

Phonons in a one-dimensional crystal

Let us consider the following problem: we have a one-dimensional crystal, which we can think of as a linear chain of equally-spaced identical atoms of mass m . Let a be the equilibrium distance between consecutive atoms. Then, at equilibrium, the position of the n^{th} atom of the chain will be

$$x_n^{(0)} = na$$

Let us assume that there are N atoms in the chain, so that $n = 1, 2, \dots, N$.

We would like to answer the following question: if the atoms are constrained to move along the x -axis, what are the normal frequencies of oscillations of this system? These are called longitudinal phonons, where longitudinal (as opposed to transversal) shows that we are only looking for oscillations along the x -axis. “Phonons” is the name given to such oscillations of a solid. Strictly speaking, one needs to treat them quantum mechanically, but classical mechanics already tells us what their allowed frequencies are, just like we discussed for small molecules. Understanding these phonons is very important in solid state physics. For example, as you may know, when the solid is heated up, its atoms start oscillating around their equilibrium position – for instance, this is what is responsible for an increased resistance of a metal, as the temperature is increased. As the electrons that make up the electric current try to move through the material, if the motion of the atoms is more violent (which is true at higher temperatures), the chances for electrons to scatter off these moving atoms increase. After such a scattering, the electron will generally move in a different direction than the one of the current. If there was no applied voltage, the current would become zero very fast because after a very short time the electrons would be moving every which way and the average current in any direction would be zero. If we want a current, we need to apply a voltage, so that even if an electron is scattered in a “wrong” direction after it hits a vibrating nucleus, the applied electric field will re-accelerate it in the desired direction so that we do have an overall current. If we know the phonon frequencies and have some ideas about the scattering processes, we can calculate how the resistance should increase with temperature (and test to see whether experiments agree with the calculations). For simple metals at fairly high temperatures, resistance increases linearly with temperature, as one can show quite easily. Figuring out such properties of materials is part of the condensed matter, or solid state physics – something very near and dear to my heart. In fact, in recent years my main research interest has been to understand precisely such interactions between electron and phonons (it turns out that sometimes these quantum objects can combine into a new object, which is called a polaron, and which is a superposition of the electron plus various numbers of phonons. But I digress).

Back to classical mechanics – let’s find these frequencies. The Lagrangian of this system is

$$\mathcal{L} = \sum_{n=1}^N \frac{m\dot{x}_n^2}{2} - U(x_1, \dots, x_N)$$

Let us use a simple model for the interaction potential. First, we assume that each atom interacts only with its two neighboring atoms, which implies

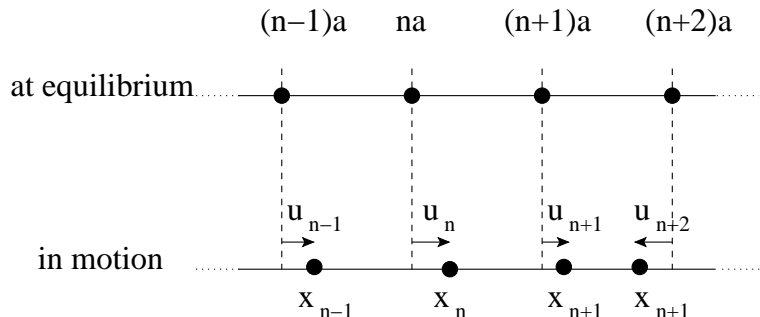
$$U(x_1, \dots, x_N) = \sum_{n=1}^{N-1} U_{\text{pair}}(x_{n+1} - x_n)$$

where $U_{\text{pair}}(x_{n+1} - x_n)$ describes the interaction between atoms n and $n + 1$. Now, we know that if we are interested in small oscillations, we can Taylor expand this to obtain

$$U_{\text{pair}}(x) = \frac{K}{2} (x - a)^2$$

which, indeed, has a minimum at the equilibrium length $x = a$. Then we have a simplified version of the Lagrangian, valid near the equilibrium positions:

$$\mathcal{L} = \sum_{n=1}^N \frac{m\dot{x}_n^2}{2} - \sum_{n=1}^{N-1} \frac{K}{2} (x_{n+1} - x_n - a)^2$$



We can make things easier if instead of x_n , we use the generalized coordinates to be $u_n = x_n - x_n^{(0)} = x_n - na$, i.e. the displacement of each atom from its equilibrium position (see the figure for an illustration). With these new variables, we have

$$\mathcal{L} = \sum_{n=1}^N \frac{m\dot{u}_n^2}{2} - \sum_{n=1}^{N-1} \frac{K}{2} (u_{n+1} - u_n)^2$$

The EL equation for u_n then is:

$$m\ddot{u}_n = -K(2u_n - u_{n-1} - u_{n+1})$$

or, if we define $\omega_0 = \sqrt{K/m}$, we have:

$$\ddot{u}_n = -\omega_0^2(2u_n - u_{n-1} - u_{n+1})$$

and we have one such equation for each value of $n = 1, 2, \dots, N$. In fact, this is not quite true: you can convince yourselves that for $n = 1$ and $n = N$ (i.e. the end atoms of the chain) the equation must be somewhat different, simply because these end atoms are missing the neighbor either to left, or right. We will see a bit later how we deal with those two particular atoms.

We have already discussed in class how to deal with the time dependence: in each normal mode all atoms will oscillate in phase, and therefore we must have

$$u_n(t) = a_n \cos(\omega t + \phi)$$

where the allowed values of ω are the natural frequencies we are looking for. If we plug this “guess” into the equation of motion, we find that $\ddot{u}_n = -\omega^2 u_n$, and therefore the equation of motion can be rewritten as

$$(2\omega_0^2 - \omega^2)a_n = \omega_0^2(a_{n+1} + a_{n-1})$$

This is a recurrence relation, and we need a way to solve it. Some of you may be familiar with Fourier transforms and then you already know what we should do. If you are not familiar with those, look at the end of these notes for a way of dealing with such recurrence relations. We assume the solution to be of the form

$$a_n = A \cos(nqa + \beta)$$

where q is a number called “wave-vector”, and β is some phase. With this “guess”, the recurrence relation becomes

$$(2\omega_0^2 - \omega^2)A \cos(nqa + \beta) = \omega_0^2 \{A \cos[(n+1)qa + \beta] + A \cos[(n-1)qa + \beta]\}$$

Using the relation $\cos \alpha + \cos \beta = 2 \cos \frac{\alpha+\beta}{2} \cos \frac{\alpha-\beta}{2} \rightarrow \cos[(n+1)qa + \beta] + \cos[(n-1)qa + \beta] = 2 \cos(nqa + \beta) \cos(qa)$ and therefore we find:

$$2\omega_0^2 - \omega^2 = 2\omega_0^2 \cos(qa) \rightarrow \omega^2 = 4\omega_0^2 \frac{1 - \cos(qa)}{2} \rightarrow \omega = 2\omega_0 \left| \sin \frac{qa}{2} \right|$$

Thus, we found that for a given value of q , the frequency of the oscillations is

$$\omega_q = 2\omega_0 \sin \frac{qa}{2} \rightarrow u_n^{(q)}(t) = \cos(\omega_q t + \phi_q) \cos(qna + \beta_q)$$

(we use the superscript to remind ourselves that this is the normal solution for a given q). The last question we need now to answer is what values can q take? The answer to this comes from the condition that this solution describes properly the behavior of the end atoms of the chain. There are several possibilities for these end atoms; for instance, periodic boundary conditions are very popular and useful in solid state – in this case we would ask that the chain is circular and atom 1 has atom N as its left-side neighbor. This imposes certain periodicities satisfied only by certain q values – if you take the intro to solid-state course, you’ll find out how to do that.

However, for today, let us consider the case where the end atoms are not allowed to move, i.e. $u_1(t) = u_N(t) = 0$. In this case, only the rest $N - 2$ atoms move, i.e. there are $N - 2$ degrees of freedom (for longitudinal motion) and we expect $N - 2$ distinct natural frequencies. (If you wonder why we don’t have a pure translational mode, the reason is that we fixed the ends of the chain). From

$$u_1(t) = \cos(\omega_q t + \phi_q) \cos(qa + \beta_q) = 0 \text{ for all times} \rightarrow \cos(qa + \beta_q) = 0 \rightarrow \beta_q = \frac{\pi}{2} - qa$$

This condition, therefore, fixes the value of β . The second condition is now:

$$u_N(t) = \cos(\omega_q t + \phi_q) \cos(Nqa + \frac{\pi}{2} - qa) = 0 \text{ for all times} \rightarrow (N-1)qa = j\pi \rightarrow q = \frac{j\pi}{(N-1)a}$$

where j can be any non-zero integer (if $j = 0 \rightarrow q = 0 \rightarrow \omega_q = 0$ which is not a vibration). Since the allowed values of q are indexed by the integer j , we can rewrite the normal modes in terms of it. Collecting all results, we have the motion of the n^{th} atom, in the j^{th} mode, to be:

$$u_n^{(j)}(t) = \sin \left(j\pi \frac{n-1}{N-1} \right) \cos(\omega_j t + \phi_j), \text{ where } \omega_j = 2\omega_0 \left| \sin \left(\frac{j\pi}{2(N-1)} \right) \right|$$

where j is an integer number. This might suggest that there is an infinite number of solutions, one for each possible j . We know this cannot be true; the problem has only $N - 2$ degrees of freedom (there are N atoms, but only $N - 2$ of them are allowed to move in the x -direction). Careful considerations show that indeed only the values $j = 1, 2, \dots, N - 2$ give distinct solutions. You can convince yourselves that the solution given by any other j is equivalent to one of these because sin and cos are periodic functions.

To conclude, the chain with N atoms and fixed ends has $N - 2$ distinct frequencies of longitudinal oscillations, given by ω_j with $j = 1, 2, \dots, N - 2$.

Such calculations can be generalized to 3-dimensional crystals, and one can consider more complicated unit cells as well. These normal frequencies are called “phonons” and they can be measured experimentally, for instance by scattering neutrons off the lattice and looking at what happens (mind you, we need to use some quantum mechanics because atoms and neutrons are quantum objects, but things proceed in a fairly similar fashion there). Such measurements were pioneered by (amongst others) the Canadian Bertram Brockhouse, who won a Nobel prize in 1994 for this work.

Recurrence relations:

Let us consider recurrence relations of the general form $\alpha a_n = a_{n-1} + a_{n+1}$. In particular, for our problem we have $\alpha = (2\omega_0^2 - \omega^2)/\omega_0^2$. There are many ways to deal with such equations. One possible way is to the following: let’s form the system of equations

$$\begin{cases} a_{n+1} = \alpha a_n - a_{n-1} \\ a_n = a_n \end{cases} \rightarrow \begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = \begin{pmatrix} \alpha & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix} \rightarrow \begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = \begin{pmatrix} \alpha & -1 \\ 1 & 0 \end{pmatrix}^n \begin{pmatrix} a_1 \\ a_0 \end{pmatrix}$$

Let λ_+ and λ_- , respectively \hat{u}_+ and \hat{u}_- be the eigenvalues and eigenvectors of this 2×2 matrix:

$$\begin{pmatrix} \alpha & -1 \\ 1 & 0 \end{pmatrix} \hat{u}_{\pm} = \lambda_{\pm} \hat{u}_{\pm}$$

(you can easily find them by standard linear algebra methods). We know then that any vector can be written as a linear combination of these 2 eigenvectors. In particular, we must have

$$\begin{pmatrix} a_1 \\ a_0 \end{pmatrix} = a_+ \hat{u}_+ + a_- \hat{u}_-$$

where a_+ and a_- are some constants. If we now put this into the recurrence relation and use the fact that every time the matrix acts on one of its eigenvectors, it just multiplies it by the corresponding eigenvalue, we find the general solution of the recurrence relation to be:

$$\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = a_+ \lambda_+^n \hat{u}_+ + a_- \lambda_-^n \hat{u}_- = a_+ e^{n \ln \lambda_+} \hat{u}_+ + a_- e^{n \ln \lambda_-} \hat{u}_-$$

There are two possibilities now: depending on the value of α , the two eigenvalues are both real numbers, in which case the recurrence relation shows that a_n increases or decreases exponentially with n . This is not an acceptable solution, generally speaking, except maybe near ends of the chain.

The more interesting case is when $\lambda_+ = (\lambda_-)^* = e^{i\phi}$, i.e. the eigenvalues are complex conjugate numbers (they must have unit amplitude since the determinant of the 2×2 matrix is 1, which means that $\lambda_+ \lambda_- = 1$). In this case, $\ln \lambda_+ = -\ln \lambda_- = i\phi$, and you see that

$$a_n \sim a e^{in\phi} + b e^{-in\phi} \sim A \cos(n\phi + \beta)$$

which is precisely the type of solution we used. All we did was to “rename” $\phi = qa$ in the notes, this being a useful thing to do, as you’ll find out when you take a course in solid-state physics. You see that the value of ϕ depends on the value of α which enters the 2×2 matrix. This gives the relation between ω_q and q , which is also called a “dispersion relation”.