in the chain and u(Na)=u(0). Equivalently, u([N+1]a)=u(a).

Plugging this into the wave-like solution, we get:

$$e^{i(kNa-\omega t)} = e^{i(0-\omega t)}$$

$$e^{ikNa} = 1$$

$$kNa = 2\pi n \text{ (where n is an integer)}$$

$$k = \frac{2\pi n}{aN}$$

Thus, k is not a continuous variable, but it only takes on quantized solutions. However, for large N, the spacing between adjacent values is very small.

Phonon momentum

The horizontal axis of the $\omega(k)$ plots we have been drawing is alternately called 'momentum' and 'wavevector'. It is connected to the reciprocal lattice via the concept of the 'Brillouin zone' which sets the minimum range of k needed to capture all of the information contained in $\omega(k)$ without redundancies. It should be noted that reciprocal space is also called 'momentum space.'

The momentum of a phonon is similar to a free-space momentum in some ways, but different in other ways.

Similar: if a phonon makes a collision with a particle, such as a neutron or electron, it can impart its momentum and energy to that particle and vis versa. This is how phonon dispersions are measured experimentally. Typically, a beam of neutrons with a known incoming momentum and energy is fired at a crystalline material, and the distribution of momenta and energies of the diffracted beam gives information about energy and momentum that was lost/gained from colliding with phonons. This property of phonons highlights the particle-like nature of their duality.

Different: a phonon cannot take on any arbitrary momentum and its available momentum states are subject to the periodicity of the reciprocal lattice. For example, a momentum **k** is equivalent to **k+G** where **G** is any vector of the reciprocal lattice. As a corollary, if a phonon encounters a collision with a particle with momentum **K** such that the phonon momentum becomes **k'=k+K** and **k'** falls outside of the first Brillouin zone, its final momentum will be equivalently be expressed as **k''=k-G**, where **k''** is in the first Brillouin zone.

In the next chapter, we will use the concept of phonons and their sometimes particle-like nature to understand thermal phenomena in real materials such as heat capacity and thermal conductivity.