3

Crystal Vibrations

Vibrations of atoms in a crystal give us waves (sound waves). This lecture studies these sound waves.

Model: consider atoms as points (sites) and consider a crystal as points connected by springs.

3.1. Vibrations of crystals with monotonic basis

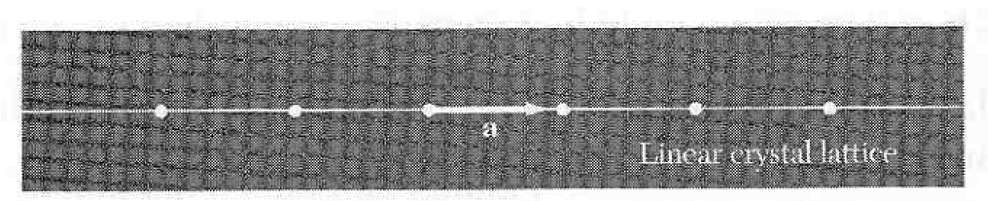

Fig. 1. a 1D crystal

3.1.1. Displacement and Force

Consider a 1D crystal with one atom per unit cell. Here we label the sites (atoms) using an integer $s = 1,\ 2,\ \ldots,\ N$

Displacement of site s: how far the site moves away from its equilibrium position: $u_s = R_s - R_s{}^{(0)}$ where R_s is the position of the site s and $R_s{}^{(0)}$ is the equilibrium positions.

Force on site s: F_S

$$F_S = C\,(u_{s+1} - u_s) + C(u_{s-1} - u_s) \tag{3.1}$$

Here we assume each spring follows the Hooke's law and C is the spring constant $F = C\,\Delta\mathrm{L}$ (assuming higher order terms are small)

3.1.2. Equation of motion

$$m\,\frac{d^2 u_s}{d t^2} = F_S = C\,(u_{s+1} - u_s) + C(u_{s-1} - u_s) = C(u_{s+1} + u_{s-1} - 2\,u_s) \tag{3.2}$$

3.1.3. Sound waves

To solve this equation, we consider a plane wave:

$$u_s = u \exp(i\,K\,s\,a) \exp(-i\,\omega\,t) \tag{3.3}$$

This u_s is complex and the real part of it is the true displacement.

Here the amplitude of this wave is u. The wavevector is $K = 2\,\pi/\lambda$. a is the lattice constant. The frequency of this wave is ω. For this wave, the equation of motion turns into

$$-m\,\omega^2\,u \exp(i\,K\,s\,a) \exp(-i\,\omega\,t) = C[\exp(i\,K\,a) + \exp(-i\,K\,a) - 2]\,u \exp(i\,K\,s\,a) \exp(-i\,\omega\,t) \tag{3.4}$$

Here we used the following relations:

$$u_s = u \exp(i K s a) \exp(-i \omega t) \tag{3.5}$$

$$u_{s+1} = u \exp[i K (s+1) a] \exp(-i \omega t) = u \exp(i K s a) \exp(-i \omega t) \exp(i K a) \tag{3.6}$$

$$u_{s-1} = u \exp[i K (s-1) a] \exp(-i \omega t) = u \exp(i K s a) \exp(-i \omega t) \exp(-i K a) \tag{3.7}$$

$$\frac{d^2 u_s}{d t^2} = u \exp(i K s a) \frac{d^2}{d t^2} \exp(-i \omega t) = -\omega^2 u \exp(i K s a) \exp(-i \omega t) \tag{3.8}$$

We can simplify the EOM:

$$-m \omega^2 = C[\exp(i K a) + \exp(-i K a) - 2] = 2 C[\cos(K a) - 1] \tag{3.9}$$

So

$$\omega^2 = 2 \frac{C}{m}[1 - \cos(K a)] \tag{3.10}$$

and thus

$$\omega = 2 \sqrt{\frac{C}{m}} \sqrt{\frac{1 - \cos(K a)}{2}} \tag{3.11}$$

Using the trigonometric identity $\sqrt{\frac{1-\cos\alpha}{2}} = \left|\sin\frac{\alpha}{2}\right|$

$$\omega = 2 \sqrt{\frac{C}{m}} \left|\sin\frac{K a}{2}\right| \tag{3.12}$$

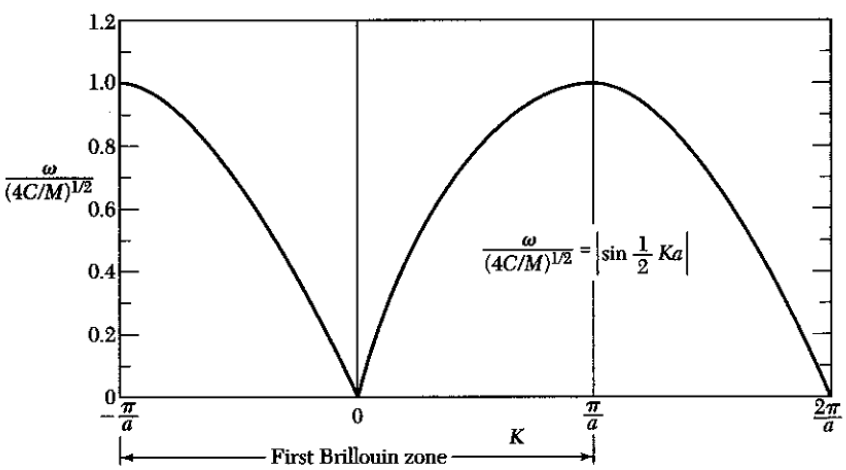

Fig. 2. ω as a function of K.

3.1.4. the long wave length limit

At small momentum (very small K, $K a << 1$), $\sin\frac{K a}{2} = \frac{K a}{2} + O\left(\frac{K a}{2}\right)^2$, so

$$\omega \approx a \sqrt{\frac{C}{m}} K \tag{3.13}$$

This limit is known as “the long wavelength limit”, becomes small K means very large wavelength ($\lambda = 2\pi/K \to \infty$ when $K \to 0$)

Here, the frequncy is a linear function of the wavevector and at $K = 0$, ω=0. This type of sound waves with $\omega \propto K$ are known as “acoustic sounds”.

For an acoustic sound mode, the relation between ω and K is very similar to the corresponding relation for light. For light, we have $\omega = c\, K$ where c is the speed of light. Here, we have $\omega = v\, K$ where $v = a \sqrt{C/m}$ is the speed of this sound wave.

3.1.5. the continuum limit

If we set the lattice spacing to be very small ($a \to 0$), when this lattice model should recover the continuum limit. Here, the continuum limit is the same as the long wave length limit, because both these two limit have $k\, a << 1$, so

$$\omega = 2 \sqrt{\frac{C}{m}} \left| \sin \frac{K\, a}{2} \right| \approx a \sqrt{\frac{C}{m}}\, K \tag{3.14}$$

3.1.6. Brillouin zone boundary $K = \pi / a$

At $K = \pi / a$

$$u_s = u \exp(i\, K\, s\, a) \exp(-i\, \omega\, t) = u \exp(i\, \pi\, s) \exp(-i\, \omega\, t) = (-1)^s\, u \exp(-i\, \omega\, t) \tag{3.15}$$

This is a standing wave, where even sites and odd sites move in the opposite way.

3.2. Quantization of sound waves

Quantum mechanics tells us that for a wave with frequency ω and wavevector k, we can consider it as a beam of particles with energy $E = \hbar\omega$ and momentum $P = \hbar\, K$.

For EM waves (light), the corresponding particles are photons.

For sound waves, the corresponding particles are called "phonons".

The energy of a phone is E=$\hbar\omega$ and we know that

$$E = 2\, \hbar \sqrt{\frac{C}{m}} \left| \sin \frac{P\, a}{2\, \hbar} \right| \tag{3.16}$$

At small momentum (very small P, $P\, a / 2\, \hbar << 1$), we have

$$E = a \sqrt{\frac{C}{m}}\, P \tag{3.17}$$

3.3. Sound velocities: phase velocity and group velocity

3.3.1. Phase velocity

The phase velocity of a wave is

$$v_p = \frac{\omega}{K} \tag{3.18}$$

For this sound wave, $\omega = 2 \sqrt{\frac{C}{m}} \left| \sin \frac{K\, a}{2} \right|$, so we have

$$v_p = \frac{\omega}{K} = 2 \sqrt{\frac{C}{m}} \frac{\left| \sin \frac{K\, a}{2} \right|}{K} \tag{3.19}$$

at small K (the long wavelength limit),

$$v_p = \frac{\omega}{K} = 2\sqrt{\frac{C}{m}}\,\frac{\left|\sin\frac{K a}{2}\right|}{K} \approx 2\sqrt{\frac{C}{m}}\,\frac{\frac{K a}{2}}{K} = \sqrt{\frac{C}{m}}\,a \tag{3.20}$$

3.3.2. Group velocity

The group velocity measures the velocity of a wave packet. It is defined as:

$$v_g = \frac{d\omega}{dK} \tag{3.21}$$

For this sound wave, $\omega = 2\sqrt{\frac{C}{m}}\left|\sin\frac{K a}{2}\right|$. For the first Brillouin zone $(-\pi/a < K < \pi/a)$, $\omega = 2\sqrt{\frac{C}{m}}\sin\frac{K a}{2}$, because in this region $\sin\frac{K a}{2} \geq 0$

$$v_g = \frac{d\omega}{dK} = 2\sqrt{\frac{C}{m}}\,\frac{d}{dK}\sin\frac{K a}{2} = a\sqrt{\frac{C}{m}}\cos\frac{K a}{2} \tag{3.22}$$

At small K (the long wavelength limit), $v_g \approx v_p$

$$v_g = a\sqrt{\frac{C}{m}}\cos\frac{K a}{2} \approx a\sqrt{\frac{C}{m}} \tag{3.23}$$

which is the same as v_p at small K

At the edge of the Brillouin zone, $K = \pi/a$,

$$v_g = a\sqrt{\frac{C}{m}}\cos\frac{\pi}{2} = 0 \tag{3.24}$$

Zero group velocity means that there is no energy flow. As discussed above, $K = \pi/a$ has a standing wave, which indeed has no energy flow.

3.4. two atoms per primitive basis

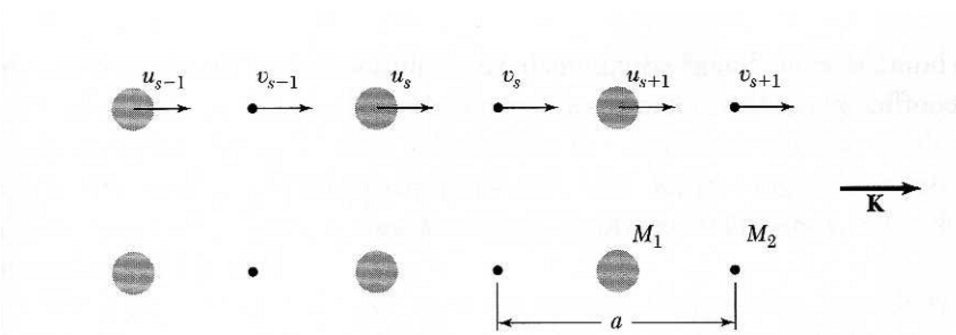

Fig. 3. a 1D crystal formed by two different types of atoms

3.4.1. Equations of motion

Two types of atoms. ABABABABAB...

- Use an integer s to label each unit cell (each unit cell contains two atoms: 1 A tome and 1 B atom)
- Use u_s to describe the displacement of A atoms
- Use v_s to describe the displacement of B atoms

The equations of motion is

$$M_1 \frac{d^2 u_s}{d t^2} = F_S = C\,(v_s - u_s) + C(v_{s-1} - u_s) = C(v_s + v_{s-1} - 2\,u_s) \tag{3.25}$$

$$M_2 \frac{d^2 v_s}{d t^2} = F_S = C\,(u_{s+1} - v_s) + C(u_s - v_s) = C(u_{s+1} + u_s - 2\,v_s) \tag{3.26}$$

Here M_1 and M_2 are the masses for atoms A and B respectively.

So we have

$$M_1 \frac{d^2 u_s}{d t^2} = C(v_s + v_{s-1} - 2\,u_s) \tag{3.27}$$

$$M_2 \frac{d^2 v_s}{d t^2} = C(u_{s+1} + u_s - 2\,v_s) \tag{3.28}$$

3.4.2. Sound wave solutions

Let’s consider sound waves

$$u_s = u \exp(i\,K\,a\,s) \exp(-i\,\omega\,t) \tag{3.29}$$

$$v_s = v \exp(i\,K\,a\,s) \exp(-i\,\omega\,t) \tag{3.30}$$

Here, a is the lattice constant (the size of a unit cell. NOT the distance between neighboring A and B atoms).

Now, the EOM will take the form

$$-M_1\,\omega^2\,u \exp(i\,K\,a\,s) \exp(-i\,\omega\,t) = C\left(v_s + v_s\,e^{-i\,k\,a} - 2\,u\right) \exp(i\,K\,a\,s) \exp(-i\,\omega\,t) \tag{3.31}$$

$$-M_2\,\omega^2\,v \exp(i\,K\,a\,s) \exp(-i\,\omega\,t) = C\left(u_{s+1}\,e^{i\,k\,a} + u_s - 2\,v\right) \exp(i\,K\,a\,s) \exp(-i\,\omega\,t) \tag{3.32}$$

So

$$M_1\,\omega^2\,u = -C\left(v + v\,e^{-i\,K\,a} - 2\,u\right) \tag{3.33}$$

$$M_2\,\omega^2\,v = -C\left(u\,e^{i\,K\,a} + u - 2\,v\right) \tag{3.34}$$

So

$$\left(M_1\,\omega^2 - 2\,C\right) u + C\left(1 + e^{-i\,K\,a}\right) v = 0 \tag{3.35}$$

$$C\left(e^{i\,K\,a} + 1\right) u + \left(M_2\,\omega^2 - 2\,C\right) v = 0 \tag{3.36}$$

We can write these two equations into a matrix form

$$\begin{pmatrix} M_1\,\omega^2 - 2\,C & C(1 + e^{-i\,K\,a}) \\ C(e^{i\,K\,a} + 1) & M_2\,\omega^2 - 2\,C \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3.37}$$

where u and v are the two unknowns for these two equations.

For this type of linear equations, to have nontrivial solution (u and v being nonzero), we must have

$$\det\begin{pmatrix} M_1\,\omega^2 - 2\,C & C(1 + e^{-i\,K\,a}) \\ C(e^{i\,K\,a} + 1) & M_2\,\omega^2 - 2\,C \end{pmatrix} = 0 \tag{3.38}$$

This condition give us a relation between ω and K

$$\begin{aligned}\det\begin{pmatrix} M_1\,\omega^2 - 2\,C & C(1 + e^{-i\,K\,a}) \\ C(e^{i\,K\,a} + 1) & M_2\,\omega^2 - 2\,C \end{pmatrix} &= \left(M_1\,\omega^2 - 2\,C\right)\left(M_2\,\omega^2 - 2\,C\right) - C^2\left(1 + e^{-i\,K\,a}\right)\left(e^{i\,K\,a} + 1\right) = \\ &\left(M_1\,M_2\,\omega^4 + 4\,C^2 - 2\,C\,M_1\,\omega^2 - 2\,C\,M_2\,\omega^2\right) - C^2\left(2 + e^{-i\,K\,a} + e^{i\,K\,a}\right) = \\ &\left(M_1\,M_2\,\omega^4 + 4\,C^2 - 2\,C\,M_1\,\omega^2 - 2\,C\,M_2\,\omega^2\right) - 2\,C^2(1 + \cos K\,a) = 0\end{aligned} \tag{3.39}$$

So

$$M_1\, M_2\, \omega^4 - (2\, C\, M_1 + 2\, C\, M_2)\, \omega^2 + 2\, C^2 (1 - \cos K\, a) = 0 \tag{3.40}$$

The solution to this equation is:

$$\omega^2 = \frac{2\, C\, M_1 + 2\, C\, M_2 \pm \sqrt{(2\, C\, M_1 + 2\, C\, M_2)^2 - 8\, M_1\, M_2\, C^2 (1 - \cos K\, a)}}{2\, M_1\, M_2} = \frac{C\, M_1 + C\, M_2 \pm \sqrt{(C\, M_1 + C\, M_2)^2 - 2\, M_1\, M_2\, C^2 (1 - \cos K\, a)}}{M_1\, M_2} \tag{3.41}$$

where the "+" solution is known as the optical branch and the "-" one is known as the acoustic branch

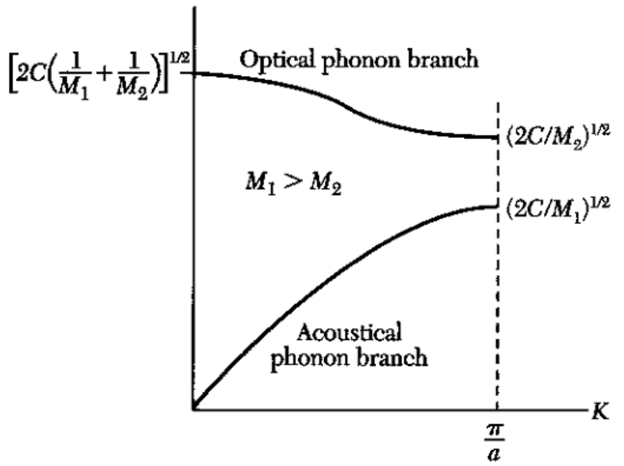

Fig. 4. ω as a function of K. Notice that there are two branches of solutions. The low branch is called acoustic branch and the upper one is the optical branch.

3.4.3. the long wave length limit ($K \approx 0$)

In the long wave length limit (or the continuum limit), where $K\, a << 1$, we can set $\cos K\, a = 1$ for the optical branch

$$\omega^2 = \frac{C\, M_1 + C\, M_2 + \sqrt{(C\, M_1 + C\, M_2)^2}}{M_1\, M_2} = \frac{2\, C\, M_1 + 2\, C\, M_2}{M_1\, M_2} = 2\, C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \tag{3.42}$$

For the acoustic branch, setting $\cos K\, a = 1$ will give us $\omega^2 = 0$, which is not good enough. So we need to keep higher order terms here and set $\cos K\, a \approx 1 - (K\, a)^2 / 2$. Then we have,

$$\omega^2 = \frac{C\, M_1 + C\, M_2 - \sqrt{(C\, M_1 + C\, M_2)^2 - M_1\, M_2\, C^2\, K^2\, a^2}}{M_1\, M_2} = \frac{C\, M_1 + C\, M_2}{M_1\, M_2} \left(1 - \sqrt{1 - \frac{M_1\, M_2\, C^2\, K^2}{(C\, M_1 + C\, M_2)^2}\, a^2} \right) \approx \frac{C\, M_1 + C\, M_2}{M_1\, M_2} \left(\frac{1}{2} \frac{M_1\, M_2\, C^2\, K^2}{(C\, M_1 + C\, M_2)^2}\, a^2 \right) = \left(\frac{1}{2} \frac{C\, K^2}{M_1 + M_2}\, a^2 \right) \tag{3.43}$$

So

$$\omega = \sqrt{\frac{1}{2} \frac{C}{M_1 + M_2}\, a^2}\; K \tag{3.44}$$

The acoustic mode has $\omega \propto K$, so we have $\omega = 0$ at $K = 0$. But the optical mode has finite ω at $K = 0$.

3.4.4. the edge of the zone $K = \pi/a$

At zone edge $K = \pi/a$, $\cos K a = -1$

$$\omega^2 = \frac{C M_1 + C M_2 \pm \sqrt{(C M_1 + C M_2)^2 - 4 M_1 M_2 C^2}}{M_1 M_2} = \frac{C M_1 + C M_2 \pm \sqrt{(C M_1 - C M_2)^2}}{M_1 M_2} = \frac{C M_1 + C M_2 \pm (C M_1 - C M_2)}{M_1 M_2} \tag{3.45}$$

So,

$$\omega^2 = 2 \frac{C}{M_1} \text{ or } \omega^2 = 2 \frac{C}{M_2} \tag{3.46}$$

Here, one of the modes only involves the motion of A atoms (with mass M_1) and the other mode only involves the motion of the B atoms (with mass M_2).

3.4.5. Energy gap

Notice that between the acoustic and optical branches, there is a range of frequency which cannot be reached, regardless of the momentum K (the equation has no solution). This range is called an "energy gap".

3.4.6. Questions: Why at K=π/a, the frequency of the accoustic phonon mode only relies on M_1, but is independent of M_2. For the optical phonon model, why it frequency only depends on M_2 but not M_1 at K=π/a?

Answer: at $K = \pi/a$, for the accoustic mode, only atoms with mass M_1 moves. For the optical modes only atoms with mass M_2 moves.

3.5. Longitudinal and transverse phonon modes

In higher dimensions, the deformation u_s becomes a vector $\vec{u}_s$ and the wavevector K becomes a vector $\vec{K}$. Depending on the angle between $\vec{u}$ and $\vec{K}$, we can distinguish two different types of sound waves:

Longitudinal modes: $\vec{u}$ is parallel to $\vec{K}$

Transverse modes: $\vec{u}$ is perpendicular to $\vec{K}$

In a D-dimensional space, there will be 1 longitudinal acoustic branch and D-1 transverse acoustic branches.

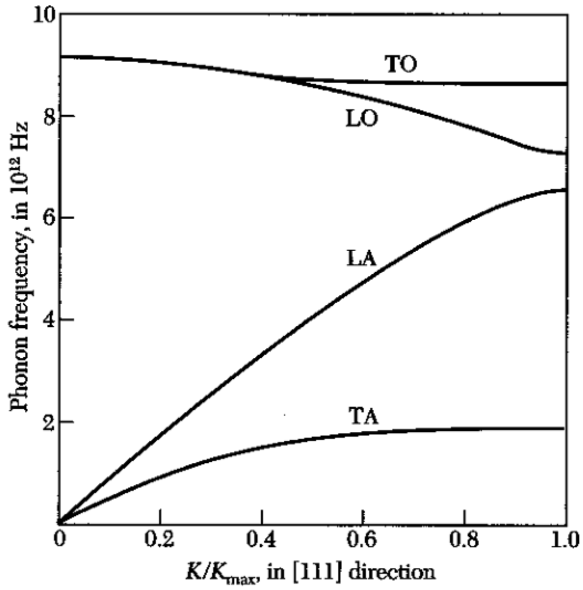

Fig. 5. Longitudinal and transverse modes. LA: longitudinal acoustic modes. TA: transverse acoustic modes. LO: longitudinal optical modes and TO; transverse optical modes.

Q: Why LA has a higher velocity than TA?

A: Will be ansewred in the next chapter.

3.6. Number of phonon modes

For a lattice with n atoms per unit cell, there are $(n-1)\,d$ optical phonons and d accoustic phonon modes.

For these d accoustic phonon modes, one of them is longidudinal and the other $d-1$ modes are transverse accoustic modes.

In each unit cell (n atoms per unit cell), there are $n\,d$ degrees of freedom, this number matches the number of phonon modes (accoustic+optical).