Normal Modes of a 1D Lattice

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The simplest case when examining a crystal structure is the approximation that the positive ions (or multi-atom bases) remain stationary at their Bravais lattice positions $\mathbf{R}$. This is not very realistic of course, so the next best approximation would be to assume that the ions can move from their equilibrium Bravais lattice positions $\mathbf{R}$ - but only across distances small compared to the interatomic spacing. This is known as the **harmonic approximation**, so the crystal structures we examine under this assumption are often called **harmonic crystals**.

Monatomic Basis

We begin with the easiest system to analyze, which is a 1D crystal with a monatomic basis. The interatomic, or Bravais lattice vector spacings are a constant a, the Bravais lattice vectors are $\mathbf{R} = na$, where n is an integer. We then denote $u(na)$ as the displacement from equilibrium of the ion oscillating about $\mathbf{R} = na$. For simplicity, we assume that only nearest neighbor ions interact via a linear force $F = Kx$ where x is the instantaneous separation. Newton's third law thus gives:

$$\begin{aligned} m\frac{\partial^2 u(na)}{\partial t^2} &= -K\left[u(na) - u([n-1]\,a)\right] + K\left[u([n+1]\,a) - u(na)\right] \\ &= -K\left[2u(na) - u([n-1]a) - u([n+1]a)\right] \end{aligned} \tag{1}$$

where M is the mass of each ion. If there is only a finite number of atoms N, we would need to specify the behavior of the atoms at the ends of the chain. One way of doing this would be to have them interact with their inside neighbor only, but this would only complicate the analysis without visibly altering the final results. If N is large, we can approach the problem via the same method as for the free electron gas - the Born-von Karman (periodic) boundary conditions. Denoting the atoms in the finite chain by $n = 1, 2, \ldots N$, we have the boundary conditions:

$$u([N+1]a) = u(a) \quad \text{and} \quad u(0) = u(Na) \tag{2}$$

As usual the plane wave solution satisfies these conditions, which is of the form:

$$u(na, t) = Ae^{i(kna - \omega t)} \tag{3}$$

where A is an arbitrary coefficient. Plugging this solution into the boundary conditions, we find:

$$\begin{aligned} Ae^{ika}e^{-i\omega t} = Ae^{ikNa}e^{ika}e^{-i\omega t} &\rightarrow e^{ikNa} = 1 \\ Ae^{-i\omega t} = Ae^{ikNa}e^{-i\omega t} &\rightarrow e^{ikNa} = 1 \end{aligned}$$

which restricts the value of k:

$$k = \frac{2\pi\ell}{Na} \quad \text{where } \ell \text{ is an integer} \tag{4}$$

Notice that nothing changes when we change k by $\frac{2\pi}{a}$:

$$u(na,t) = Ae^{i\left[(k+\frac{2\pi}{a})na-\omega t\right]} = Ae^{i(kna-\omega t)} \tag{5}$$

Thus, only k within a range $\frac{2\pi}{a}$ yield distinct solutions - in this case N distinct solutions for k. We thus only consider the values $-\frac{\pi}{a} < k < \frac{\pi}{a}$, which is the first Brillouin zone. Substituting our assumed solution into the equation of motion:

$$-M\omega^2 = -K\left[2 - e^{-ika} - e^{ika}\right] = -2K(1 - cos(ka))$$

Solving for $\omega(k)$:

$$\omega(k) = \sqrt{\frac{2K(1-cos(ka))}{M}} = 2\sqrt{\frac{K}{M}}\left|sin\left(\frac{ka}{2}\right)\right| \tag{6}$$

There are thus N distinct values of $\omega(k)$, corresponding to the N distinct values of k - resulting in N modes ($2N$ modes if we consider longitudinal and transverse modes which are discussed at the bottom of the page).

These modes describe waves with frequency $\omega(k)$ and phase/group velocities:

$$v_p = \frac{\omega}{k} \quad \text{and} \quad v_g = \frac{\partial\omega}{\partial k} \tag{7}$$

There are two interesting cases - when $k \ll \frac{\pi}{a}$ and $k = \pm\frac{\pi}{a}$:

- $k \ll \frac{\pi}{a}$:

$$\begin{aligned}\omega(k) &= 2\sqrt{\frac{K}{M}}\left|sin\left(\frac{ka}{2}\right)\right| \\ &= 2\sqrt{\frac{K}{M}}\left|\frac{ka}{2} - \frac{1}{2!}\left(\frac{ka}{2}\right)^3 + \dots\right| \\ &\approx 2\sqrt{\frac{K}{M}}\left|\frac{ka}{2}\right| = a\sqrt{\frac{K}{M}}|k|\end{aligned} \tag{8}$$

  the frequency is thus linear with respect to k, which is the typical behavior of light and sound waves. The group and phase velocities are thus equal ($v_g = v_p$) and are constants.

- $k = \pm\frac{\pi}{a}$:

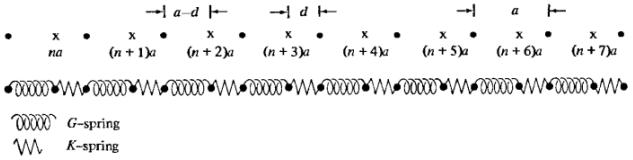
$$\omega\left(\pm\frac{\pi}{a}\right) = 2\sqrt{\frac{K}{M}} \tag{9}$$

  the frequency thus reaches a maximum value and $v_g = 0$.

Notice that we haven't specified the direction of the displacement $u(na)$. There are two possible directions of motion - along the line (longitudinal) or perpendicular to the line (transverse).

Diatomic Basis - Identical Mass, Different Spacing

We now consider a slightly more complicated problem, which is a 1D lattice with a diatomic basis. We still assume all ions are identical, but now the equilibrium spacing between atoms alternates between $a - d$ and d. The interatomic forces change depending on the equilibrium spacing, which we account for by imagining springs of different spring constants G and K connecting the atoms:



Since we now have two different "types" of atoms - one that oscillates about position na and one that oscillates about position $na + d$ - we denote the displacement from equilibrium of each type by $u_1(na)$ and $u_2(na)$ respectively. Writing Newton's third law for both types of atoms:

$$M\frac{\partial^2 u_1(na)}{\partial t^2} = -K\left[u_2(na) - u_1(na)\right] - G\left[u_1(na) - u_2([n-1]a)\right] \tag{10}$$

$$M\frac{\partial^2 u_2(na)}{\partial t^2} = -K\left[u_2(na) - u_1(na)\right] - G\left[u_2(na) - u_1([n+1]a)\right] \tag{11}$$

Again applying the same boundary conditions, we assume solutions of the form:

$$u_1(na) = \epsilon_1 e^{i(kna-\omega t)} \tag{12}$$

$$u_2(na) = \epsilon_2 e^{i(kna-\omega t)} \tag{13}$$

where ϵ_1 and ϵ_2 are coefficients that give the relative amplitude and phase of the motions. Also, for a finite lattice of N atoms we again obtain N values of k that provide distinct solutions. Substituting our solutions into the equations of motion, we obtain two coupled equations:

$$\left[M\omega^2 - (K+G)\right]\epsilon_1 + (K + Ge^{-ika})\epsilon_2 = 0$$

$$(K + Ge^{ika})\epsilon_1 + \left[M\omega^2 - (K+G)\right]\epsilon_2 = 0$$

For a nontrivial solution, the determinant of the coefficients must vanish:

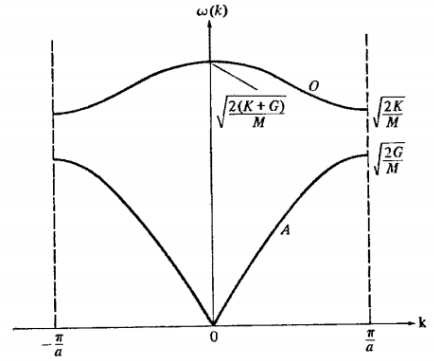
$$det\begin{vmatrix}\left[M\omega^2 - (K+G)\right] & (K + Ge^{-ika}) \\ (K + Ge^{ika}) & \left[M\omega^2 - (K+G)\right]\end{vmatrix} = 0 \tag{14}$$

Solving this equation gives:

$$\omega^2 = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2 + G^2 + 2KGcos(ka)} \quad \text{and} \quad \frac{\epsilon_2}{\epsilon_1} = \mp\frac{K + Ge^{ika}}{|K + Ge^{ika}|} \tag{15}$$

Notice that the $\pm$ in the expression for ω^2 gives *two* values of ω for each k. Since there are N nontrivial values of k, we thus have $2N$ normal modes - unsurprising since there are $2N$ degrees of freedom. Again, if we allow movement perpendicular to the line there are $4N$ transverse/longitudinal modes since each atom now has an additional degree of freedom perpendicular to the line.

Plotting the two solutions for $\omega(k)$:



The two ω vs. k curves shown are referred to as the **branches** of the dispersion relation. The lower curve resembles the curve found earlier for a 1D monatomic lattice, and is called the **acoustic branch** because of its small k behavior ($\omega \approx vk$) characteristic of sound waves. The upper curve is called the **optical branch**, since these modes tend to interact with electromagnetic radiation. Another notable feature is a gap in allowed frequency - a **phononic gap**.

We now examine the limiting cases again:

- $k \ll \frac{\pi}{a}$:

$$\omega \approx \sqrt{\frac{2(K+G)}{M}} \quad \text{and} \quad \epsilon_2 = -\epsilon_1 \quad \text{(Optical Branch)} \tag{16}$$

$$\omega \approx a\sqrt{\frac{KG}{2M(K+G)}}|k| \quad \text{and} \quad \epsilon_2 = \epsilon_1 \quad \text{(Acoustic Branch)} \tag{17}$$

  From the relative sign of ϵ_1 and ϵ_2, we see that, at low k, the optical branch describes neighboring motion 180° out of phase with each other and the acoustic branch describes neighboring motion completely in phase.

- $k = \frac{\pi}{a}$:

$$\omega = \sqrt{\frac{2K}{M}} \quad \text{and} \quad \epsilon_1 = -\epsilon_2 \quad \text{(Optical Branch)} \tag{18}$$

$$\omega = \sqrt{\frac{2G}{M}} \quad \text{and} \quad \epsilon_1 = \epsilon_2 \quad \text{(Acoustic Branch)} \tag{19}$$

  Again, the optical branch describes neighboring motion 180° out of phase, and the acoustic branch describes neighboring motion completely in phase.

We now see the difference between the optical and acoustic branches for a 1D lattice. The acoustic branch describes all ions within a primitive cell moving in phase, in which the inter-cell interactions dominate. The optical branch describes all ions within a primitive cell vibrating in place against each other.

Diatomic Basis - Different Mass, Identical Spacing

We examine the final example for a 1D lattice, in which each Bravais lattice site refers to two atoms of different mass M_1 and M_2 and displacements $u_1(na)$ and $u_2(na)$ respectively. The equations of motion are:

$$M_1 \frac{\partial^2 u_1(na)}{\partial t^2} = -K\left[2u_1(na) - u_2(na) - u_2([n-1]a)\right] \tag{20}$$

$$M_2 \frac{\partial^2 u_2(na)}{\partial t^2} = -K\left[2u_2(na) - u_1(na) - u_1([n+1]a)\right] \tag{21}$$

Again assuming solutions of the form:

$$u_1(na) = \epsilon_1 e^{i(kna-\omega t)} \tag{22}$$

$$u_2(na) = \epsilon_2 e^{i(kna-\omega t)} \tag{23}$$

we obtain the coupled equations:

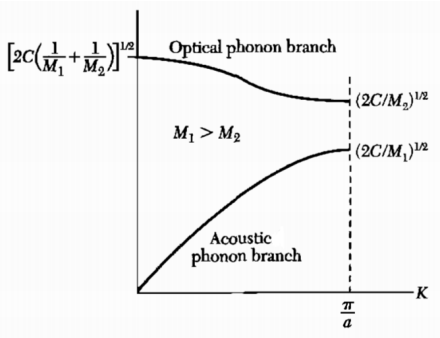
$$(2K - M_1\omega^2)\epsilon_1 + \left[-K(1+e^{ika})\right]\epsilon_2 = 0$$

$$\left[-K(1+e^{ika})\right]\epsilon_1 + (2K - M_2\omega^2)\epsilon_2 = 0$$

The determinant of the coefficients must again vanish, which gives the equation:

$$M_1 M_2 \omega^4 - 2K(M_1+M_2)\omega^2 + 2K^2(1 - cos(ka)) = 0 \tag{24}$$

To avoid repeating the same analysis, we simply provide the dispersion plot:



The limiting cases are:

- $k \ll \frac{\pi}{a}$:

$$\omega^2 \approx 2K\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \quad \text{(Optical Branch)} \tag{25}$$

$$\omega^2 \approx \frac{K}{2(M_1+M_2)}k^2a^2 \quad \text{(Acoustic Branch)} \tag{26}$$

- $k = \pm\frac{\pi}{a}$:

$$\omega^2 = \frac{2C}{M_2} \quad \text{(Optical Branch)} \qquad \omega^2 = \frac{2C}{M_1} \quad \text{(Acoustic Branch)} \tag{27}$$