**Excitations**

So let’s return to:



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



I’m going to copy the work we did in the Quantum Mechanics/Distinct Particles folder. In that folder we solved this problem a few different ways, and did a few examples of 1D harmonic lattices, but I’m just going to reproduce one of those solutions. So to find the eigenstates of H we make the canonical substitutions (suppressing the Greek index for now)



Note that periodic boundary conditions restrict the q’s to N distinct values. For instance, if we’re dealing with a paralleliped with side lengths Lx­ = Nxax, Ly = Nyay, Lz = Nzaz (where ai are the lattice spacings), then periodic boundary conditions require:



We’ll choose the Ni distinct values of qi to be:



Basically we’re choosing the q’s within the first Brillouin zone (BZ). We can invert the ‘transform’ to get:



Note that the Hermiticity of xR and pR imply:



This is a canonical transformation so we also have, as one can verify:



Now plug this substitution into H:



Define:



Then we have:



Note Kαβ(q) is a real symmetric 3×3 matrix with non-negative eigenvalues that we denote MionΩqλ2, and real eigenvectors εqλ (see K Matrix Properties file). Given Kαβ(q) = Kαβ(-q) (see file again), we can expect that a similar relationship holds for the eigenvalues: Ω**q**λ = Ω-**q**,λ. And also for the eigenvectors. But, we can also make the following actually more convenient choice,



which admits the possibility **ε**qλ = **q**, which is useful for isotropic crystals’ longitudinal vibrations. Now make an eigenvector expansion (with a certain prefactor choice to keep things canonical):



Then we still have canonically conjugate variables,



and our H comes to:



Finally, we can diagonalize H by defining,



which satisfy bosonic commutation relations, as we can verify,



Solving for x and p we get:



And filling these in we get:



And then finally we have,



Thus the excitation spectrum of the harmonic lattice can be described as a set of non-interacting bosonic excitations or phonons, having energies Ωqλ created and destroyed by aqλ†,

aqλ respectively. If need be, we can recover the ionic displacements and momenta as



and:



Can also rewrite these using ρion = MionN/V. We have implicitly assumed that the lattice has one ion per unit cell. If there are Nb ions in the basis, then there will be 3Nb phonon branches which we can label λ = 1, 2, …., 3Nb. So we have the same frequency spectrum as in the classical case. Each oscillation frequency can have n phonons in it, for an energy of (n+1/2)ωk.

*\* I’ll call the results we have for x(R) and p(R) to be the one’s using the CMT phase convention (see QFT folder/photon quantization too).*

**Characteristic Features of the Phonon Eigenfrequencies**

The dispersion relation Ωkλ consists of this: for every k (and recall k is restricted to a BZ basically, because the number of oscillation wavevectors matches the number of lattice sites), there are 3 acoustic modes and 3(p-1) optical modes, where p is the number of atoms in the basis. The acoustic modes are characterized by having all the ions in the basis oscillate in phase with each other. The optical modes are characterized by the ions in the basis oscillating out of phase (to varying degrees) with each other. In an isotropic system, 2 acoustic modes will be perpendicular and 1 will be parallel to q. The ones perpendicular to q are called transverse acoustic modes. And the one parallel is called the longitudinal acoustic mode. Similarly, we would talk about longitudinal and transverse optical modes. Otherwise, the directions of the vectors would be different (see later files for calculations).

If the interactions between the atoms are long-ranged (and they would be at this point, since the effect of electron screening is not yet taken account of), then the acoustic modes will have a finite minimum, ΩE, at k = 0 🡪 basically they will have a kind of optical-looking dispersion relation. It *might* actually resemble the dispersion relation we got in the Thermodynamics/Plasma file, ω(k) ~ √(ΩE2 + ck2). And ΩE would be the lattice vibrational equivalent of the plasma oscillation frequency, Ωp. This is about (faux Gaussian units):



(recall this is the same frequency that we encountered in the Electrodynamics folder – see Plasma oscillations). Just to make connection with the electron plasma frequency, if we had e-‘s in the picture (which we don’t yet) then overall charge neutrality would require.



So the ionic ‘plasma’ frequency is much smaller than the electronic one, Ωp, owing mainly to the greater inertia. Now Ωp ~ 1015 Hz, so, that would make ΩE ~ 1013Hz. I guess that puts it in the infrared range.

Apropos the optical phonons, as aforementioned, these are frequencies that result from the atoms in the basis oscillating out of phase with each other. One can think of them as just the eigenfrequencies of the basis/molecule, broadened out into a band due to nearest neighbor interactions. In much the same way the free electron spectrum is basically (vis a vis the tight binding model) the electrons’ atomic states, broadened into a band thanks to nearest neighbor interactions. Can check out the Classical Mechanics or Quantum Mechanics folders for rudimentary calculations of the optical branch frequency spectra. The optical frequencies will lie above the acoustic branch dispersion relation. Altogether, for p = 2 atoms in the basis, the dispersion relation will look like this (top three = optical, bottom three = acoustic):

Chart, surface chart

Description automatically generated

A general excited state of the system would be specified by counting the number of phonons in each allowed mode.

