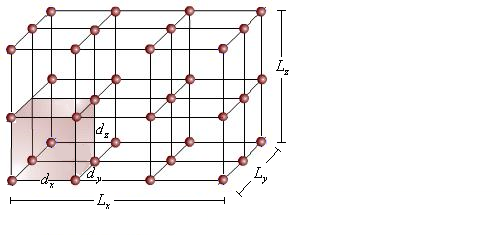
**Coupled Harmonic Oscillators**

**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. But to get the equations of motion we’ll write down the Lagrangian again. We’ll work this out in general I guess. So we start by considering a set of N atoms, each of mass M. Let the position of the jth atom be **r**j = **R**j + **x**j where **R**j­ is its equilibrium position and **x**j­ is the deviation from equilibrium. The {**R**j} forms a complete basis provided that we assume periodic boundary conditions. So the atoms in the lattice we’re modeling above each forms covalent bonds, etc, with its neighbors, resulting in the cohesive force of attraction holding the solid together. The actual potential between the atoms is probably pretty hard to figure out. If we’re dealing with a metal, then we might be able postulate that each of the atoms contributes one or two electrons to the conduction band, and so is left with a +|e| or +2|e| ionic charge. And so each atom exerts an ionic Coulomb force on every other. But for semiconductors or insulators, this doesn’t happen, and so the interatomic force is a little more nebulous. But in any event, it obviously creates a potential well in the neighborhood of each atom. Let V({**r**m}) be the total potential energy of all the ions together as a function of their positions. We can expand the potential in a Taylor series about the atoms’ equilibrium positions **r**j = **R**j.



where i = 1…N, j = 1…N, k = 1…N each label the ion, and α = x,y,z, β = x,y,z, δ = x,y,z each denote the components of the respective vector in the x, y, z directions. A more concise way to write this might be:



where the **:** indicates a generalized dot product between tensors. Either way, the first term is a constant, and so neglectable apropos dynamics. By presumption, the particles are in a stable potential minimum, experiencing no net force at equilibrium, so the second term is zero. We keep the third term, but neglect the fourth, and all others, for simplicity [well also presuming the deviations from equilibrium are small enough that these terms don’t matter appreciably]. So we’ll define the spring constant tensor which gives the ‘spring constant’ between the two ions located at **R**i and **R**j:



where **e**α and **e**β are the unit vectors in the respective x,y,z directions. And we’ll write the displacement of the ith ion as,



where again α refers to the x,y,z component. So then we have, for our potential:



FYI, sometimes we’ll write xi(α) as xα(**R**i). So then our total Hamiltonian would be:



Or we can write it more concisely as…



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,

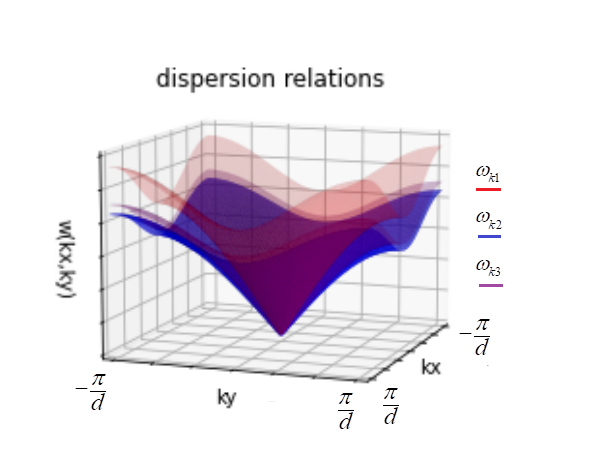


The usual caveat about the k = 0 harmonic applies. Plotted below are the typical frequency spectrums. Again, there will be 3 sets of frequencies, corresponding to oscillations along the direction **ε**k1, **ε**k2, and **ε**k3. The dispersion relation will be one of two varieties (I think). If the interactions between ions are long ranged, meaning that decays as a power law 1/rn, like the Coulomb interaction, then they’ll look like this the plot below is for a two dimensional lattice, and Python sucks at rendering multiple 3d images on same axes so this is best I can do).

Chart, surface chart

Description automatically generated

What notable about this spectrum is that it has a finite minimum at kx = ky = 0. The minimum is known as the plasma oscillation frequency (see EM folder perhaps, and I *kind of* worked out an example in the Thermodynamics folder/Plasma file). This kind of spectrum would be expected to predominate in ionic crystals and substances without a lot of conduction electrons running around. If there are enough conduction electrons in the material, then these electrons tend to ‘screen’ the interionic forces, making them exponentially damped, effectively acting only over nearest neighbors, or next nearest neighbors. Metals are one prime example of this sort of material. And we’d get this kind of dispersion relation for them,



The salient property here is that the spectrum goes to zero at kx = ky = 0, instead of a finite value. And the spectrum near the origin is approximately cone-shaped with a constant slope. Since all of the examples we’ll be dealing with, and have dealt with, are ones where the oscillators exert forces only on their neighbors, it is *this kind* of spectrum that we’ve been seeing.

**Properties/Symmetries of K**

Okay, so first, let’s recall K’s primary definition:



And we can observe that due to equality of cross-partials, we have:



If we have a periodic crystal, then we should be able to make the mapping xα(**R**i) → xα(**R**i + **a**), where **a** is any lattice vector which points from one lattice site to another, without fundamentally changing anything – in particular, the energy. That is to say, we can replace the displacement of every atom with the displacement of the atom **a** away from it, w/o changing the energy. This implies,



Now this must be true for all xi(α) and xj(β). And this means we must have, for every **Ri**, **R**j:



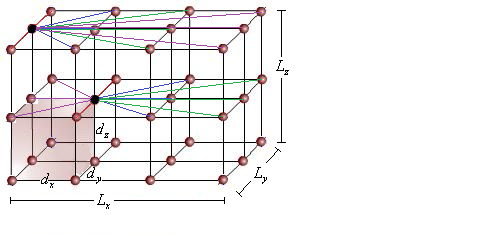
But say we made **a** = **R**j. Then we’d have:



Therefore **K** is a function only of the relative displacement of the ions. So we can write:



Quick note on Kαβ(**Ri**-**R**j). For fixed **R**j, there are N possible values for Kαβ(**R**i – **R**j). But it would seem that the set of possible values Kαβ(**R**i – **R**j) can take on would be depend on what **R**j is. But that’s not actually so, thanks to the periodicity condition. Consider a lattice below, and the two black atoms in particular. The colored lines are position vectors. And identical colors are identical sets. So in particular, the purple ones which up top traverse the entire crystal are equivalent to the purple ones in the middle which go backwards one unit cell.



Okay, moving on, we can say that every (repeating) crystal lattice has an inversion center so that if take that point as our origin, and make the mapping xα(**R**i) → -xα(-**R**i), we will end up with the same crystal and displacements, relative to each other. And so the potential energy won’t change under such a transformation. So that means:



Since this must be true for every xi(α), xj(β), it follows that we must have:



which, in light of the previous equality, means,



And so **K** is a symmetric matrix. There are a few other properties of note. If we translate all the ions by a uniform displacement, **a**, this shouldn’t change the energy, as the relative orientations of the ions wouldn’t have changed. We can see what the consequence of this is for our **K**. Technically, **a** will have to be a small displacement, since our expansion of V is only good in a small neighborhood about all the **R**’s, out to second order in **x** (we’re not moving the equilibrium positions of the atoms, just the atoms themselves). So we should have:



Since this should be true for any **a**, and **x** for that matter, we must have:



There should also be rotational symmetry – i.e., if we rotate all particles by an angle **θ**, this shouldn’t change the energy, as it wouldn’t change the relative orientations of the particles. Our angle **θ** must be small, since again our V approximation is only good to second order in **x** (we’re not rotating the equilibrium positions of the atoms – just the atoms themselves). If we rotate the crystal by θ, then the positions of all the particles will change to **r**i → **r**i + **r**i×, i.e., **x**i → **x**i + (**R**i+**x**i)× **≈ xi** + **R**i× (since x is first order, we can only keep terms to first order to be self-consistent). Well filling this into V, we have:



This must be zero for all **x**’s, and all **θ**’s. Everything will be zero if we just require:



We can leave it like this, or if we place our origin at **R**i, then we can write this as:



which looks slightly prettier. Now let’s consider **K**(q):



And consider two properties of Kαβ(q). First,



And second, we said Kαβ(**R**) = Kαβ(-**R**). And so we can say,



So this makes **K**(q) a real matrix. Further, it is symmetric, as we saw. And this guarantees that it has real eigenvalues. The eigenvalues have to be positive too, in order for the potential to be ‘concave up’. Else, the potential landscape would be a relative maximum, instead of minimum. So these are the main properties of concern for Kαβ(Ri,Rj) and Kαβ(q). Note this means that Kαβ(q) has only 6 d.o.f., since it’s a real symmetric matrix. Last thing. Note that:



So we can use these symmetries to write Kαβ(q) in a nice way,



So we have, making cosmetic change **R** → Δ**R**.



Well I guess we can exclude the ΔR=0 term from the sum, since we get zero. So,

