**Phonon Interaction**

Going back to (and see maybe Quantum Mechanics/Distinct Particles/Harmonic Lattice something for more on the lattice interaction):



We’ll focus on just the lattice/ion part,



I’m just going to pretty much copy the work we did in the Quantum Mechanics/Distinct Particles file. Let’s start by considering a little more how we end up with that interaction term (1/2)Kxx. We start by considering the Hamiltonian for a set of N ions, each of mass Mion. Let the position of the jth ion 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. We are considering that the ions each have a positive charge of + because I assume that one of each atoms e-‘s is mobile and floating around in the material. Excluding these mobile electrons, there is a net attractive force between each of the ions obviously, if they’re stuck together in a lattice. Each forms covalent bonds, etc. And on top of this there would be the repulsive Coulomb interaction between each of their + charges. Let V({**r**m}) be the total potential energy of all the ions together as a function of their positions. Appropos the repulsive Coulomb part at least, we could say the total potential energy between the ions is something like:



where Z would be the net charge of the ion (Z = 1 or 2 at most). The actual potential between the ions is probably pretty hard to figure out. But in any event, it obviously creates a well in the neighborhood of each atom. We can expand the potential in a Taylor series about the atoms’ equilibrium positions **r**j = **R**j.



where ∂/∂**r** is short for the gradient operator, ∂2/∂**r**2 would be the outer product of two gradient operators, etc., the **:** indicates dot product with a tensor (that’s what the ∂2V/∂**r**2 and ∂3V/∂**r**3 term is, and the third term is). The first term is a neglectable constant. 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, though, turns out that to describe compressibility we do need the anharmonic, i.e., 4th, term]. So we have:



where **e**α and **e**β are the unit vectors in the respective x,y,z directions. The displacements we’ll call the displacement (position) operators of the individual ions:



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



We often assume that **K** depends only on the difference between **R**i and **R**j. So



So then our total Hamiltonian would be:



We can rewrite this as:



where **x**(**R**) and **p**(**R**) denote the displacement and momentum of the oscillator at position **R**, and satisfy,

