**Crystal Excitation Properties**

Now going to calculate some things in particular,

**Free particle ρ(E)**

Starting from the first definition, we have,



and so in the various dimensions we have,



(this includes spin) Via the second formulation we have,



where,



and so we have,



and so we have the same thing. Another way is to count the number states within the sphere of radius ε + dε, i.e., Φ(ε+dε), subtract Φ(ε) and divide by dε, and the volume. In other words, just take the derivative of Φ(ε), and divide by volume. This would be:



and this is the same, assuming Ωd = dVd. And we see that it is the case in all three dimensions (Vd is the volume of the unit d-dimensional sphere, and Ωd is its surface area).

What if the Fermi surface has a saddle point? Some 2D semiconductors have this property. Then if we rotate our coordinate system a certain way, we can write it as this:



(assume band masses are same in each direction for simplicity) Then our density of states would be (I’ll assume ε > 0):



Guess I’ll introduce some bounds of integration for the 1st BZ. We’ll say it’s square,



So,



Can see there is a log singularity near ε = 0. Another way to do this is with the velocity formula. Note the surface of costant ε becomes a line of constant ε.



**Ground State Properties**

Now let’s work out the ground state energy of our Fermi gas. This is easy to do now that we have the density of states. We integrate the density of states up to the Fermi energy EF and set equal to N/V. So the density of states is:



and then,



Solving we have:



Parenthetically, we have the Fermi wavevector to be:



which reduces to, in the various dimensions:



(this includes spin) Fermi energy is ~ eV. And the Fermi wavevector would be:



(n includes spin) kF is, as we can see, on the order of the reciprocal of the lattice spacing ~ 1/a. Copper, for instance, has 8.5×1028 electrons/m3. And so kF ~ 0.7nm. Then, the ground state energy is just:



In the various dimensions this reduces to:



(includes spin) It’s useful to observe that the density of states can be written in terms of the Fermi energy,



In various dimensions,



(includes spin) where n is N/V of course. Might also go ahead and calculate the density of states at the fermi energy. This is:



In 3D, in particular, we have:



(includes spin) By the way, we’ve been setting ℏ = 1. To put in SI units, we should multiply density of states by ℏ to some power p. To find out what p we just need to make the units work out as they should.



clearly need p = -2. So it would be, for instance,



Or if we go back to the (3D) formula:



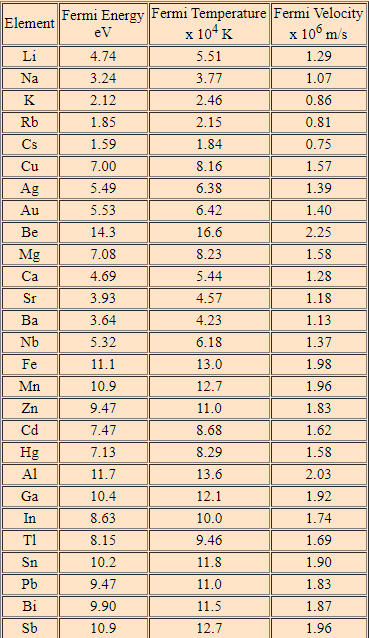
Then we see we actually need a different power. Cause,



So p would have to be -3. Guess these annoyances are the cost of leaving out h.

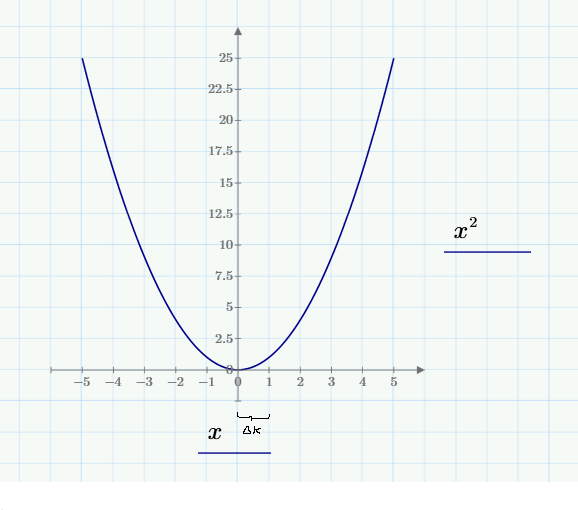
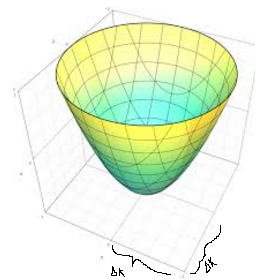
**Table of Values**

Here’s a nice table of values, stolen from the Hyperphysics website.



**Appendix 1. Trying make ρ(E) calculations for realistic bands (not just parabola)**

This has nothing to do with the stuff above, butI’d like to understand how to draw the density of states, given knowledge of E(k). First I’d like to examine the continuum approximation we’re going to make when counting states. So I’ve drawn the 1D and 2D energy spectrum for a free particle.

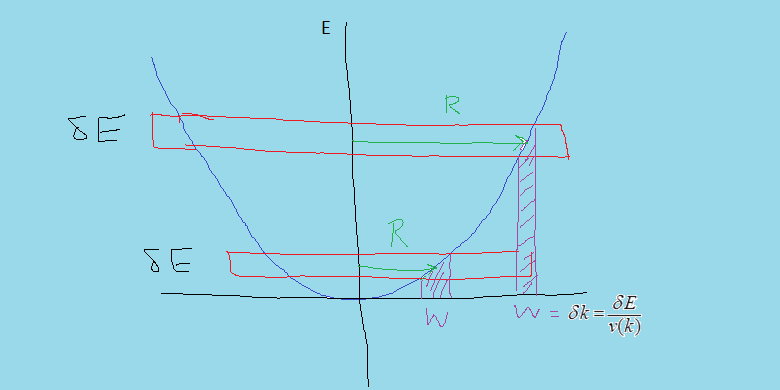
 

So note that there is only one state per grid. But nonetheless we will be making the approximation that the states are smeared out evenly throughout all k-space. So we can have a region with 0.2 states, or 3.7 states, etc. Let’s say that each grid corresponds to a distance Δk. Now consider commensurate regions in both dimensions. A region of width ℓ would cover a number of states equal to ℓ/Δk in 1D, but ℓ2/Δk2 in 2D. When ℓ is small, this would clearly cover fewer states in 2D, which seems a little counterintuitive. But this is because in 1D, a single state is merely smeared out over Δk, whereas in 2D a state is smeared out over Δk2. So a state is much more sparsely smeared in higher dimensions.

So to start, let’s consider the free particle density of states – well results are above. So why does density of states at E = 0 go infinite, finite, zero for the three cases? ρ(E) = limδE→0 δstates/δE. Generally speaking, as dimension increases E increases faster, since E ~ dk2, where d is the dimension. The gradient of E vs. k increases.



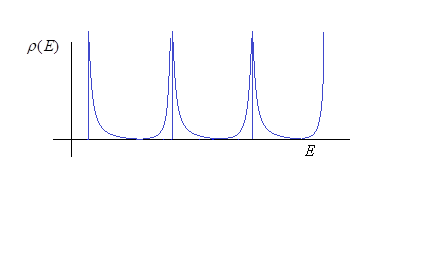
Well consider the energy windows below (in blue). We can think of the density of states as the number of states within window E±δE/2 ÷ by δE ~ volume of phase space within window E±δE/2 ÷ δE = surface area of constant E surface ∙ δk ÷ δE = surface area of constant E surface ÷ v(k). It’s true that as slope of energy curve gets steeper, fewer k-states would tend to be found inside the window on that account, but note also that the radius of the window increases, and so that means that the radius of the circle of k-states within the window will increase as well, meaning that more states will be available to the window. So there are two competing effects: larger E means wider circle within energy window, but also narrower circle since slope of energy curve gets steeper.



Now let’s consider the tight-binding model. E(k) = VΣcos(k∙δ), where δ is vector pointing to nearest neighbors. In 1D, this would look like this: E(k) = 2Vcos(ka), where a is lattice spacing, and k would run from –π/a to π/a. What is ρ(E) here?



So we would see something like this…



where there are singularities on either end of the band gaps (i.e. energies -2V, +2V. In 2D, E(k) would look like E(k) = 2Vcos(kxax) + 2Vcos(kyay). So what would this density of states look like?



This cannot be done exactly per se΄. Singularities occur when E/2V – cos(kyay) = ±1 → cos(kyay) = ±1 – E/2V → ksin = cos-1(±1-E/2V)/ay. So there will always be a singularity in the integral. These are called Van Hove singularities I think. What type? Well, expanding about this point we have:



So the singularity is first order under the √ which means it is integrable and therefore ρ(E) is finite…what if E = ±2V? Then we get

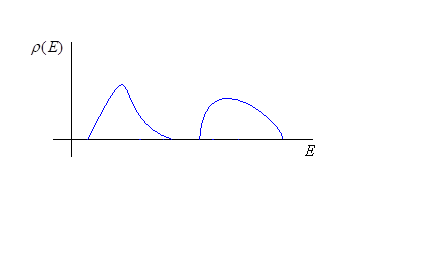


and so is finite still. Note that this mimics the behavior of the free-particle 2D spectrum (it is finite where the slope of the energy spectrum is zero). What if E = 0?

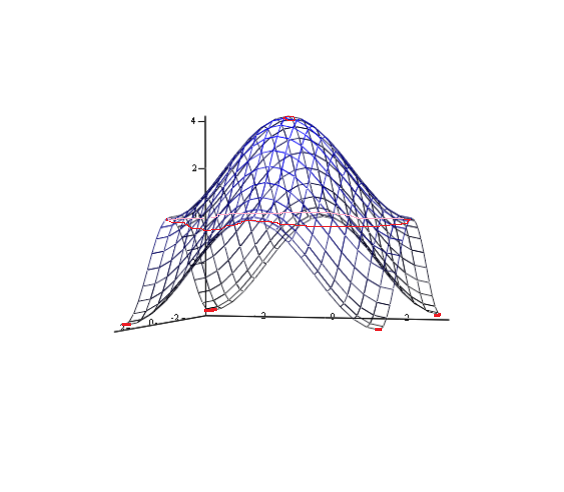


So the singularity would be non-integrable. So ρ(E) would go infinite in middle of band apparently.

In 3D, E(k) would look like: E(k) = 2Vcos(kxax) + 2Vcos(kyay) + 2Vcos(kzaz), for a certain type of lattice anyway. The result would be something like this (makes sense b/c 3D smoothed out the singularity in the free particle case)… for notice that, in 3D, as slope of free-particle spectrum goes to 0, the density of states goes to 0 as well. And so it should make sense that for the tight-binding model, as the slope of the energy spectrum goes to 0, the density of states will as well, and this will happen at the top and bottom of the band.



Perhaps the best way to see these behaviors is directly from the formula ρ(E) = ∫dS/v = 1/v, ∫dℓ/v, ∫dS/v in 1,2,3 dimensions. For free particles, in 1D this would just be 1/k. And in 2D this would be k/k = constant. And in 3D it would be k2/k = k. This is all as expected. For tight-binding models, in 1D we’d blow up at beginning and end of spectrum where v goes to 0. In 2D, according the formula proffered for Eks, v looks like it would go to zero at the top, middle, and bottom of the band. At top the integral would go as ∫dℓ/v = ∫2πkdθ/k and so would be finite. At the middle, our integral goes as ∫2πkdθ/v and v would go to 0 four times along the perimeter it appears, and so it appears we’d get ∞, but I suppose we’d need to know how v → 0 w/r θ because the singular *could* be integrable. At the bottom, it doesn’t appear that v is zero at all, but since these are just finite points, we’d not get any contribution to the surface/line integral, and so we should get zero.



In 3D, our integral would be a true surface integral. And I expect that at the top, the energy will be quadratic in k as usual, and so ∫dS/v should be ∫4πk2/k which ought to be zero. In the middle of the band, ∫dS/v would be finite as long as singularities occur at isolated points again (and simply go as 1/k). And then at the band minimums, I would expect to get zero again, just like in 2D.

**Example**

Let’s consider the limit of infinite dimension. Oddly, this problem then becomes a little more tractable. So let’s revisit our tight-binding excitation spectrum. Let’s suppose we have a hypercube with side lengths *a*, and dimension *d*, and our spectrum is something like this, therefore:



If d is large, we can think of the sum over cos( )’s as a sum over random variables. The average of cos() is 0, and its variance is ½. Consequently, the average and variance of ε(**k**) is:



Therefore, we can approximate ε(k) as a Gaussian with the same mean and variance,



Would have to multiple this by the total number of states and then divide by the volume to really get the density of states. Total number of states should be (L/a)d. So then,



In order to not have a pathological limit d -> ∞, which is what’s necessary to make this approximation scheme work, we have to scale the strength of the interaction down, with dimension. One scaling I’ve seen is (obviously it must go as 1/√d to work):



Filling this in, we’d have:



So we see the expected Gaussian profile of the density of states – largest in the middle of the band (ε = 0). And we see that the width of the density of states is proportional to the interaction strength. This makes sense because larger t’s increase the width of the energy spectrum. But this doesn’t evince any of the singularities we saw that we run into above. And this is because the infinite dimension limit we took removes them.

**Appendix 2. Translating integrals over k to integrals over ε and the like**

Say we have an integral like,



where f is a function of only the magnitude of k, or equivalently, can be considered a function of the energy ε(k) = k2/2m, say. And let’s define a density of states (not going to bother with spins and stuff):



Then we can put this integral in terms of an integral over ε via:



What if f(k) = f(**k**) so that it isn’t a function purely of energy? Well we can introduce new coordinates: ε, u, v. ε will define a surface of constant energy, ε = ε(**k**), while u(**k**) and v(**k**) will run along the surface of constant energy. We could invert the coordinate transformation and say **k** = **k**(ε,u,v).

Chart

Description automatically generated

Anyway, then a 3D k-space volume element would be, as above, given by,



Presumably dSε(u,v) would look like some g(ε,u,v)dudv. And ∇ε would also depend on ε,u,v. Okay and of course ∇ε = **v** (not the coordinate v, but the velocity **v**):

