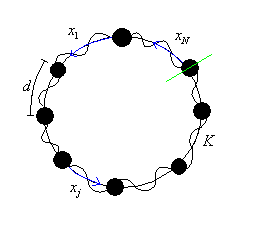
**Coupled Harmonic Oscillators**

Let’s generalize our discussion to N harmonic oscillators. We’ll find this to be a good model of the oscillations of the atoms in a lattice. We’ll space these atoms/oscillators a distance *d* apart, with the last one coupled to the first, like our ring in the last lecture. Let’s also assume that there is some tension in the springs, such that the equilibrium length of the springs is ℓ which is different from the actual length of the springs in the solid, d. In other words, each spring is stretched or compressed a distance d-ℓ. This is realistic since all materials are usually under some sort of tension from the likes of atmospheric forces, hanging weights or loads, etc. In any event, it is necessary to realistically model the solid since the actual forces involved are electric in nature and a naïve spring approximation to these forces, where d = ℓ turns out to be too simple because it doesn’t allow transverse waves.

This model is also important pedagogically because it provides a first glimpse of the behavior of the atoms in a metal’s crystal lattice. Such a model, when continuumized will also lead to a description of how sound waves propagate through a material, and how the electromagnetic field propagates through space. Such a continuum model is often used as an introductory quantum field theory model (the green line denotes the beginning of the origin of the coordinate system).



**Longitudinal oscillations of lattice**

Let’s assume purely longitudinal motion for now. The differential equation for the j’th atom is:



This, together with the boundary condition that:



provides a complete description of our system. Now we look for the harmonic modes again, since a linear combination of these provides the general solution to our system of masses. So recalling the general form of such harmonic modes, we will assume a solution of the form,



Plugging this in…



And in terms of the u’s, our boundary condition reads:



So what we have here is an eigenvalue *difference* equation (as opposed to *differential* equation) for the frequencies (squared) λ, and amplitudes uj. Unlike before, it is not explicitly a matrix equation – though it could be turned into one as the book does. Still, I think the difference equation format is the easier way to solve this equation. Either way, the goal is the same: to find the λ’s that enable non-zero values of the uj’s. And to find out what those uj’s are. To that end, we employ the standard technique of solving linear difference equations. We will assume that the uj follow the form: uj = eqj where q is some number (this is just like the ansatz used for linear *differential* equations). First, the boundary conditions require that:



Now n only ranges between 0 and N-1 because these are the only terms which give distinct values of amplitudes ui = eqi. For instance, if you plug n = N into the equation for q, you’ll just get the same value for eqn as when n = 0. So n can only range over N values, but we needn’t choose n = 0→N-1. In fact, a different choice is usually made: n = -N/2 → N/2-1. And I’m going to choose that range. So our eigenvectors would be uj = eqj, which is:



It turns out these uj *are* the eigenvectors (solutions to our difference equation). We will verify below that these are indeed the eigenvectors. So let’s plug this into our difference equation:



So we have that the allowed eigenvalues and eigenvectors are:



The ωn are the possible frequencies of oscillation. And the Re(uj(n)) are the eigenvectors/amplitudes corresponding to these frequencies. Altogether these define the N normal modes of the set of harmonic oscillators. Explicitly the nth normal mode consists of this. If we displace each of the oscillators xj by Reuj(n), where j ∈ 1, 2, …, N, then they will oscillate back and forth at the single frequency ωn. Now that we have the eigenfrequencies and eigenvectors we can write down the general expression for the displacement of each oscillator as a function of time. So the position of the jth oscillator as a function of time will be:



where we have considered An complex in the second line, and split it up into magnitude/phase in the third. Also we take into account the fact that when n = 0 we get the constant solution, which must be modified to include a the linear time part, just like in the example above. And in the last line we redefine the constant |An| as just An. So the sum doesn’t include the n = 0 term.

**Writing our solution in prettier wave-number notation**

Before we consider this solution in more detail though, we will find it useful to rewrite it in a more perspicuous format. To that end, let’s define the equilibrium coordinate of the oscillator, Rj. In terms of d and j this is:



And let’s define the wavenumber of the nth normal mode, kn, as:



where L = Nd is the total length of the circle of oscillators. Keeping in mind that

n ∈ [-N/2, 1,…, N/2-1) we would have that:



which means that kn runs from -π/d (inclusive) to π/d (exclusive) in steps of 2π/L. In Condensed Matter Physics parlance, this range is called the first Brillouin zone. So for short, often we just write:



Now observe that we can write the exponent of the uj(n) as…



And so the eigenvectors can be written:



And the eigenfrequencies can be written as:



So we have the eigenvectors and frequencies to be the following. We’re going to switch the index from n to k now to put it in line with conventional notation.



With these definitions, we can write our solution as:



In the last line we’ve extracted the kn = 0 case and handled it separately as in previous problems. And of course we separated An into its magnitude and phase in the 3rd line, and then renamed |An| as just An in the last line. So our solution is:

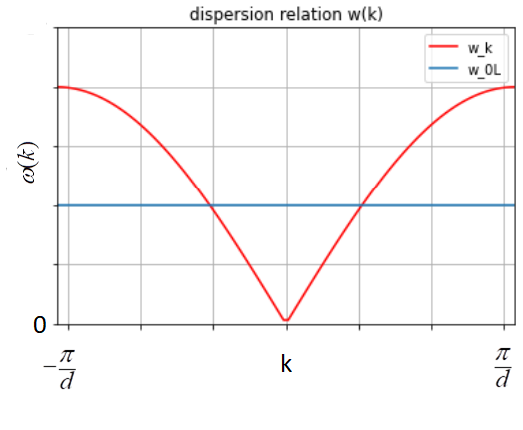


**Interpreting our result**

Now let us observe that the term in the sum is of the form of a traveling wave. Each of the N normal modes forms a traveling wave with wavevector kn and frequency ωn. The positive kn travel rightwards, and the negative kn travel leftwards. The wavelength of each normal mode is λn = 2π/|kn| which works out to be:



Since |n| goes from 1 (excluding 0 ‘cause that term is handled separately) to N/2, λn ranges from L to L/(N/2) = 2L/N = 2d. So the allowed wavelengths make the wave periodic over the length of the ring. Now let’s take a look at the allowed frequencies ωn = 2πfn corresponding to each of the wavenumbers kn.



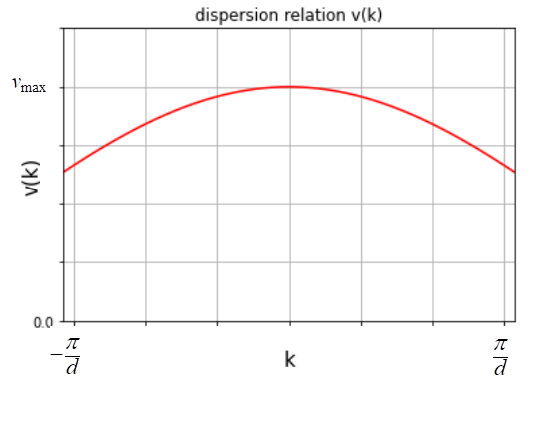
The maximum allowed frequency is twice the natural frequency of the springs and occurs at wavenumbers |kn| = π/d, which is wavelenth λn = 2d. The velocities of these normal wave modes is vn = λnfn = ωn/kn, given by:



The maximum velocity occurs for small k’s, large λ’s. Using the fact that sin(x) → x in small x limit, this max v is given by:



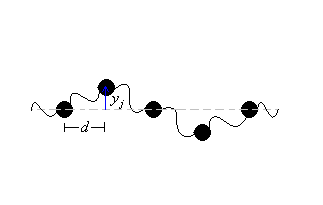
These are plotted below:



Since the velocity of the waves obviously depends on their wavelengths (frequencies), the medium would be said to be *dispersive*.

**Modeling transverse oscillations of a crystal lattice (in the ‘y’ direction)**

Now let’s consider the case whereby the masses are oscillating up and down (i.e. transversely in the y-direction) rather than longitudinally – a side view of the ring is shown since can’t really depict this from top-down perspective.



We want to examine the motion of these oscillators in the y-direction. So to that end, we have:



Now taking the limit that the y’s are small, we have to first order:



Let’s define,



Then we can write our equation as:



This, together with the boundary condition that:



provides a complete description of our system. Now to solve it, we will assume a solution consistent with what we found before – namely:



And we will find, as before, that:



where kn is as before. And the eigenfrequencies, ω­n, will be:



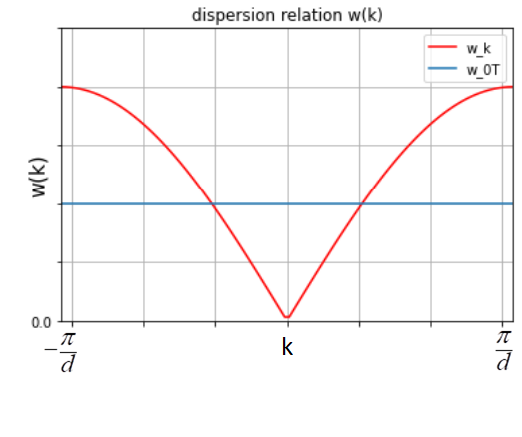
So we have the eigenvectors and frequencies to be:



With these definitions, just like we did before, we can write our general solution as:



Below we plot the frequencies vs. the wavenumber. The general shape is the same as before.



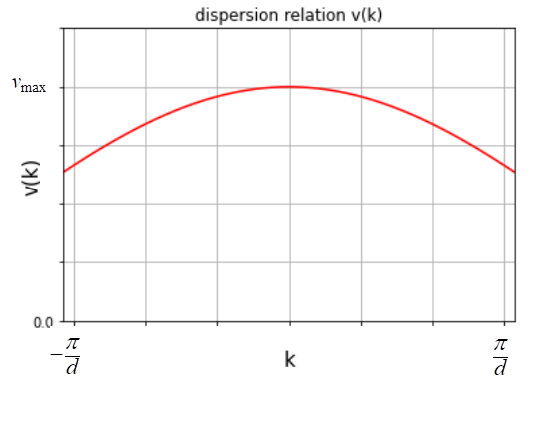
But for this model, the transverse frequencies are a little less than the longitudinal frequencies, as KT < K. Generally speaking this may not always be the case for a real crystal. Nonetheless, the general shape of the curve is definitely realistic. Now, the velocities of these normal wave modes is given by:



and vmax will be for small kn’s as before, and given by:



These are plotted below. Again, same general shape.



Let’s look at vmax­ a little further. If we fill in what ω0T is from above we’ll have:



Now m/d is the mass density of the ‘string’, and (*d*-ℓ) is approximately the stretch of the spring since y is assumed quite small. Therefore K(*d*-ℓ) is the force each individual spring is exerting. In other words, this is the tension in the ‘string’. Therefore we have:



which you’ll recall is what we had obtained from Physics 1 by other means!

**Modeling transverse oscillations of a crystal lattice (in the ‘z’ direction)**

Now let’s consider the case whereby the masses are oscillating into and out of the page (i.e. transversely in the z direction). Since this is into and out of the page can’t really show it. Nonetheless, the mathematics is the same. Writing down the force equation we have:



Now taking the limit that the z’s are small, we have to first order the same equation we got for the y’s. We can write this as:



This, together with the boundary condition that:



provides a complete description of our system. Now to solve it, we will assume a solution consistent with what we found before – namely:



And we will find, as before, that:



where kn is as before. And the eigenfrequencies, ω­n, will be:



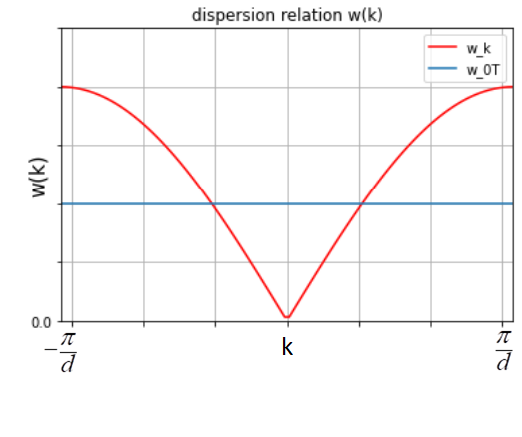
So we have the eigenvectors and frequencies to be:



as before. With these definitions, we can write our solution as:



Below we plot the frequencies vs. the wavenumber, and compare to the longitudinal frequencies too.



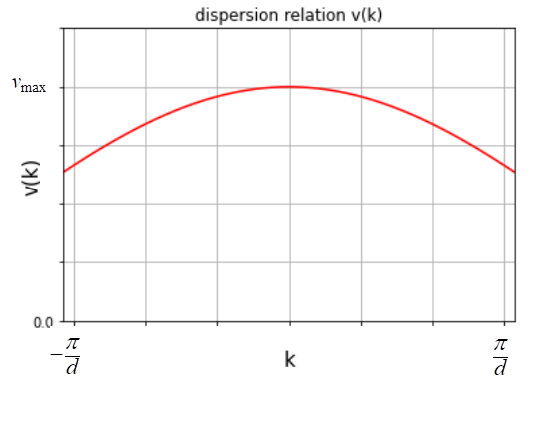
For this model, the transverse frequencies in the z direction are the same as those in the y-direction. They are shown slightly displaced from the y-frequencies though for clarity. Generally speaking, however, the frequencies may be different. Now, the velocities of these normal wave modes is given by:



where,

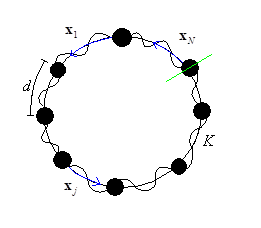


And these are plotted below:



**Modeling more general oscillations of a crystal**

Now let’s consider arbitrary oscillations of our crystal, where the atoms can oscillate in the x, y, or z directions simultaneously. We’ll label the position of each particle with the vector **x** = x + y + z.



Let’s use the Lagrangian to obtain the equations of motion. We have:



Let’s simplify the Lagrangian before taking derivatives. Start with:



And **1** is unit tensor, **:** is double dot product (see Tensor file). Now we will expand the root out to 2nd power in |**x**j+1 – **x**|­j.



Now we can discard irrelevant constants, and note the linear terms drop out of the sum since j = 2 cancels out the j = 1 term, and j = 4 cancels out j = 3 term, etc. So we have:



And now recognize KT = K(1-ℓ/d), which implies Kℓ/d = K – KT. So we can write:



Finally, in the 3rd line, **x**j2 + **x**j+12 = 2**x**j2 because the j = 1 term will add with the j = 2 term, etc. Now let’s write out the equations of motion. We have:



Since **x**i is a vector, we have to modify our ansatz a little. Mindful of the past, let’s suppose that:



Plugging this in we have:



So our matrix equation is:



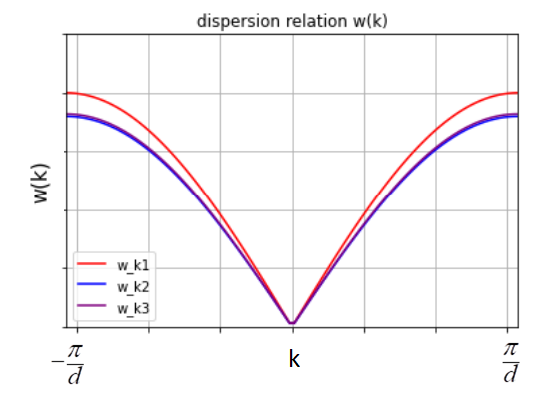
The eigenvalues and eigenvectors are obvious. They are:



And these are of course the eigenvectors and frequencies found above, when we considered oscillations in each direction separately. So we can write our solution as:



The usual caveat about the k = 0 harmonic applies, but I’m not bothering to be explicit about it anymore. And below we plot the eigenfrequencies and velocities together for comparison. Note that the frequencies and velocities for oscillations along the y and z axes are the same, but displaced a bit for clarity. Again note how this solution is just the linear combination of all possible periodic waves.



and,

