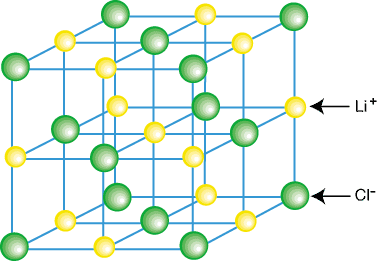
**Coupled Harmonic Oscillators**

Now going to do sample calculation of phonon dispersion relation when we have a basis. In the Quantum Mechanics/Many Particles file, I solved some simple 1D examples to get the eigenvectors and energies of a lattice of ions. Instead of reproducing that analysis here, I’m going to instead reach back to the Classical Mechanics/Coupled Harmonic Oscillators files and such. We can use that analysis to the same effect, since, as discussed in the QM folder/Foundations file, the energies of a system are the frequencies at which wavefunctions and operators undergo periodic motion. And of course QM operators obey the same equations of motion as their classical real number counterparts. So to determine the energies of a lattice it suffices to solve the associated equations of motion of the position operators involved in the Hamiltonian. So I’m going to reprise that discussion, just about word for word, below.

**Modeling a crystal lattice with a basis in 3D**

Now let’s consider a crystal with a basis in 3D. The ionic crystal LiCl is shown below, and is such an example.



To develop the equations of motion, we will write out the Lagrangian and take the appropriate derivatives:



The sum over j goes from 1 to N – over each of the N bases in the crystal. The sum over α proceeds from 1 to p – over each of the p atoms per basis. Same for sums over k, β. So then, applying the Euler-Lagrange equation…



The matrix **K** should be symmetric about switching **R**i and **R**j, as well as the indices α and β so we have:



Again, assume an expression of the form:



Applying the periodic boundary conditions like before will require that ui take the form:



Filling this into the equations of motion we get:



If we define:



then we can write this equation as:



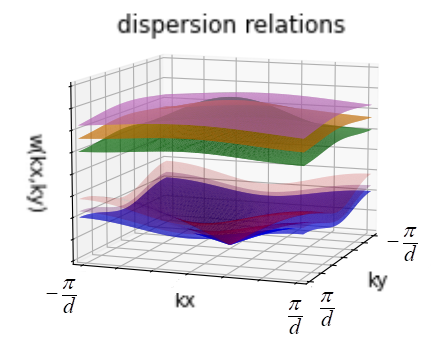
This is a matrix equation for the eigenvectors **εα**. Since this is a 3p dimensional matrix. As such there will be 3p such eigenvectors. And correspondingly there will be 3p such eigenvalues.



And so the general solution to the equations of motion would look like,



The caveat about **k** = 0 applies. We’d find the oscillators would have 3 acoustic modes – one for each direction of polarization: one longitudinal and two transverse (in a homogeneous system). Additionally, upon diagonalization of the 3p dimensional matrix we’d find 3(p-1) optical modes for a total of 3p modes. In the acoustic modes, all the oscillators in the basis oscillate in phase. In the optical modes, otherwise. The spectrum would look something like this (illustrated for case of 2 oscillators in basis (p = 2)) in a 2 dimensional system:



The bottom three dispersions are acoustic modes, and the top three the optical modes. Anyway, so the quantum mechanical energies would be:



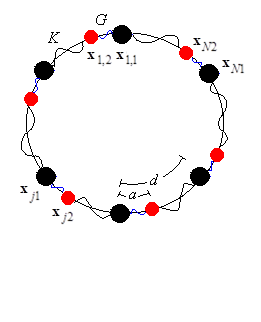
where λ runs from 1 to 3p. It bears recalling the example in the Classical Mechanics/N 1D Coupled HO w/ basis file, where we found approximate expressions for the dispersion relation for small k,



We can argue similarly that in the small k limit, we can find a rough formula for the acoustic modes by examining the equation of motion of the basis as a whole (call it mass M). And we should find that we get something of the sort above, generalized to 3D [kd → kxdx, kydy, kzdz or something, and K → some overall restoring force constant for the basis as a whole). And then also for the optical modes, we should be able to find their frequencies by in the small k limit by ignoring the motion of the lattice, and just looking at the relative motion of the atoms w/in the basis. We can verify these formulas explicitly in the example below, taking k → 0 and presuming, as is usual, that G >> K. We can consider the optical specttrum as just the basis frequencies of oscillation, broadened into a band by the restt of the lattice, like as happens for the electron excitation levels in the tight binding model. Going to apply these concepts to two illustrative examples.

**Example: Applying this formalism to our 1D crystal**

Consider a 1D crystal with 2N oscillators free to slide along a ring. Well, let’s say that the oscillators can move in the x, y, z directions, but that their equilibrium points are all stuck to the ‘x-axis’, which wraps around the ring.



and let’s write the Lagrangian in the form above. Well, starting from the beginning …. our Lagrangian is:



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. Now we’ll expand 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; because j and j+1 terms in the sum should cancel each other out. This is a manifestation of the fact that the net forces on our atoms is 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,



Now we can expand the squares,



and,



Finally, can write this as:



where,



The Fourier transform is,



and our eigenvalue equation would be:



And explicitly, this matrix equation is:



where we must keep in mind that each element is technically a 3×3 matrix itself. But anyway, this is the same equation (actually the complex conjugate of the equation – so I might have messed up a minus sign somewhere, but pretty sure that doesn’t matter as we should get real number results) we had in the N 1D coupled harmonic oscillators w basis file (in Classical Mechanics folder). So good. Not going to try to solve it though. Let’s content ourselves with solving it presuming we only have longitudinal oscillations. Then we basically ignore the y and z components of the tensors in our matrix equation, and we’re left with:



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 (well we don’t, but…). 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:



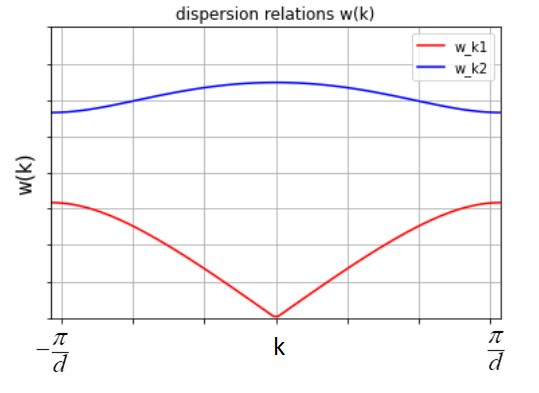
Therefore the eigenfrequency and (unnormalized) eigenvector corresponding must be:



So the eigenvectors/eigenfrequencies are:



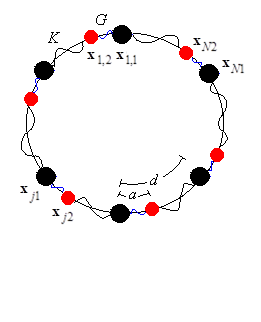
A plot of the eigenfrequencies is given below:



The lower branch is the ‘acoustic’ one, where the atoms in the basis are oscillating in unison. And the top branch is the ‘optical’ one, where the atoms in the basis are oscillating 180o out of phase.

**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.