Lecture 5 – Calculation of Normal Modes in Crystal

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1 General Form of Solution

The first thing to note is that the normal mode solutions can be given in the following form:

$$\begin{bmatrix} u_{\vec{k}}(\vec{R}) \\ v_{\vec{k}}(\vec{R}) \\ . \\ . \\ . \end{bmatrix} = \begin{bmatrix} u \\ v \\ . \\ . \\ . \end{bmatrix} \exp\left\{ i(\vec{k}\cdot\vec{R} - \omega t) \right\} \tag{1}$$

We will be able to understand later where this form comes from (Bloch's theorem). At this point, it suffices to say that the normal mode solution can be understood in two parts – one part that is a discrete wave-like modulation over the lattice points (the exp part) and the other part (the row vector part) that describes what is being modulated, i.e. the behavior of basis atoms. The row vectors above have the dimension given by the number of atoms in the basis, and each number in the row vector $u, v, ...$ describes the displacement of each atom relative to the mean equilibrium position.

2 Crystal Momentum, and Its Quantum

In Eq. 1, note that $\vec{k}$ is ambiguous up to a reciprocal lattice vector, as for any reciprocal lattice vector $\vec{G}$, $\exp\left[i(\vec{k}+\vec{G})\cdot\vec{R}\right] = \exp(i\vec{k}\cdot\vec{R})$, due to the definition of the reciprocal lattice. Thus, although $\hbar\vec{k}$ is a good label ("quantum number") of the normal mode ("eigen-state"), it is actually different from normal momentum, and is instead called the "**crystal momentum**."

Also important is the fact that crystal momentum is quantized for a finite size crystal. Let us say that there are N_a lattice points along the $\vec{a}$ direction, N_b along the $\vec{b}$ direction and so on. The wave solution such as Eq. 1 should be single-valued, which means that it should be invariant under the change $\vec{R} \to \vec{R} + N_a\vec{a}$ and similarly for $\vec{b}$ and $\vec{c}$ directions. Thus

$$\vec{k} = \frac{l}{N_a}\vec{a}^* + \frac{m}{N_b}\vec{b}^* + \frac{n}{N_c}\vec{c}^* \tag{2}$$

where l, m, n are integers. Namely, the **quantum** of $k_{a^*} = \vec{a}^*/N_a$ and so on.

Two points are worth remembering here. (1) There are as many unique crystal momentum ($\vec{k}$) values as there are lattice points in the real space. (2) Crystal momentum can be taken within a unit cell of the reciprocal space, and the volume per crystal momentum ($\frac{\vec{a}^*\cdot(\vec{b}^*\times\vec{c}^*)}{N_a N_b N_c}$). For the unit cell in $\vec{k}$ space, the first Brillouin zone, i.e. the WS cell, is the most important one to use.

3 Case of One Atom per Unit Cell in One Dimension

From now on, only one dimensional case will be discussed, although the above discussion was made in three dimensions.

For one atom per unit cell, we seek the solution, according to Eq. 1:

$$u_{\vec{k}}(n) = u \exp(ikna - i\omega t)$$

where $\vec{R} = na$ is used. Assuming that atoms have mass M and neighboring atoms interact via a spring with a spring constant K, the Newtonian equation of motion for the n^{th} atom is

$$M\ddot{u}_{\vec{k}}(n) = -K(u_{\vec{k}}(n) - u_{\vec{k}}(n-1)) - K(u_{\vec{k}}(n) - u_{\vec{k}}(n+1))$$

In simplifying this equation, note that the second derivative on $u_{\vec{k}}$ is equivalent to multiplying by $-\omega^2$. After doing that, one can simply this equation further by dividing both sides by $u_{\vec{k}}(n)$. Then, one gets

$$-M\omega^2 = -K(1 - \exp(-ika)) - K(1 - \exp(ika)) = -2K(1 - \cos(ka)) = -4K \sin^2(ka/2)$$

Thus

$$\omega = \sqrt{\frac{4K}{M}} |\sin(\frac{ka}{2})|$$

It is important to notice that

$$\omega \rightarrow \sqrt{\frac{K}{M}} a|k| \rightarrow 0, \; for \; |k| \rightarrow 0$$

$$\omega_{max} = \sqrt{\frac{4K}{M}}, \; for \; k = \pm\frac{\pi}{a}$$

Even without solving the problem we already learned these two limiting behaviors (soft and hard phonons). In particular, the first behavior defines the sound velocity $v_s = a\sqrt{\frac{K}{M}}$.

4 Case of Two Atoms per Unit Cell in One Dimension

Consider the case that the crystal looks like $---MmMmMm---$ where M, m are the masses of the basis atoms. Assume that the spring constant is K for any bonding. In accordance with Eq. 1 we associate u with the mass M and v with the mass m. The normal mode is described by

$$u_{\vec{k}}(n) = u \exp(ikna - i\omega t)$$

$$v_{\vec{k}}(n) = v \exp(ikna - i\omega t)$$

Writing down the solution in this correct form is perhaps the most crucial part. The equation of motion is

$$M\ddot{u}_{\vec{k}}(n) = -K(u_{\vec{k}}(n) - v_{\vec{k}}(n-1)) - K(u_{\vec{k}}(n) - v_{\vec{k}}(n))$$

$$m\ddot{v}_{\vec{k}}(n) = -K(v_{\vec{k}}(n) - u_{\vec{k}}(n)) - K(v_{\vec{k}}(n) - u_{\vec{k}}(n+1))$$

Simiarly as before, the second time derivative is equivalent to multiplying by $-\omega^2$ and both sides of each equation can be divided by $\exp(ikna - i\omega t)$ to make it look simple. We get

$$\begin{aligned} -M\omega^2 u &= -K(u - v\exp(-ika)) - K(u - v) \\ -m\omega^2 v &= -K(v - u) - K(v - u\exp(ika)) \end{aligned}$$

which means

$$\begin{bmatrix} M\omega^2 - 2K & K(1 + \exp(-ika)) \\ K(1 + \exp(ika)) & m\omega^2 - 2K \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = 0$$

which in turn means

$$(M\omega^2 - 2K)(m\omega^2 - 2K) - 4K^2\cos^2(ka/2) = 0$$

which in turn means

$$Mm\omega^4 - 2K(m + M)\omega^2 + 4K^2\sin^2(ka/2) = 0$$

which means

$$\omega = \sqrt{\frac{K(M+m)}{Mm}\left[1 \pm \sqrt{1 - 4\frac{Mm}{(M+m)^2}\sin^2(ka/2)}\right]}$$

So we have two branches of excitations. Note that this is expected, since there are $2N$ normal modes expected, while there are only N crystal momentum values. The lower branch is called an acoustic branch, as its long wave length behavior is the sound wave behavior:

$$\omega \approx a\sqrt{\frac{K}{2(M+m)}}|k|$$

I.e., in this case the sound velocity is given by $v_s = a\sqrt{\frac{K}{2(M+m)}}$ (how would you understand this?). The other branch – called "optical branch" – has the following long wave length behavior:

$$\omega \approx \sqrt{\frac{2K(M+m)}{Mm}}$$

(how would you understand this?). At the boundary of the Brillouin zone (BZ), $k = \pm\pi/a$, we have:

$$\omega \approx \sqrt{\frac{2K}{M}}, \sqrt{\frac{2K}{m}}$$

(how would you understand this?).