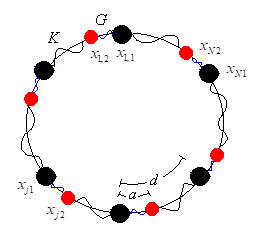
**Modeling a crystal lattice with a basis**

Let’s generalize our discussion further to a crystal with two different atoms in its ‘unit cell’. It would look like this:



There is a basis of two atoms/oscillators connected to each other via spring constant G. And these ‘bases’ are connected to each other via the usual spring constant K (capital now to distinguish from the wave-vector). The positions of the black atoms are labeled by xj1 and the positions of the red ones are labeled xj2. The equation of motion of the jth black guy is:



and the equation of motion of the jth red guy is:



So these are our differential equations. Taking our previous problem as a cue, we will try solutions of the form:



where Rj = jd is the position of the jth basis and k is to be determined. First, the boundary conditions require (α can be 1 or 2),



And of course n can run between -N/2, -N/2+1, …, N/2-1. OK, now we must plug these into the equations. Into the first reads:



Plugging into the second equation yields,



We have a matrix equation for the coefficients ε1, ε2 and eigenfrequencies ω. So let’s put these two equations together in matrix form. They then read:



In order for there to be non-zero solutions for ε1 and ε2, we must have the determinant 0. So:



Using the quadratic equation for the frequencies…



Now we need to find the corresponding eigenvectors. Filling ωk1 into the eigenvector equation we get:



Using the property of the determinant being zero, we can see that multiplying the top row by



and adding to the bottom row will give us:



Then let’s divide through by K+G – m1ωk12 – after a bit of algebra we’d get:



The bottom equation requires that ε2 be anything. And the top equation requires that ε1 = ε2. So we have, for the unnormalized eigenvector and frequency:



Then filling in the second frequency, ωk2, we can determine that the corresponding eigenvector equation reduces to:



Therefore the eigenfrequency and (unnormalized) eigenvector corresponding must be:



So the eigenvectors/eigenfrequencies are:



And the general solutions would be (ε(1)1 means first component of ε(1), etc.):



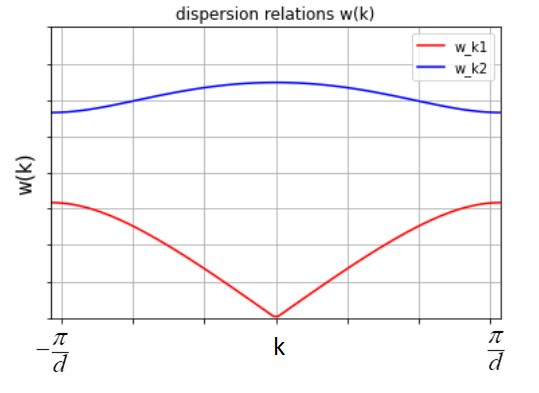
while xj2(t) is given by:



Or more compactly, these are usually written,



where xjα is the αth atom in the jth basis. In this case *α* runs from *1* to *2*. And ε(λ)α is the eigenvector of the atom α in basis j corresponding to mode λ. The usual caveat about the k = 0 harmonic applies. Now let’s examine the allowed frequency spectrum. For some random values of K = 10, G = 25, m1 = 10 and m2 = 5, we get the following typical frequency spectrum.



Observe that ωk1 gives the spectrum we saw before, and this is to be expected since the corresponding eigenvector ε(1) has each atom in the basis move in the same direction and amount. So the basis atoms never oscillate with respect to each other, and we simply have the old oscillation pattern, albeit with the basis oscillating rather than just an atom. This spectrum is called the acoustic spectrum. On the other hand, if you move the basis atoms out of phase with respect to each other, as ε(2) instructs, then you the frequency spectrum ωk2. This spectrum is called the optical spectrum. You’ll note that frequency is non-zero, even if the wavenumber k is large.

This reduces to the previous expression in the limit m1 = m2, G = K, when taking into account that d → d/2. Suppose we look at the limit k is small. Then we have,



Apropos the ωk1 guy, Taylor expanding the sin(kd/2), we could write this as:



where M is the total mass. Normally G >> K, in which case, we could write,



We’ll recognize this as the usual HO formula for ω = √(k/m), with the spring constant being K and mass being the total mass of the basis, M. So in the small-ish k approximation we can ignore the inner workings of the basis, and just treat the oscillations of the basis as a whole. Apropos the ωk2 guy, we could rewrite it as:



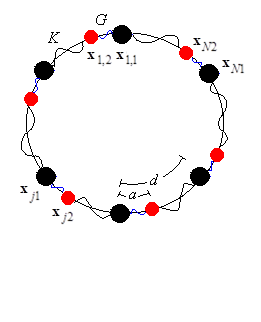
which is just usual HO formula ω = √(k/m) where we replace k with the total spring constant G + K, and the mass with the reduced mass μ. Normally G >> K, and so we can say



which is to say we can ignore the rest of the lattice entirely and just look at the oscillations within the basis itself, at least in this limit. We’re a litle early for Bloch’s theorem, but you can see how the rest of the crystal broadens the optical (ωk2) frequency from a single value into a spectrum.

**Modeling general oscillations of a crystal with a basis**

Generally speaking, the atoms in our basis can oscillate in the x-y-z directions. Taking this into account, let’s see what the frequency spectrum of such a system would be. So we start with our previous model, but allow the oscillations to be in any arbitrary direction.



We’ll start by writing out the Lagrangian:



where a and d-a are the lengths of the springs G and K when the masses are at rest, and ℓG, ℓK are the equilibrium lengths of the springs. Before taking derivatives and everything, we’ll first simplify the Lagrangian, by expanding it out to only second order, as usual. So for instance,



and so we’d have, correspondingly,



We can discard the constants. The linear term should go away; it did in the previous file because j and j+1 terms in the sum canceled each other out. This was a manifestation of the fact that the net forces on our atoms was zero in equilibrium. In order for this to happen here, we need:



which we can see is just a statement that the spring forces on both sides of any atom cancels out. So we’ll presume this to be so of course. And now let’s define:



(last equality follows from the force equilibrium equation) and we can say,



Well I guess we’ll take a derivative now:



and for the other one we have:



So our equations are:



FWIW, these match the ones at the top of the page when we set GT = KT = 0. Now assume a solution of the form:



Plugging these into the equations of motion we get:



which simplifies to:



and,



Keeping in mind that the **ε**ε’s are themselves vectors, and the coefficients multiplying them are matrices, we can write this in ‘super-matrix’ notation as:



which is,



The only non-zero solutions to this 6 dimensional equation occurs when the determinant is 0. Written out in matrix form, this amounts to:



Now, each of the 4 matrices commute, so we can use the formula,



where A, B, C, D are block matrices. So we have:



Obviously this splits into three separate equations,



which are each just independent copies of the equation we solved at the top of the page. So we have (pretty sure):



(the **ε**’s don’t depend on k, as they didn’t above, but they could in general depend on **k**) Dispersion curves look something like this (artifically displaced the green and blue guys so they’re separately visible). Note made KT, GT smaller than K, G.

Chart, line chart

Description automatically generated

Note I’m using notation A1, A2, A3 to stand for the commonly designated acoustical modes which go to 0 as k → 0, and O1, O2, O3 to stand for the commonly designated optical modes, which go to a constant as k → 0. One more comment: mode A1 is also called longitudinal acoustic, while A2,3 are called tranverse acoustic. And mode O1 is called longitudinal optic, while O2,3 are called tranvsere optic. And so the general solution to the equations of motion would look like:



where α can run between 1 and 2, and λ runs between 1 and 3p = 3(2) = 6. We also introduce the notation that p stands for the number of atoms in the basis. So in this case p = 2 clearly. The caveat about k = 0 applies. Might note that in the purely 1D example at the top of the page, the **ε**’s corresponding to these here would be pure numbers, or well, I guess you could say they’d be vectors, but they’d only point in the x direction.