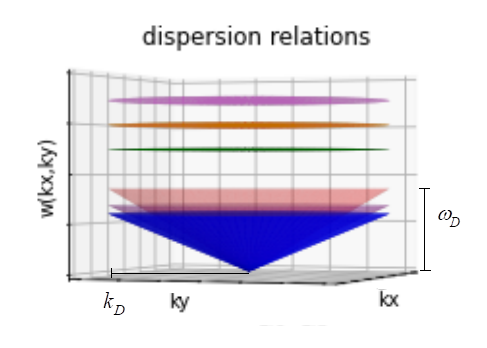
**Heat Capacity**

**Phonon Contribution**

Let’s use the Debye Model to work out the heat capacity of a solid, just focusing on the contributions from the screened phonons. Recall we said,



(s labels the branches) depicted below:



Also, for what it’s worth, the acoustic wave velocities are ~ 100m/s. And so that makes the upper limit of the acoustic branches, called the Debye energy ωD = kDvs ~ (100K)kB ~ 10-2eV. Which means at room temperature we expect all k modes in the acoustic branches to be well populated. The optical branch frequencies ω0s are typically much higher, being near the optical frequency range. Seems like it’s usually closer to infrared. So ω0s ~ c/1000nm ~ 3×1014Hz ~ eV ~ (104K)kB, where c is speed of light. So we would not expect the optical modes to be populated at room temperatures. And in fact, the solid would probably have melted by the time they would be populated. But I guess targeted application of infrared/visible EM fields can excite a few. 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, 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



Now note,



So we can write



Let’s go to the high T limit. We’ll presume we’re at high enough T so that kT >> ωks for all branches. Then we have:



And so we find:



where p is the number of atoms in the basis and is implicitly accounting for the 3 acoustic modes and 3(p-1) optical modes. Note energy doesn’t saturate because we can always keep adding phonons (which are bosons) to the energy levels indefinitely. But as aforementioned, we’d expect the solid to have melted at such temperatures. Let’s lower the temperature to ωD << kBT << ωksoptical. Then for the acoustic branches we can still say:



and for the optical branches, we’d have:



in the grossest approximation. So repeating our analysis, we’d have:



Now let’s go to even lower temperatures whereby kBT << ωD << ωksoptical. For simplicity I’ll take the 3 acoustic branches to have the same dispersion relation (i.e. vs is same for both). And I guess we’ll include all the optical branches, just for kicks, even though they will negligibly contribute, as estimated above. So now we’ll have:



If we specialize to the small T limit, we’ll observe the integral’s upper limit will go to ∞, and also that we can safely neglect the 1/[eβω – 1] term in the last bracket. So then we’d have, borrowing the boson function definition (see Stat Mech folder free boson file thing),



this comes to:



So altogether we have:



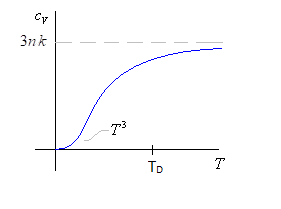
Now let’s consider the specific heat.



We’ll see that in the asymptotic limits we have:



And in general, it will look something like this:



The crossover from T3 to constant behavior is roughly at the Debye temperature, TD = ED/kB = kDvs/kB. This is typically ~ 100K or so. So at room temperatures we’re usually in the saturated constant regime. Not displayed is what happens at T ~ ∞, if the solid is still around, then cV would begin to rise and approach the T ~ ∞ asymptote. Actually I guess it would approach intermediate asymptotes as each individual optical branch gets ‘thermally’ activated.

**Phonon + Electron contribution**

So now we have electrons and phonons interacting. The total heat capacity would just be the sum of the two heat capacities. If we presume the phonons are effectively screened by the electrons, then the phonon spectrum becomes linear in the small q regime, and we find the phonon specific heat goes as T3 in the small T limit and asymptotes to 3nkB. But we’ll recall the electron contribution went as ~ T in the small limit, thereby dominating the phonon specific heat, and then asymptoted to 3nkB/2. So we expect the following behavior:

