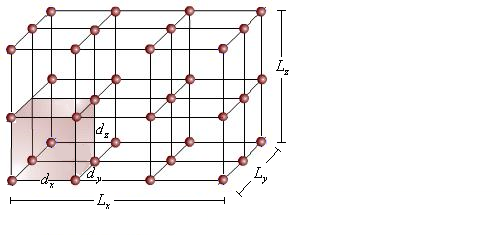
**Coupled Harmonic Oscillators**

Just going to reproduce some sample calculations of the phonon spectrum given a screened ion-ion interaction. 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.

**3D crystal lattice**

Now let’s extend our analysis to a three dimensional crystal lattice, with dimensions Lx ×Ly×Lz, lattice spacing dx×dy×dz, and spring-like forces between the constituent atoms. Such an arrangement is displayed below. This arrangement is known as a cubic lattice,, for obvious reasons. Other lattice structures are possible, and can in general be kind of complicated. But this simple one will be enough to demonstrate the qualitative features of 3D systems that we wish to explore.



The mathematics is more complicated in this case. But the result will be familiar. We would write down, in principle, the forces acting on a random atom in the lattice, and attempt to solve the equation of motion. To get the equations of motion we’ll write down the Lagrangian again…



Applying the Euler-Lagrange equation…gonna do it all at once, as vectors. We’re going to use the fact that **K** is a symmetric matrix, i.e., that Kαβ(**R**i,**R**j) = Kβα(**R**i,**R**j). Also going to use fact that **K**(**R**i,**R**j) = **K**(**R**j,**R**i). See the properties of the **K**-matrix section for details on that.



(in second line, can switch the order of the two r terms b/c they’re contracting against a symmetric tensor, K, and in the penultimate line, we use fact that K(Ri,Rk) = K(Rk,Ri), and in line before that we change a label of summation from k to j) Maybe a little more on that funky derivative that gives us the unit tensor, although it’s in the Tensor file. For instance,



So in any event, we have the kind of expected equation. Now going to use fact that **K**(**R**i,**R**j) = **K**(**R**i-**R**j) – see Properties of K matrix section. So we can write out equation of motion as:



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:



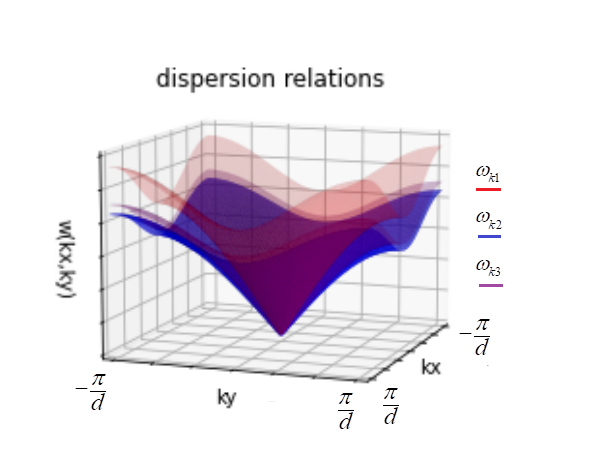
(it seems that we still have d.o.f. associated with Ri d because we’re not summing over i, but in reality, due to the periodicity of the crystal, there are only N distinct Ri – Rj values – see Properties section) This is a matrix equation for the eigenvectors **ε**. Since this is a three dimensional matrix, there will be three such eigenvectors. And correspondingly there will be three such eigenvalues.



In a homogeneous medium, one of the eigenvectors will be parallel to the direction of propagation of the wave, i.e., along **k**, and the other two will be perpendicular to **k**, as was the case for the 1D crystal we looked at above. That is, there will be a longitudinal wave and two transverse waves. For crystals that aren’t homogeneous – meaning the couplings are not the same in all spatial directions the eigenvectors won’t generally work out like this, and the waves won’t be purely transverse or longitudinal. The general solution to the equations of motion would look like,



The usual caveat about the k = 0 harmonic applies. Plotted below are the typical frequency spectrums. Again, there will be 3 sets of frequencies, corresponding to oscillations along the direction **ε**k1, **ε**k2, and **ε**k3. The plot below is for a two dimensional lattice (Python sucks at rendering multiple 3d images on same axes so this is best I can do).



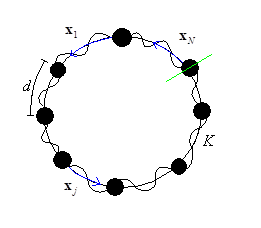
So the quantum mechanical energies would be:



where λ runs from 1 to 3.

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

Let’s apply this formalism to our 1D crystal, just to verify that everything checks out.



We have:



We’ll expand to 2nd order in the displacements. Note,



So we can say,



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/define 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. And we want to write our 1D crystal Lagrangian in the following form,



So here we go…



(the second line isn’t the most straightforward translation to δ’s, but using it because it’ll match previous results better) So we have:



And we saw in previous file that the solution is:



where the **ε**(kλ) and ωkλ are the eigenvectors and frequencies of the Fourier transformed K-matrix (again, there are just N distinct ΔRj’s),



Therefore the eigenvectors and eigenvalues of the system are determined by the equation:



which gives us identical results to what was found earlier. As so it follows that the eigenvectors and eigenvalues are:



and then that the general solution is:

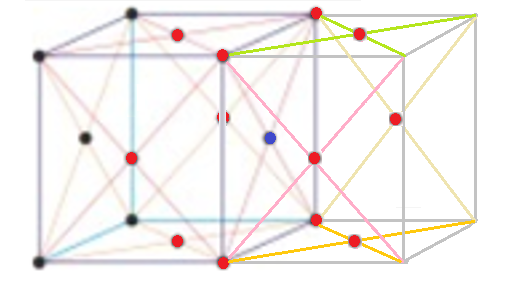


where the **ε**(λ) are just the Cartesian unit vectors **e**λ. Just as we’d found before. But anyway, main point is we have found the harmonic frequencies of oscillation, and so energy levels of the system.

**Example. FCC crystal nearest-neighbors interaction**

Might refer back to the Free Day/Phonons/Excitations/K-matrix properties for more background on this. Let’s consider a face-centered cubic crystal,

Chart, radar chart

Description automatically generated 

And consider that a typical ion has interactions only with its nearest neighbors. In this case, there’s 12 of them. I drew a blue guy, and its 12 n.n. in red. What is the **K** matrix for this guy? Let the blue guy above be the origin of our coordinate system, for these purposes. And say that each of the red n.n. interacts with the blue guy via a potential energy φ(ΔR) which is only dependent on the magnitude of ΔR = d. A Coulomb interaction would be one such example. All twelve Δ**R**’s are (points to right, points into page, and points up):



and we can work out K in different ways. But let’s go with our general pair-wise potential formula,



and restricting the sum over k, for a given i, to the nearest neighbors, we get:



where z = 12 is the number of nearest neighbors. Now we have to work out that tensor sum over all these guys.



Well, here’s all 12…



The sum of the squares:



So now we have:



Now let’s work out the Fourier transform. From previous file, recall we found,



The same colored Δ**R**ij’s above result in the same summand, so just doing unique terms, we have:



I don’t feel like we can simplify further. Say **q** = q. Then this does simplifies to:



which simplifies to:



The eigenvalue/vector equation,



tells us the polarizations and frequencies of the oscillatory modes of the given wavevector. So for us, in this direction we clearly have:



So one mode (longitudinal) is parallel to **q**, and the other two (transverse) are perpendicular. Plus the two transverse ones are degenerate in frequency. I imagine that if we chose a different **q**, less symmetrically oriented, we’d find the ωλ(**q**) to be completely non-degenerate and the **ε**λ(**q**) to be not necessarily longitudinal and transverse w/r to **q**.