**Excitations**

So general dispersion relation looks something like this, one acoustic spectrum and one optical spectrum, for case of two atoms in a basis. If we have 3 atoms in the basis, then we’d get one acoustic spectrum and two optical ones. In the three acoustic branches, the atoms in the lattice site basis oscillate in unison like a single atom, and the lattice site as a whole participates in the wave motion of the entire lattice. The 3 branches correspond to three different directions the lattice site can oscillate in (x,y,z basically). In the optical branches, the different atoms in the basis oscillate out of phase with each other.

Chart, surface chart

Description automatically generated

The precise dispersion relation ω(k) for these guys is rather complicated. A few simple examples were calculated in the Excitations folder. But a rough phenomenological approximation is usually attempted as follows. For the acoustic branches, though clearly the dispersion fills up the bounds of the first BZ of the reciprocal lattice, for simplicity we approximate the 3d k-space cubic BZ as a simple sphere (or circle in 2d k-space, as would be appropriate for the plot shown above). Of course each branch contains N (N being number of lattice ions) modes, and so our spherical BZ will have to too. The radius of such a sphere is called the Debye wavelength (or wavenumber in this case), kD. Since each mode takes a region in k-space equal to (2π/Lx)(2π/Ly)(2π/Lz) = (2π)3/V, we must have approximately,



and so we have:



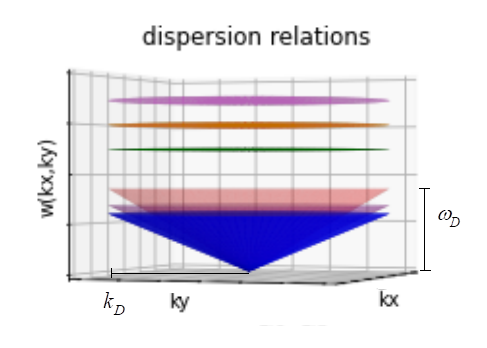
which puts the Debye wavelength at about the Fermi wavelength, kF = (3π2n)1/3, for what it’s worth (only difference being a factor of two inside the ( ) owing to factor two spin degeneracy of electrons). Or, another way to look at it, if we had a cubic lattice, then we’d need:



which makes sense, as the diameter of the sphere (2.5π/d) is just a little over the width of the cube (2π/d). Anyway, so then as for the dispersion relation(s) ω(k) itself, we make the following simple approximation:



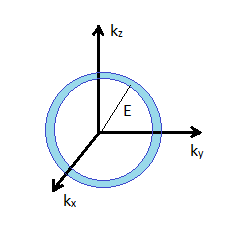
(s labels the branches) depicted below:



Do note that the domain of our (2D for illustration’s sake) Debye model approximation is a *circle* in k-space, with radius kD. In contrast, the *actual* domain is a *square* in k-space with side lengths 2π/d (at least if we have a square lattice). Likewise a 3D Debye model would be a sphere, as opposed to a cube (or whatever else the BZ might be for some other lattice structure).

**Density of States**

For *an* acoustic branch model (3D), where (customary to call Ω as ω when acoustic spectrum) ωks = |**k**|vs and vs is the slope (velocity) of the branch (of the excitation wave), there will of course be many states/modes with the same energy. We’d like to calculate the density of states (per unit volume). This would be:



as follows,



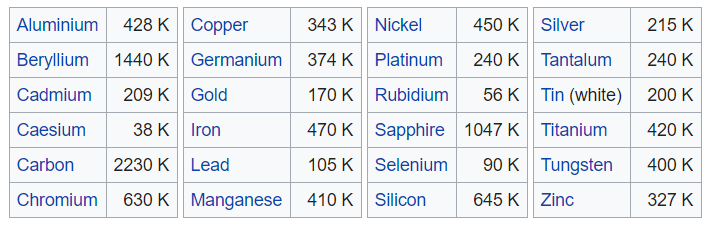
(ED = ωD) We have to impose the step function to cut off the distribution past ED, which is defined such that there are N modes within that range, i.e.,



And is this more like a density of excitations, rather….? We’d multiply n by 3 if we want to include all acoustic branches.

**Table of Debye Energies**

A table of Debye temperatures (ED = kBTD) is given below:



Evidently ED << EF, even though kD ~ kF. In terms of eV’s, we have kBT/eV = (1.38×10-23T)/(1.6×10-19) ~ 10-4eV to 10-3eV. Compare to EF which is around 1eV to 10eV. So these are 104 times smaller.