**Excitations**

**Mean Field Theory**

So going back to:



Now we’ll try to use the GS wavefunction analysis as a spring board to analyze the full excitation spectrum (or thermally averaged excitation spectrum, kind of), from which we could then get the thermodynamic properties of the metal. Our prior use of MFT – see tight binding model of electron-electron interactions – took the number operator per site as the quantity which we could take as having relatively few fluctuations (fluctuations over what? I guess thermal fluctuations? and as elaborated on later, in the grand canonical ensemble).



We *could* do the same here, but I wonder if we don’t because our wavefunctions have been sort of built up from the grand-canonical ensemble and so particle fluctuations might actually be large (or maybe not large, but still, too large). Of course we don’t have ‘sites’ here either. Well anyway, instead we take another quantity as being non-fluctuatey, namely, the Cooper pair destruction/creation operators,



whose average value, at least in the GS, we calculated in the previous file. I’m not sure what basis we have to consider fluctuations of this guy(s) to be small. But if we are to consider its average value a sort of order parameter, as we argued in the previous file, then it is typically the case that fluctuations of such are rather small, unless we get *really* close to the phase transition. So let’s jump into it. We’ll define:



and then we can write:



Filling this in,



where in the last we ignore the (δg)2 term. Filling the guys back in we have:



Now let’s recall from the last file, or maybe *define*, in the *present* context:



So we can write:



Then ignoring the constant, we have:



**Mean Field Theory for K**

Now instead of doing a mean field calculation of H, we do one of K. I think this is because we are not dealing with states of definite particle number and so using the ensemble where N is specified isn’t self-consistent. For instance, in the past instances of MFT, we dealt with states of definite N and so set about calculating F = -kTlnZ, where Z = Tre-βH. Basically, then, we just had to diagonalize H. But now we do not, for better or worse, work with states of definite particle number. Rather, we are operating in the grand canonical ensemble, effectively, and so in that case we’d try to get a mean field theory for L = -kTlnΞ, where Ξ = Tre-βK. And so correspondingly, we need to diagonalize K.



Since it’s bilinear in the creation/annihilation operators, we could brute force work out the linear combination of these c’s which will diagonalize K – see the 4He calculation in the Quantum Fluids file perhaps. We will find the requisite combination to be (the Bogoliubov-Valantin transformation) (well, see Appendix for more straightforward solution):



We won’t presume the u’s, υ’s to be the same as before – though they will be. For now we’ll just say that these guys are just arbitrary complex numbers which constitute the most general unitary transformation we can make (so we presume the two column vectors satisfy the normalization requirement |uk|2 + |υk|2 = 1, and also that they’re orthogonal – as can see they are). Accordingly, we’ll observe these guys satisfy the typical (anti) commutation relations. For example,



Let’s invert this and plug it into H, and work out what u and υ actually are.



And so then,



Then we can switch k → -k in the some of the sums…to convert u-k, υ-k → uk, υk…and I’ll also invoke anti-commutation relations to get γγ† in preferred order.



Can combine a few terms – recall these guys anti-commute.



Think this is right. 3rd time is not the charm.



Now we need the γγ and γ†γ† terms to go to zero. One’s the conjugate of the other so need only check the γγ term. In previous file we had that uk, υk and Δk were real. I’ll presume so here too. Then,



And now we are effectively demanding that φk be related to Δk in this fashion. That makes the uk, υk have the properties requisite to make those undesirable cross-terms in H vanish. And this is precisely the equation that these quantities obeyed in the previous file. So we’re good. These expressions will make our constant at the end look like this:



Now we have,



Where in the last line we presume symmetry w/r to k → -k. Let’s work out the prefactor, using results from previous file (well, they follow from φk = (1/2)tan-1(Δk/ξk) a few lines up):



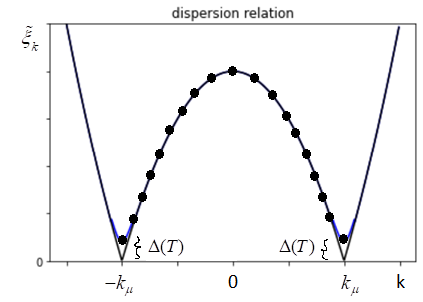
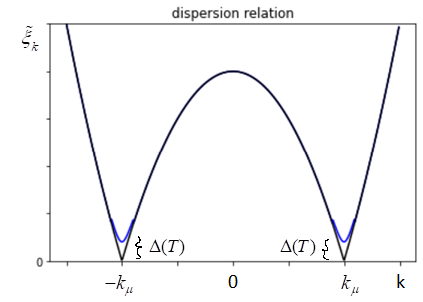
We get:



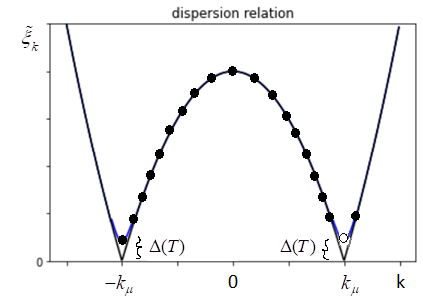
and so (restoring possibility of complex Δ),



This form energy dispersion formula seems a common occurrence. I plotted the spectrum below. The free particle dispersion relation is the black curve…might recall from the free electron folder how the spectrum looked like |ξk| = √(ξk2) for the formulation of Hamiltonian in terms of excitations above the N-particle fermion ground state and energies measured from εF (basically μ). Overlayed on top of this curve, though indistinguishable outside |ξk|>ωD, is the superconducting spectrum. Of course we’ll note the gap that has developed. The blue curve exists in the region |ξk|-ωD of course. Outside this region, Δk = 0, and so the two dispersion curves are identical.



On the right, I’m borrowing from the Free Electron dispersion curve (when measuring excitations w/r to GS), to the GS by filling in particles up to chemical potential. Not sure how kosher this is, since the particles don’t really have well defined single particle states probably. Also, in the prior file where we calculated the GS wavefunction we saw that within the |ξk| < ωD region there were some particles that were occupying states with k > kF, and compensatory dearth of particles occupying states with k < kF. So again not sure that our picture of filling in k-states up to kF only, and treating these as particles, is warranted. But…if we can, then we see that excitations are created by adding holes to the region |k| < kμ, and particles to the region |k|>k­μ. A particle-hole excitation is illustrated below:

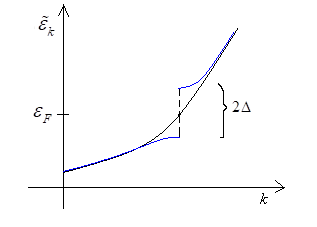


and we can see that the minimum energy cost of such an excitation is 2Δ. Since adding a hole costs at least Δ (maybe check out that Free Electrons/particle-hole file again), and adding a particle also costs at least the same (more than Δ in my picture above).

What k represent is perhaps a *little* ambiguous. It’s definitely the excitations of K above the GS, but it could be a 0, 1, 2, 3, etc., particle excitation, because γkσ† does not create a definite particle number. And if k is the change in energy that we get from adding a single particle vs. two particles, or more, to the GS then that makes a conceptual difference. By comparison with the non-interacting spectrum, we can at least surmise that in the large |k| >> kF limit, γk† becomes particle like, and in the |k| << kF limit, γk becomes correspondingly hole-like. And so in these limits we may interpret the k as single particle excitation energies (measured from chemical potential). And so we could say:



which looks like this:



Since we have the excitations, we can construct the eigenstates as well. The ground state, and excited states, would be given by:



Vis a vis the first equation, will get the same old |ψGS> we got in the previous file (at least at T = 0 – because T is bound up in our definition of Δκ and hence uk, υk, as we see below). But won’t pursue it. It is clear, by the way, that these states are superpositions of states with different particle numbers. Remember that the second line is an Nth order excitation, but it would constitute a superposition of particle numbers still.

But these states are orthogonal to each other, moreover, as can be proved from the anti-commutation relations. Also, it follows from the anti-commutation relations of γkσ that the thermal average occupation number of the kσ excitation would be nF(kσ), where nF(x) = 1/(eβx + 1) – note no ‘extra’ μ here. Just check out the statistical mechanics file for reassurance – there is no requirement to consider the γ’s as particles per se´.

**Working out the Δ equation**

Now we’re not quite done, as we do not know what Δk is. We have:



And we can solve for gk self-consistently, via:



So here we’re commiting to a thermal average calculation for gk = <c-k↓ck↑>. So I guess this means we’re getting a sort of thermal averaged set of excitations. We can cross out those expectations because states with different numbers of excitations are orthogonal. Plugging this into the Δ equation we have:



We’ll observe that when T = 0, we get nF(x) = 0, and so this reduces to:



which is the gap equation we worked out in the last file. Now let’s fill in the potential:



We may presume,



and then our equation reduces to:



Now we’ll note,



And we’ll do our usual density of states approximation on the integral. Then we have:



Goal would be to solve this for Δ(T). Could simplify somewhat,



We’ll observe that at the lower end of the integration limit, the argument of tanh is βΔ/2. And at the upper end, it’s βΔ√(1+(ωD/Δ)2)/2 ~ βωD/2 (since ωD >> Δ). If we were to say T >> Δ, ωD, then both limits are small, and a Taylor series approximation to tanh is appropriate. So then we’d have:



which, well, isn’t true ‘cause all of these are given constants. So that tells us there is no solution in the really large T range. On the other hand, if T << Δ, ωD, then the argument of tanh is large and we can approximate by its asymptotic value, 1. And we have:



This is what we found for the ground state in the previous file. So there is some critical temperature Tc, above which we have no solution. We may surmise that Δ starts finite at the T = 0 value above, and then goes to 0 as T increases to Tc, and remains at zero thereafter. What is Tc? Let’s go back to the original equation.



As T → Tc, we have Δ → 0. And so then the upper limit is ∞. In that case, for the overwhelming majority of the integral ξ >> 1. And so we can say,



Then integrate by parts:



For large βcωD/2, it’s appropriate take the limit to ∞. Then,



The value of the integral is apparently -γ + ln(π/4), where γ = 0.577…is Euler’s constant. So now,



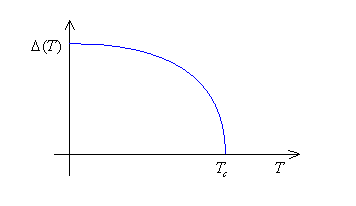
so (setting kB = 1), we get:



The numerical prefactor works out to about 1.13. This isn’t too far away from the most naïve approximation of all, which is to equate kBT with the ‘bound’ state energy of a Cooper pair found from our analysis of the two-body BCS Schrodinger equation.



(factor of 2 in numerator of exponent is due to different definition of Vs(k-k´)). So all in all, Δ(T) graphically looks like this:



Can we get the behavior near T = Tc? Let’s go back to the gap equation:



In the T → Tc limit, Δ is again small. This time we’ll write T = Tc + T – Tc = Tc + δT, and expand our integrand in powers of δTc. And simultaneously, while presume ξ >> 1, we won’t replace ξ2 + 1 with ξ2, but rather expand this in powers of 1/ξ. We’ll keep just the first non zero terms in δT and 1/ξ. First we’ll expand the arguments of tanh and that denominator.



Now use Taylor series on the tanh,



Now keeping just the (four) first order terms in this product,



Next, we can change variables to factor out a bunch of stuff,



Amazingly, the middle term is non-singular, net, at ξ = 0, and so even though our approximation was only valid for ξ > 1, it is safe to integrate even down to 0. OK, now we take the upper limit of the last two integrals to ∞ as ωD is ~ room temperature, and Tc is ~ couple Kelvin, and they will converge. This means we’ll be missing a term ~ (ωD/2Tc)-2 coming from the tanh guy in the middle integral, and terms ~ exp(-2ωD/2Tc) coming from the sech2ξ guys. But that’s okay. So,



Apparently,



where ζ(x) is Riemann function or something I think. So now,



The integral remaining is just 1/λρ(εF), as this was how Tc was defined, basically. So now we have:



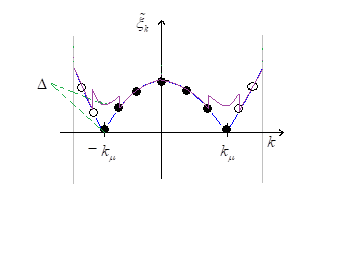
So finally,



So the order parameter, as it turns out to be, goes to 0 as √(ΔT). This is consistent with the previos results from mean field theory.

**Density of States**

Now let’s examine the density of states. I guess this is more like density of excitations above the N-particle ground state (I suppose even the usual free density of states would be density of particle excitations above the vacuum). Anyway, we’re actually going to analyze the density of states near the Fermi surface, or chemical potential, and approximate Δk as simply Δ. Recall the spectrum looks something like:



and so,



Proceeding,



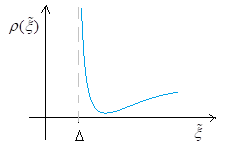
So evidently,



Near → Δ, we have:



where ρ(μ) is the free particle density of states (spinless) at the chemical potential. So we see a singularity at the gap, and certainly, no states below the gap, as expected [ = excitation – μ, roughly].



**Appendix**

Going back to K,



There was a quicker way to diagonalize the interaction. Define:



and then we can write our H as:



Now we need to find the eigenvalues of this matrix:



That was fast. And now eigenvectors:



and so the normalized eigenvector(s) is:



I’m presuming the Bogoliubov-Valantin transformation:



is equivalent to:



I don’t want to work this out. But then filling this into our H, and taking advantage of the orthonormality of our eigenvectors, we’d have:



Now anti-commute the γ’s and change the -k → k in second γ product.



And so we get:



which is the same as we got before. Well maybe the constant term is different? Not sure? Hope it’s the same.