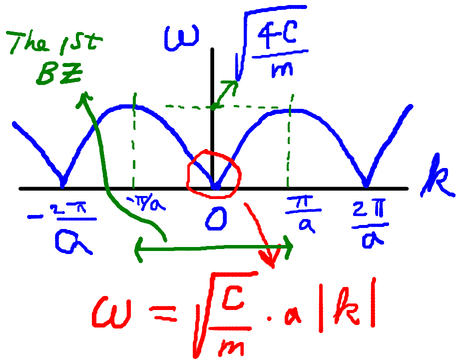
Lecture 07

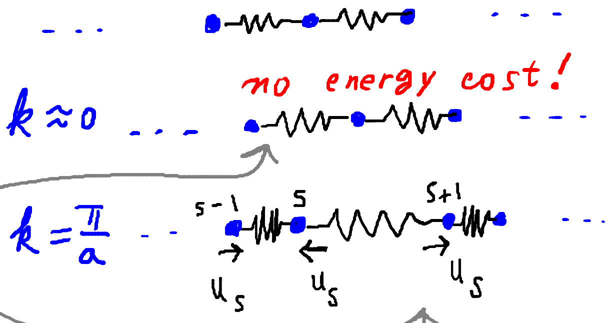
Tuesday, January 31, 2012

Note on notation:

In the phonon part, Kittel uses $\vec{K}$ for $\vec{k}$ (or K for k). Later on Kittel uses $\vec{k}$ to mean the same thing, i.e. a general wave vector, for the electron! This is a bit non-standard (cf. A&M). It seems better to use the small letter $\vec{k}$ to mean a general wave vector for any wave in a crystal, be it phonon, electron or something else like neutron. Thus, I will stick to the notation that $\vec{K}$ or $\vec{G}$ refers to the reciprocal lattice vector, and $\vec{k}$ refers to the general wave vector.

Phonons in 1D (monatomic crystal)





Important Physics

- $\omega \to 0$ as $k \to 0$ (long wave length sound wave).
  - Why? Because on a local scale, it is just a translation.
  - This fact often goes by the name of "Goldstone theorem/boson." When a continuous symmetry broken, then a long wave length zero energy boson **emerges**.
  - Similar to how **Debye** thought of phonons.
  - Group velocity $\frac{d\omega}{dk} = \pm\sqrt{\frac{C}{m}}a$. **Speed of sound** = $\sqrt{\frac{C}{m}}a$.
- $\omega = \sqrt{\frac{4C}{m}}$ at the BZ boundary, i.e. $k = \pm\pi/a$.
  - Why? $u_s = ue^{ikas}e^{-i\omega t}$ means u_s at near neighbors are completely out of phase ($u_s = -u_{s\pm1}$).
  - Thus, force on atom at index $s = -2Cu_s - 2Cu_s$, from left and right springs. The effective spring constant = $4C$.

- ○ As though vibrations are all localized, with that effective spring constant.
- ○ Similar to how **Einstein** thought of phonons.
- ○ Group velocity $\frac{d\omega}{dk} = 0$. **Standing wave**! Often the case for waves in crystal: standing waves tend to form at the **BZ boundary** (more about this later).

Phonons and the emergence

The long wave length phonon is a collective phenomenon that arises only because a large number of particles form a crystalline state. The details of microscopic interactions are not important at all or far less important, in comparison to the fact that *when we have any crystal, no matter what kind it is, we know that there must be long wave length phonons with zero energy*. Such sure quality that emerges out of the many body character, or the statistical nature, of a system is often called an **emergent phenomenon**.

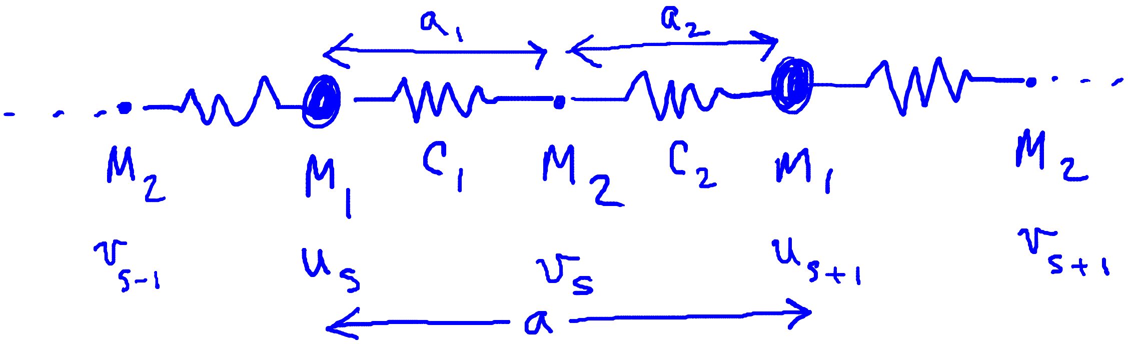
There are many examples that can be called emergent phenomena (http://emergentuniverse.org/). Condensed matter physics is essentially a study of emergent phenomena, of which we will discuss several important examples in this course. The long wave length phonons (and the associated elasticity) are perhaps the simplest example of all, and thus the most classic example.

It is worth noting that in the case of phonons, there is a theorem (Goldstone theorem) that says that if a continuous symmetry is broken then there must be a long wave length emergent excitation, whose energy goes to zero as k goes to zero. Why this is so should be obvious in the above diagram ("no energy cost!").

Thus, the fact that the phonon energy approaches zero at wave length, while derived from the simplest model of a crystal, a monatomic 1D crystal with the nearest neighbor interaction only, should be viewed as a much more general property, which is valid as long as the interaction between atoms or ions in the crystal are reasonably short-ranged, so that a the long wave length mode costs essentially no energy, as pictured in the above diagram.

In this respect, it is not surprising that $\omega_k \to 0$ as $k \to 0$, even if one includes next neighbor interactions and so on (i.e. the interaction between atoms that are more than one lattice point away). However, the functional form can deviate from $c|k|$ (cf. Ashcroft and Mermin, Prob. 22.1, and Kittel pages 94-95 "Derivation of Force Constants …").

Phonons in a 1D crystal with two atoms per unit cell



The most important thing here is that the travelling wave solution can be written as

$$u_s = ue^{iksa}e^{-i\omega_k t}$$

$$v_s = ve^{iksa}e^{-i\omega_k t}$$

Why? The short answer is that this fits with the general form of "waves in crystal" that I presented before. Amplitude $= P(\vec{r})e^{i\vec{k}\cdot\vec{r}}$, where P is a lattice periodic function. In this case, $P(x) = \sum_s \left(u\delta_{x,sa} + ve^{-ika_1}\delta_{x,s(a+a_1)}\right) e^{-i\omega_k t}$, i.e. a series of periodic spikes at the atomic positions.

That the waves in crystal can be written in this form is the content of the important **Bloch's theorem**. We will prove it later in this course.

Possible cases:

1. $M_1 \neq M_2$ and $C_1 = C_2 = C$ (and $a_1 = a_2$ if the crystal is inversion symmetric).
2. $M_1 = M_2$ and $C_1 \neq C_2$ (and $a_1 \neq a_2$ most likely).

Once you correctly write down the wave function, then the rest is mostly "just math."

Let us consider case 1.

$$M_1 \ddot{u}_s = C\left(v_s + v_{s-1} - 2u_s\right)$$
$$M_2 \ddot{v}_s = C\left(u_{s+1} + u_s - 2v_s\right)$$

$$-\omega^2 M_1 u = C\, v(1+e^{-ika}) - 2Cu$$

$$-\omega^2 M_2 v = C\, u\,(1+e^{ika}) - 2Cv$$

$$\begin{bmatrix} 2C - M_1\omega^2 & -C(1+e^{-ika}) \\ -C(1+e^{ika}) & 2C - M_2\omega^2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = 0$$

We have a set of linear equations defined by a 2 × 2 matrix. It is straightforward to calculate the determinant of the matrix. Set it to 0 for non-trivial solutions of u, v. And, voila, the eigenvalue, ω, and the eigenvector, $[u, v]$, come out. The result for the eigenvalue is:

$$\boxed{\omega_k = \sqrt{\frac{C}{M_1 M_2}\left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos ka}\right)}}$$

basis

- **2** is the degrees of freedom within a primitive unit cell (u and v).
- The problem became a **2** × **2** matrix problem.
- The solution gives **2** branches.

all same 2's!

lattice

- $\omega_{k+G} = \omega_k$ since $\cos(ka + Ga) = \cos\left(ka + \frac{2\pi n}{a}a\right) = \cos(ka)$. This is of course the general property of waves in crystal.
- If $M_1 \to M_2$, the solution becomes that of the monatomic chain: $\omega_k = \sqrt{\frac{4C}{M}}\left|\sin\left(\frac{ka/2}{2}\right)\right|$ where the lattice constant $a/2$ for the monatomic chain is noted. Question: what happens to the other branch, $\omega_k = \sqrt{\frac{4C}{M}}\left|\cos\left(\frac{ka/2}{2}\right)\right|$ as $M_1 \to M_2$?

The limiting cases, $k \to 0$ and $k = \pm\frac{\pi}{a}$ (BZ boundary) are interesting.

For $k \to 0$, the two branches behave as

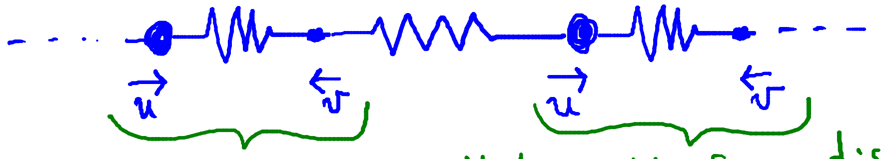
$$\omega_k \approx \sqrt{\frac{C}{2(M_1 + M_2)}}\; a|k| \leftarrow \text{acoustical}$$

$$\omega_k \approx \sqrt{2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}$$

← optical

These long wave length behaviors distinguish between acoustical and optical branches.

- Acoustical branch: $\omega_k \to 0$ as $k \to 0$ (Goldstone mode).
- Optical branch: $\omega_k \to$ a finite frequency as $k \to 0$.



$k=0$ means that each cell has the same distortion.

Optical mode : u is out of phase with v.

$uM_1 + vM_2 = 0$

Acoustical mode : $u \sim v$

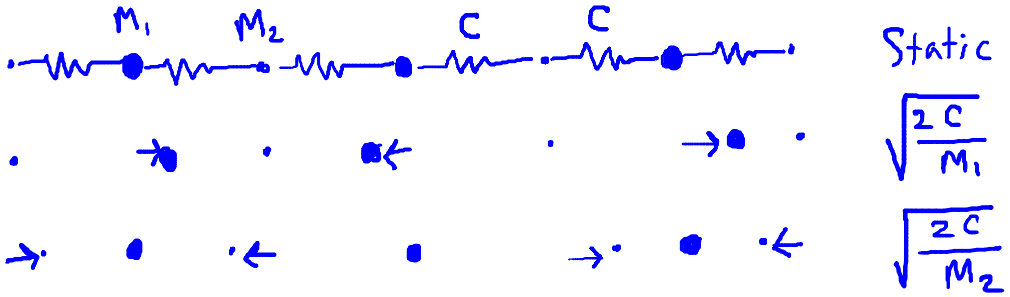
The optical mode corresponds to the fixed center of mass of the two atoms in the basis ($uM_1 + vM_2 = 0$) and the reduced mass $\mu = (M_1^{-1} + M_2^{-1})^{-1}$ oscillating with the effective spring constant is $2C$.

The name "optical" means that this is the mode that will couple to light, if different atoms carry opposite charges, as is often the case.

At $k = \pm\frac{\pi}{a}$, the two frequencies are

$$\omega_k = \sqrt{\frac{2C}{M_1}}, \sqrt{\frac{2C}{M_2}}$$

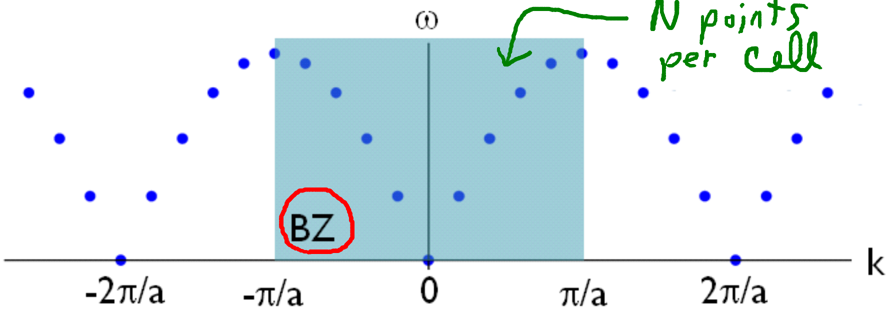
The smaller of these two frequencies belong in the acoustical branch, and the other in the optical branch. These are modes in which one kind of atom is completely at rest, while the other kind of atom vibrates out of phase in the nearest neighbor cells.

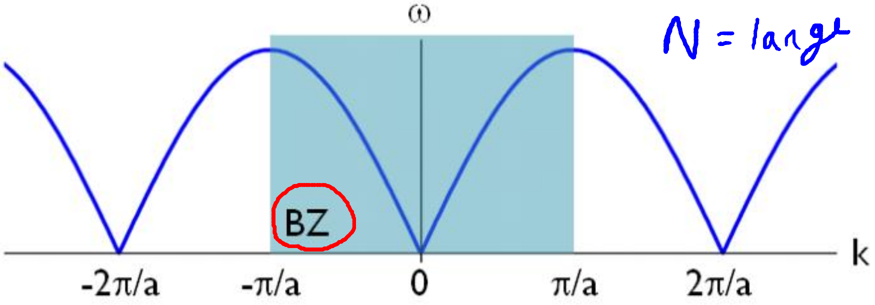


Summary: "Tuning" monatomic 1D crystal to di-atomic 1D crystal

Let us summarize by looking at some graphs.

Monatomic 1D Xtal. N = 10





Monatomic → Diatomic by "tweaking" mass

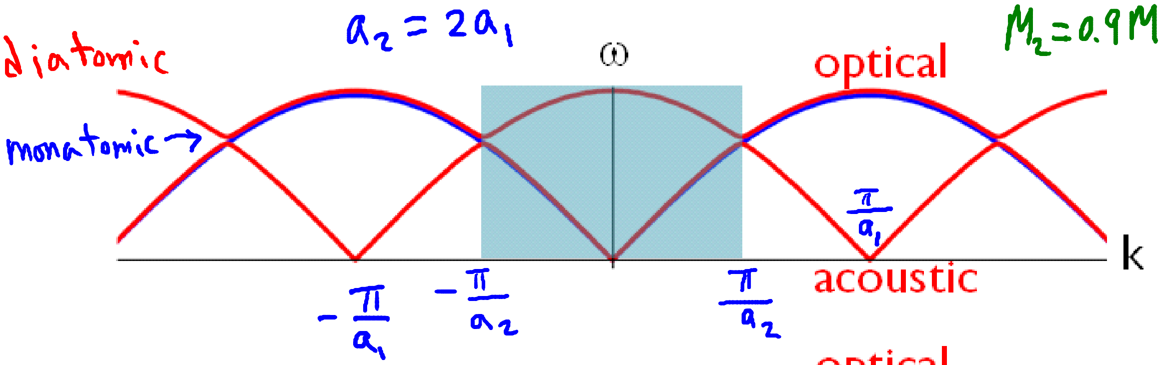
a_1 = lattice const. for

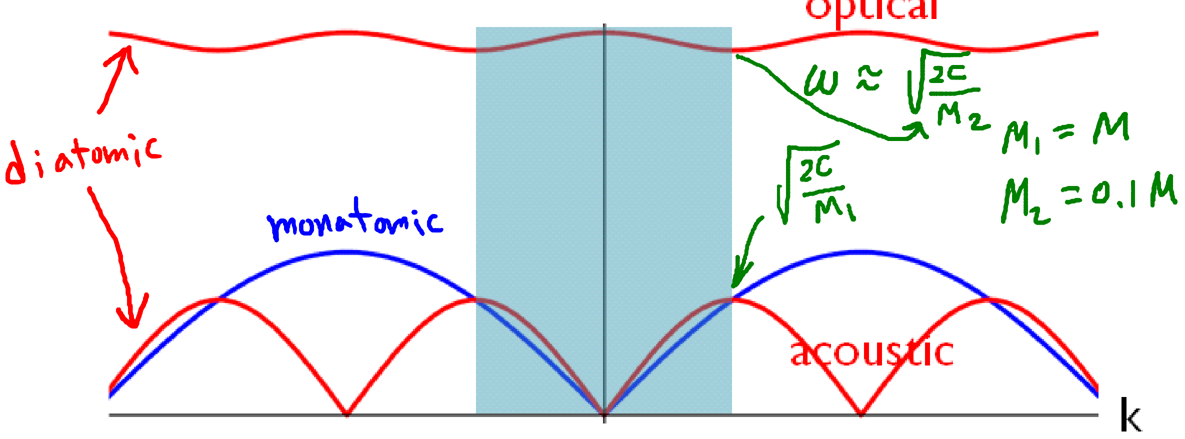
a_2 = lattice const. for

$M_1 = M$

$M_2 \neq M$

$a_2 = 2a_1$





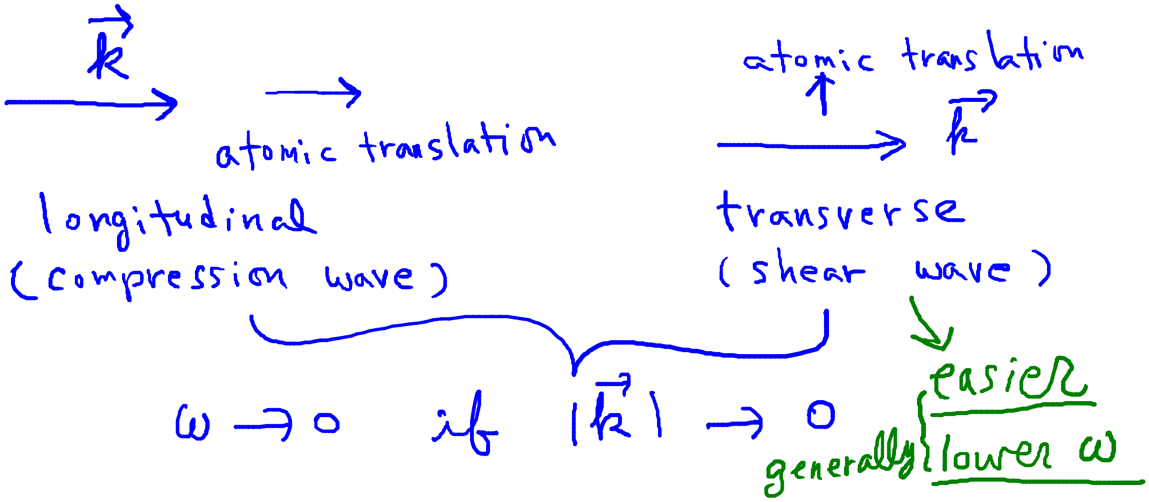
Counting and phonons in 3D or general dimensions

Let us generalize our problem to that of a D-dimensional problem with an arbitrary number (m) of atoms in the primitive basis.

1. The number of normal modes $= DmN$.
2. The number of distinct wave vectors $N_{\vec{k}} = N$ (last lecture).
3. The number of phonon branches $n_b = Dm =$ the number of degrees of freedom per cell. (Why? (1) # of branches = # of phonon modes for a fixed $\vec{k}$ = # of phonon modes for $\vec{k} = 0$, i.e. when all cells are identically vibrating. Or, (2) Divide DmN by $N_{\vec{k}} = N$.)
4. $n_a = D$ (Goldstone theorem). One longitudinal mode. The rest are

transverse.

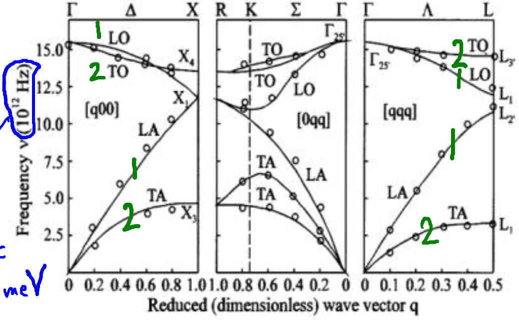
The last point can be understood easily since a D dimensional crystal breaks the translational symmetry in each of D directions. This corresponds to different **polarizations** for a given wave vector $\vec{k}$.



★★★		In one dimension	In D dimensions
m	Number of atoms in the primitive basis		
N	Number of bases in crystal		
n_b	Number of phonon **branches**	m	Dm
n_a	Number of acoustical phonon branches	1	D
n_o	Number of optical phonon branches	$n_b - n_a$	$n_b - n_a$
$N_{\vec{k}}$	Number of distinct $\vec{k}$ values	N	N
N_m	Number of phonon **modes** (i.e. normal modes)	$n_b N_{\vec{k}}$	$n_b N_{\vec{k}}$
N_p	Number of phonons (each phonon mode can have 0, 1, 2, … phonons excited)	Depends on temperatue, energy,…	Depends on temperatue, energy,…

Example of phonon spectra

Si



THz = 4.1 meV

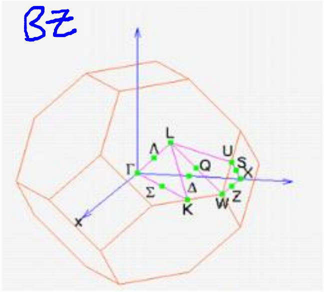
http://www.ioffe.rssi.ru/SVA/NSM/Semicond/SiGe/mechanic.html

green #'s = branch degeneracy

TA
LA
TO
LO

acoustic
optic

transverse
longitudinal



http://cst-www.nrl.navy.mil/~mehl/phonons/fcczone.png