Physics 0551 Lecture #10

Title: Lattice vibrations of a monoatomic lattice.
Justification: So far we have considered *two* fundamental properties of a system composed of a periodic arrangement of atoms.

1. The interaction of our lattice with incident plane waves (i.e., Diffraction)
2. The self-energy of this array and the forces between array members. In either case we have assumed that the ions are *fixed* at their equilibrium positions (T=0). Furthermore we have ignored the zero point motion.

Today we will investigate the vibrational properties of this lattice. It is the next "logical" step in our course of study. Since we want to examine well-conditioned non-pathological problems:

Lattice constituents are *very close* to equilibrium. Thus a *harmonic approximation* is valid.
We will examine a single constituent:

(ith atom)
equilibrium position r_0

Examine r_i potential as a function of displacement from equilibrium for $V(r_i - r_0)$. Using a Taylor series expansion:

$$V(r_i - r_0) = V(0) + \frac{dV}{dr_i}|_{r_i=r_0}(r_i - r_0)\frac{1}{2}\,\frac{d^2V}{dr_i^2}|_{r_i=r_0}(r_i - r_0)^2 + ...$$

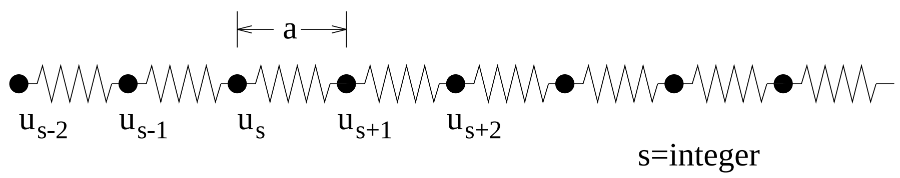
if $r_i \approx r_0$, then $\frac{dV}{dr_i} \approx 0$, since r_0 is the equilibrium position. Also if $r_i \approx r_0$, $r_i - r_0$ is small and $(r_i - r_0)^2 >> (r_i - r_0)^3$. Thus

$$V(r_i - r_0) \approx V(0) + \frac{1}{2}\,\frac{d^2V}{dr_i^2}|_{r_i=r_0}(r_i - r_0)^2$$

Note: The absolute displacements can be large, but relative displacements must be small if we are to have harmonic restoring forces
V(r) $\propto r^2 \rightarrow$ Hooke's Law relationship or a *harmonic* approximation

So let us examine the simplest periodic system within the context of the harmonic approximation. A sequence of masses m, connected with springs of force constant c, and separation a

Mass m



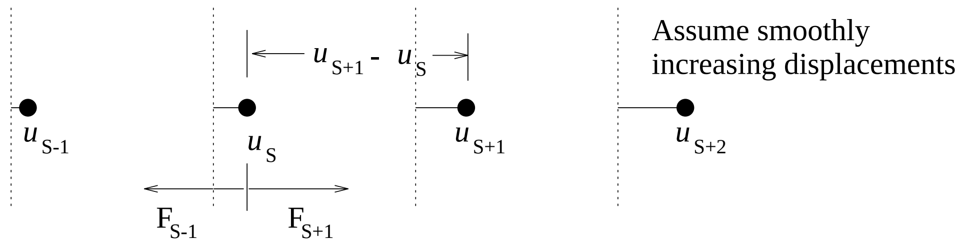
The collective motion of these springs will correspond to solutions of a wave equation. It is with this property we will focus.

Note: By construction we can see that 3 types of wave motion are possible,
2 Tranverse, 1 Longitudinal (or Compressional)

Tranverse $\rightarrow$ Displacement is perpendicular to the direction of motion of the wave

Longitudinal $\rightarrow$ Displacement is parallel to the direction of wave motion.

How does the system appear with a longitudinal wave:



The force on u_s due to the interaction with u_{s-1}, u_{s+1}

F_s = Total force $= c[(u_{s+1} - u_s) - (u_s - u_{s-1})] = F_{s+1,s} - F_{s-1,s}$ or

$m\ddot{u}_s = c[u_{s+1} + u_{s-1} - 2u_s]$

There is one equation of motion for every atom. These are simply coupled difference equations with a general solution $u_s = u_0 i^{(ksa-wt)}$ (We made a good guess!)

This solution is that of a travelling wave where

u_0 is the amplitude, s is an integer,

k is the wave momentum, $p = \hbar k$, $k = 2\pi\lambda$, $E = \hbar\omega$

Recall: A wave has *two* velocities

$v_s = \frac{d\phi}{dt}$ = phase velocity $= \frac{\omega}{k}$

$v_g = \frac{d\omega}{dk}$ = group velocity $\rightarrow$ Describes the motion of energy in the wave.

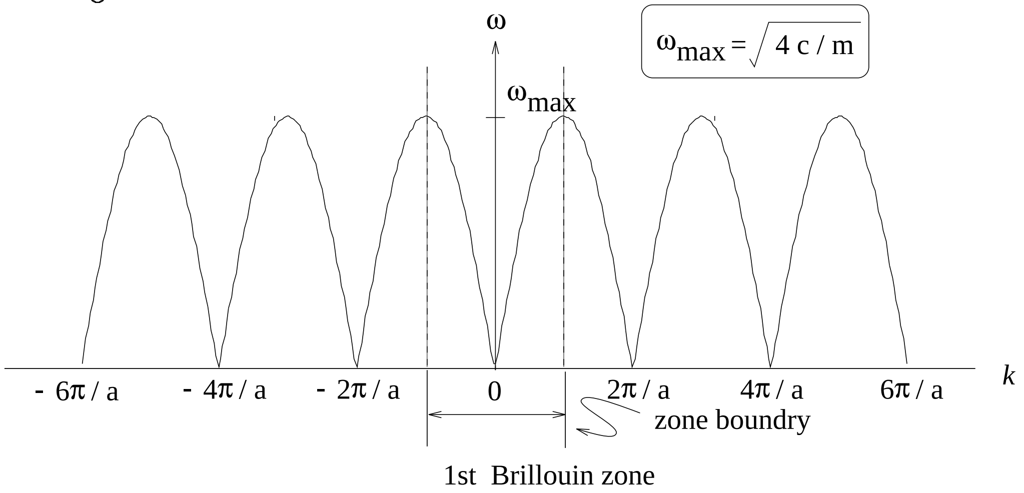
Thus $u_{s-1} = u_0 e^{i(k(s-1)a-\omega t)}$ and $u_{s+1} = u_0 e^{i(k(s+1)a-\omega t)}$

and $\ddot{u}_s = -\omega^2 u_0 e^{(iksa - \omega t)}$

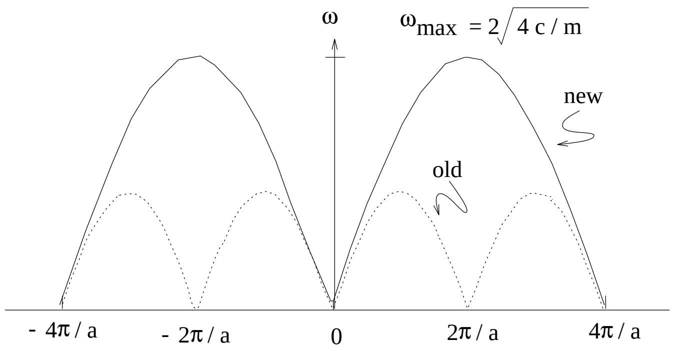
Substitute these into the initial force expression

$$\begin{aligned}
-m\omega^2 u_0 e^{i(ksa-\omega t)} &= cu_0[e^{ik(s+1)a} + e^{ik(s-1)a} - 2e^{iksa}]e^{i\omega t} \\
-m\omega^2 &= c(e^{ika} + e^{-ika} - 2) \\
m\omega^2 &= c(e^{ika/2} - e^{-ika/2})^2 \\
m\omega^2 &= -c(2i \sin ka/2)^2 \\
\omega^2 &= 4c/m[\sin^2 ka/2] \\
\omega &= \sqrt{4c/m}\,|\sin(ka/2)| \rightarrow \text{ This is a very important result} \\
\omega &= f(k)
\end{aligned}$$

Plotting:



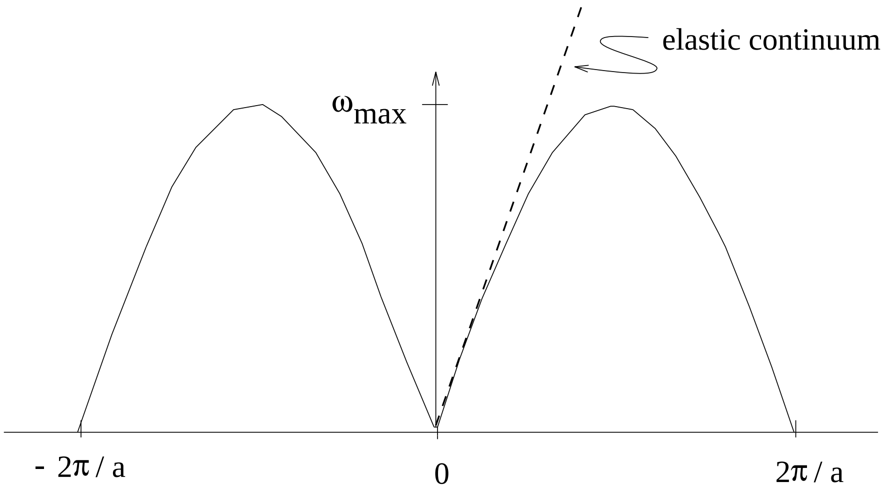
1) Notice the replication, *all* pertinent information is contained within the first zone.
2) Notice what happens if let $a' = a/2$, $m' = m/2$ and $c' = 2c$ and compare the new solution with the previous one:



And so on....., this is called the *elastic continuum*.

The solution $\omega = \sqrt{4c/m}\ |\sin\ ka/2|$ relates the frequency (or equivalently the energy of the wave) to the wave-vector or (momentum of the wave) .

This relationship is called a dispersion relation. It is important to look at the limiting cases



$k \to 0$ (long wavelength) $\lambda >> a$

$$v_s = \frac{\omega}{k} = \frac{1}{k}\sqrt{\frac{4c}{m}}\ \sin\ ka/2 \approx \frac{1}{k}\ \sqrt{\frac{4c}{m}}\ \left(\frac{ka}{2}\right) = \sqrt{\frac{ca^2}{m}} = \text{elastic continuum}$$

$$v_g = \frac{d\omega}{dk} = \sqrt{\frac{4c}{m}}\ \frac{a}{2}\ \cos\left(\frac{ka}{2}\right) = \sqrt{\frac{ca^2}{m}} = v_s,\ \text{no } k \text{ dependence}$$

No "dispersion" at long wavelengths

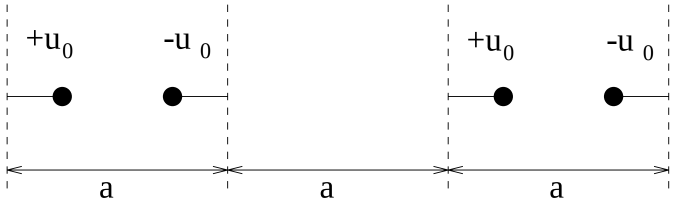
One way to think about it: All waves travel at the same speed and therefore do not spread out (or disperse), this is identical to the elastic continuum.

Back to the one dimensional array of springs:

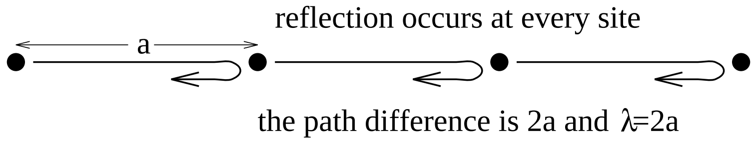
$$\begin{aligned}
\text{At } k &= \pi/a\ \ \omega = \sqrt{4c/m}, \\
v_s &= \frac{\omega}{k} = \frac{a}{\pi}\ \sqrt{4c/m}\ \text{ the phase at a point changes} \\
v_g &= \frac{d\omega}{dk} = 0\ \text{ thus no energy can travel through the lattice.}
\end{aligned}$$

Let us examine the solution at $q = \pi/a$ in more detail

$$\Delta u_s = u_0\ e^{(iksa-\omega t)} = u_0\ e^{i\omega t}(-1)^s$$



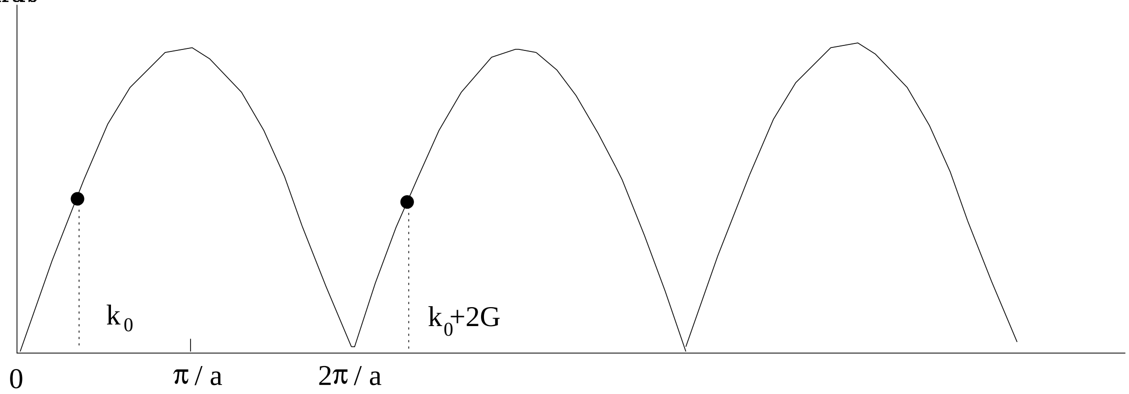
This is just a standing wave with adjacent atoms moving out of phase. A standing wave is composed of 2 waves of equal amplitudes, frequency and wavelength which travel in opposite directions. These waves result from constructive interference of wavelets reflected from each atom.



Recall the periodic nature of the ω vs k relationship. The only k vectors (for lattice vibrations) which have physical meaning are those within the range

$\left(-\frac{\pi}{a} \leq q \leq \frac{\pi}{a}\right)$ or in the 1st Brillouin zone.

So what does this mean graphically. Let us examine $k = k_0 + 2G \quad G = 2\pi/a$ thus



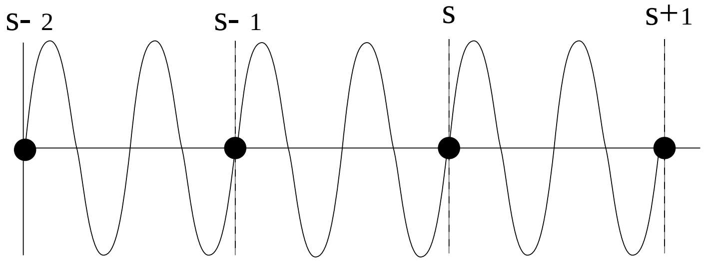
$$\text{if } k = k_0 + 2G \quad \lambda = \frac{2\pi}{k_0 + 4\pi a}, \quad \text{wavelength is short,}$$

$\lambda < a/2$! The lattice cannot support this wave

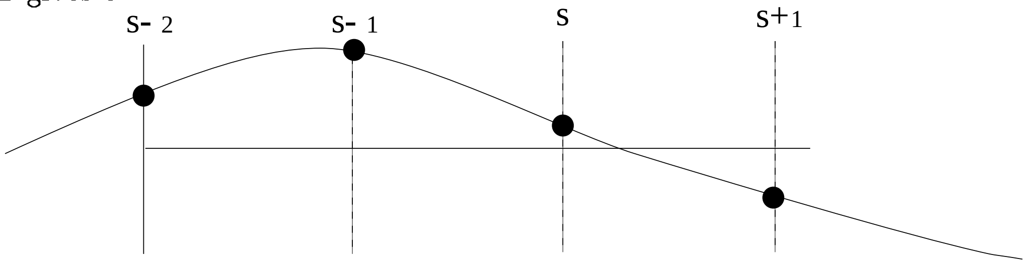
Our wave solution gives

$$\begin{aligned} u_s &= u_0\ e^{i((k_0+2G)sa+\omega t)} \\ &= u_0\ \underbrace{e^{ik_0 sa}}_{A}\ \ \underbrace{e^{i4\pi s}}_{B}\ \ e^{i\omega t} \end{aligned}$$

A gives e$^{i4\pi}$



B gives e^{ik_0}



The product gives a superposition with no new information.