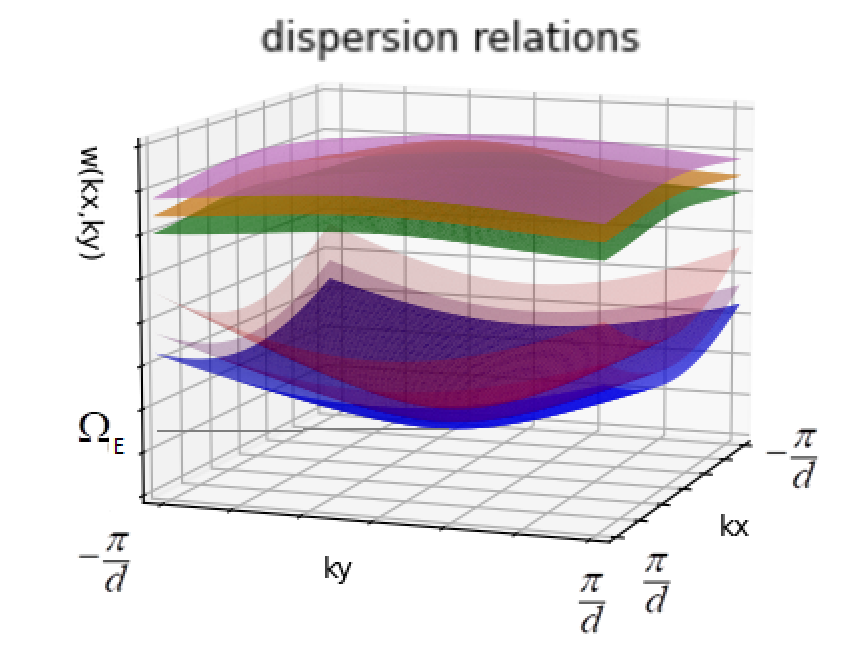
**Heat Capacity**

So general dispersion relation looks something like this, one acoustic spectrum (three branches) and one optical spectrum (three branches), 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.



The precise dispersion relation ω(k) for these guys is rather complicated. I think the acoustic spectrum goes as something like ω(k) ~ √(ΩE2 + ck2), and the optical spectra goes as some Ω02. In the Einstein model, we just approximate the acoustic branches as all having the same dispersion relation, ωs(k) = ΩE (where s = 1,2,3 is the given branch of the acoustic spectrum). Okay so let’s proceed. There are a few ways to do it. We can just calculate the system’s partition function:



And so our free energy, F = -kTlnZ, would be:



Can also write this as:



which puts it in ‘L’ form. And it makes sense that it should since phonons are bosons. Only difference is the extra constant term which comes from the fact that the lattice has energy in the zero-phonon state, whereas regular bosons have no energy if there aren’t any present. Now let’s consider the internal energy (density). This is simply



and we’ll end up with:



Well anyway, all of our ωks’s are just ΩE. So noting we have the same number of k modes as lattice sites, i.e., N, and we have 3 branches:



In the low T limit, this goes to



And in the high T limit, we have:



So altogether,



Now ΩE is around the infrared range, 1013Hz, which corresponds to an energy (we’ve been setting ℏ → 1) ℏΩE ~ 101310-33 = 10-20J ~ 103kB. So we can expect significant thermal population of our ΩE energy level around T = 1000oK, which is a little hot. So room temperture is basically the low temperature regime here. Now let’s consider the specific heat.



We can see that in the asymptotic limits we have:



Might be worried that this means c will blow up at T = 0, but in fact e-Ω/kT decreases to 0 exponentially, which beats how fast T2 blows up. And we get something like looks like this:

Diagram

Description automatically generated

We could add in the optical modes if we want, but I’m not going to here. See the heat capacity file in the Interacting Electrons and Phonons/Normal Metals file.