**Excitations**

**BCS Ground State**

Now going to use the model:



where ξk = εk – μ. The calculation before indicates that the electrons can lower their energy by pairing up in Cooper pairs. And so this attraction will change the entire ground state, first few excited states, etc. So now we’d like to work out what the many-body ground state would look like. Normally we’d posit a definite N-particle state, with parameters we could adjust to minimize the energy, H. But that’s not quite what we do here. I guess it’s easier to posit a state which comprises a superposition of different particle numbers – an infinite number in fact. And we’ll try to minimize H subject to the constraint of fixed particle expectation number, N, instead. So using the method of Lagrange multipliers, we’d construct K (μ is the Lagrange multiplier, which may be interpreted as a chemical potential as it does the same thing):



So there is an ambiguity to note. We’re presuming that N is now not fixed per se´. So then how do we locate the Fermi surface, which is crucial to the definition of Vs(q)? Well it seems that we just take the Fermi surface energy to be the same as the Lagrange multiplier. We call them both μ (or sometimes εF too, since we’re at T = 0). I guess this is the most logical choice. Maybe it’s even necessary, as they should be the same when interaction is close to zero. And here is the ansatz:



It turns out that when we do a mean field approximation on the Hamiltonian, we’ll get the same ansatz for the Ground State. But for now we’ll just accept it. The k-product runs over what? I guess over all k’s consistent with periodicity over the volume of the sample. There would be an infinite number of them. |uk|2, |υk|2 can be interpreted as being the probability that there *is not*/*is* occupation of two electrons in the ‘two-body’ state |k↑,-k↓> [take with grain of salt because the *whole* wavefunction must be anti-symmetrized, and so it is somewhat inappropriate to single out a two-body state…]. So with this interpretation we’d naturally have |uk|2 + |υk|2 = 1 (and this is necessary anyway for normalization). This two-body state should not be *unequivocally* interpreted as a Cooper-pair. Far below the Fermi surface, this state would simply be interpreted as usual: two non-interacting particles, one occupying state |k↑> and the other occupying the state |-k↓>. The energies of these particles, together, would be just (2)k2/2m. But further up the Fermi sea, as we approach the Fermi surface, where the phonon-mediated electronic attraction begins to manifest, such a pair of particles would be interpreted as a Cooper pair as their energy would now be something like ε0 ≈ 2εF – 2ωDe-2/λρ(ε\_F). And as we recede from the Fermi surface, leaving the phonon-mediated electronic attraction behind, the pair’s energy would return to (2)k2/2m I think. To be sure the energy spectrum would continuously evolve from one to the other. For example, maybe something like:



So, though the pair wavefunction of the state|k↑,-k↓> doesn’t change as k increases, the *energy* of the pair does. And it’s the energy which determines the identity of the pair.

Other thing of note(d) is that we have an indeterminate number of particles in our wavefunction. If υk were all zero, then we’d have zero particles. If υk were all one, then we’d have ∞ particles. And anything in between is a superposition of 0, 1, 2, …., ∞ particle number states. It is μ, which will implicitly enter into the solution for ψ through uk and υk, and acting like a chemical potential, that predominantly controls the number of particles. The strength of the interaction has a much smaller effect. If λ = 0, then we should just get <> = NF, where NF is the number of particles that would fill up to the Fermi surface up to chemical potential μ. But if λ ≠ 0, and presuming it has the effect of lowering the energy of the particles, then as the interaction strength increases – i.e. becomes more negative –we can fit more particles into the superconductor before getting to the μ cut-off and so <> should increase. But for a given μ and interaction strength λ, the relative fluctuation in particles is super small. One can show that σN = √(<2> – <>2) ~ √<>, and so σN/<> ~ 1/√<>. So we may, for all intents, treat N = <> as constant (meaning it’s probability distribution is something like δ(N – <>), for that given μ and λ. Either way, we can verify that for a *given* particle expectation number, our ansatz, with properly chosen parameters, will have a smaller energy than a free state with the same particle expectation number.

What should we expect for our ψGS? We should expect that when the interaction is eliminated, i.e. λ = 0, we get the normal non-interacting ground state, namely |uk|2 = 0, and |υk|2 = θ(εk < εF), where εk = k2/2m as usual, and |uk|2 = 1, |υk|2 = 0 for all k > kF. And then as we turn on the potential, if the potential were to have *no* effect, then we’d expect no change in uk, υk values. It’s *possible* to presume no change because we know from QM folder that in 3D an attractive potential requires a sufficient strength to modify the energy spectrum. But we *do* expect a change as our two-particle calculation evinced above. What we find is |υk|2 looks like (coincidence?) the T-slightly-greater-than-0 Fermi distribution function. So the k-states near below the Fermi surface are somewhat depleted, and those near above are somewhat filled. Seems odd that this would have the effect of reducing the overall energy because this clearly results in an increase in kinetic energy to pump particles up from lower to higher k-states. But I guess it is compensated for by an increase in (negative) potential energy, because by populating more states within the range μ±ωD we increase the chance for Cooper-pair bonding.

**Normalization**

Anyway, let’s set about finding the values of uk and υk that minimize the energy expectation. First thing to fix is normalization. So we need,



Note all k terms commute within themselves. All k´ terms commute within themselves. And if k ≠ k´, then these terms commute as well, even if k = q and k´ = -q. So we can group together terms where k = k´, and then we’d have:



We can take each k-term and slide it to the beginning and end of the product, because different k terms commute. Let’s slide it to the right end. What is its action on |0>?



Now let’s slide it to the left end. What is its action on <0|?



So repeating for all k terms, we can reduce the equation to:



This is satisfied, if we demand,



Given this constraint, I guess it’s useful to presume real values and parameterize the constants as:



**Particle expectation number**

What’s the expectation of particle number?



We can slide k ≠ ±q, and k´ ≠ ±q terms to the front or back, as we saw above. And so we’ll have:



The result of the last product is 1, as we saw above. Then we’re left with:



When σ = ↑, we can slide the k´ = -q term all the way to left, and the k = -q term all the way to the right. So we can combine them to get 1, ultimately, like was done above. And when σ = ↓, we can slide the k´ = q term to the left and and k = q to the right. So we combine them to also get 1. So we’re left with:



So,



where in the last we just modify the dummy summation index. μ hasn’t entered into <N> yet, but it will, through our solution to υq. Anyway, our formula here is how we come to the conclusion that |υq|2 is the occupation probability for the pair state |q↑,-q↓>. We could calculate σN. Apparently we find, eventually:



When no interaction is present, and we get (as we’ll see) |υk|2 = θ(εk < μ), this would be 0. The sum would be non-zero only in the depleted region, where |υk| is between 0 and 1. It is certainly no more than N. And so σN ~ √N at best. The relative fluction σN/N ~ 1/√N and so is negligible in the thermodynamic limit.

**K Expectation**

Now let’s consider H. We want to minimize subject to overall particle conservation. So using the method of Lagrange multipliers, we’d construct K:



and we’d take the expectation…I’ll do KE first. That’s pretty easy considering what we just went through. We’ll find:



and then PE. For simplicity, in the kk´ sum, we’ll elide the k = k´ case, as it ought to be negligible in the thermodynamic limit.



I guess this expression will require k, k´ to be equal to ±q or ±q´. The rest of terms all commute and give us 1 ultimately when the k = k´ terms are paired up and operated against both |0> and <0| (as can do because they commute with everything. So now we have:



Now I’ll consider the terms in right and left products that can slide past the potential term. So k´ = ±q,-q´ can go past to the left. And k = ±q´,-q can go past to the right. The k´ = k = -q, and k´ = k = -q´ terms can then go all the way left and all the way right to ultimately give us 1. Then we’re left with:



Cool. So now we have:



**Minimizing K expectation**

Now we want to minimize this guy by plugging in uq = cos(φq), vq = sin(φq) and differentiating w/r to φq. So,



Differentiating w/r to φk we have:



Last line because V is even function in r, and so Fourier transform should be even too. Then, presuming φk ≠ π/4, etc.,



Now let’s define:



then,



and therefore,



So our equation now reads:



We can do away with the restriction on the sum I think. Let’s fill in the potential,



And this can be solved, most simply, by the ansatz,



Filling this in, things will decouple (and I’ll start renaming μ as εF it seems):



Solving for Δ,



and approximately,



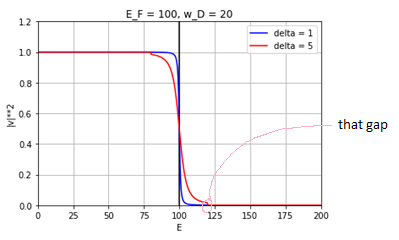
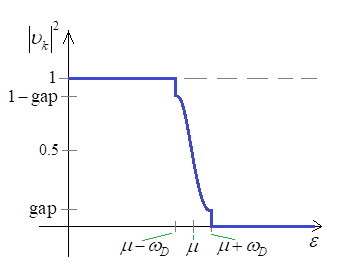
So then, we have:



It’s just a constant value, within the region where the potential is non-zero. It ranges from 0 (when λ = 0) to 2ωD (when λ = ∞). The different factor of two in the exponent has to do with our slightly different specification of the interaction potential. Then it follows:



We can see |uk|2 and |υk|2 do add up to 1. Here’s a typical, and general, plot of |υk|2 (μ = εF):

Can see also that if Δ = 0, then |υk|2 = θ(εk < εF). Will note that either way, |υk|2 = 1 for ε < εF – ωD, and |υk|2 = 0 for ε > εF + ωD, as Δε is zero in both those ranges. And likewise |uk|2 = 0, 1 in those same ranges. So for a fixed εF, increasing λ just increases the Δ gap at εF – ωD and εF + ωD. And the |υk|2 coefficient just sort of smoothly connects the gap, going from 1-Δ at εF – ωD through ½ at εF down to 0 + Δ at εF + ωD. And |uk|2 does the opposite, going from 0 + Δ at εF – ωD through ½ at εF on up to 1-Δ at εF + ωD. That gap is given by:



So the energy is lowered, evidently, by pumping electrons below the Fermi surface to the region above it, and forming Cooper pairs between the electrons below and above. The pairs have a negative potential energy, as we saw above, which will evidentally lower the energy overall.

Might note that though |υk|2 is symmetric about εF basically, higher Δ (delta) equates to higher N, because density of states is greater for greater ε, so the decrease in occupation for ε < εF is consequently overcompensated for by increase in population for ε > εF. So as we argued above, turning on the interaction will increase the number of particles. Would like to see if the energy is lowered as we increase Δ, for constant N expectation. So let’s calculate <N>.

**Expectation of N**

So let’s calculate the expectation of N. And we’ll use it to implicitly calculate εF as a function of <N>.



where ρ(ε) does not include spin. Will note that if Δ = 0, then we get:



which is indeed the relationship we’d expect between N and εF in the free particle case. What about for non-zero Δ? Then we must break it up into intervals,



In the first integral, Δε = 0 and so [ ] = 2. In the last integral, Δε = 0 again, and so [ ] = 0. So then we have:



Let’s subtract off the Δ = 0 result, which is,



so that we calculate just the change in particle number. Then,



The [ ] is an odd function. We *would* get a positive # for <δN> if we exactly carried out the integral, since ρ(ε) is larger in the (εF, εF + ωD) range than it is in the (εF – ωD, εF) range. I guess to first order we could say, recognizing Δε to be constant within the integration range:



And then,



Don’t really want to work out that integral exactly. A decent approximation is to say:



Let’s use, again,



Plugging this in,



Adding in the Δ = 0 result we subtracted off before, we now have:



As expected, increasing Δ beyond 0 does increase the number of particles. But very slightly. Now I think Δ ~ 0.1eV or lower, while εF ~ 104eV. So (Δ/εF)2 is something like 10-11. Easy to see why the ubiquitous approximation is to just approximate ρ(ε) as constant over the interval (εF – ωD, εF + ωD), which implies <δN> = 0. OK, let’s try to get εF in terms of <N>, to first order. So we’ll expand εF = εF(0) + Δ2εF(1) + … in implicit power series in Δ2. And then expand the RHS to leading order in Δ2.



Then equating order by order,



So,



**Expectation of Energy**

Let’s now calculate the energy expectation. So we have (where μ = εF):



and n = <N>/V. So now let’s get <K>.



Now we’ll convert to integrals, explicitly splitting up the intervals (0, εF – ωD), (εF – ωD, ε­F + ωD), and (εF + ωD, ∞). So then we’ll have:



The ( ) in the red guy is 2, as before. And the ( ) in the blue guy is 0, as before. The black guy is just the same integral squared too. So then we have, changing variables as well:



Let’s isolate the Δ = 0 part.



Would be nice to write this in terms of εF(0). So,



And it’d be nice to expand this out to order Δ2, so:



And now we’re left with the other part:



Since we only need to go to first order here, we’ll make the typical aforementioned approximation that ρ(ε) is roughly ρ(εF) within the interval, and recognize that Δε is just a constant Δ in the interval too.



I’ll do like before, and presume ωD >> Δ, which is justified as ωD ~ 100eV or something. Actually, we can’t do that, because we get delicate cancelations that occur at sub-leading orders. So…



Proceeding,



Now we also have:



Filling that in, we get:



Can expand for small Δ/ωD…



Now want to put this in terms of εF(0). So,



And then expanding out to first order in Δ2, this would be, since we already have a Δ2 in there,



So for <K> we now have:



And altogether for E we have (μ = εF):



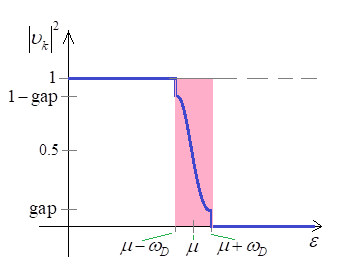
So we have:



So we see clearly the typical free fermion GS energy in the first term, and the correction due to the interaction in the second term. <E> is unambiguously smaller with the interaction turned on, so it would indeed seem that the GS *will* consist of some Cooper pairs. Since each Cooper pair has a potential energy of approximately Δ, this would seem to indicate that the number of particles forming Cooper pairs is on the order of:



This ratio Δ/εF0 makes sense as the number of particles in the pink area would be something like N(2ωD/εF0) ~ N(Δ/εF0). So we can intuitively say that it is these particles within that energy region of width 2ωD about the Fermi energy that are forming the Cooper pairs.



**Some more expectations**

With a mind toward what follows, let’s define:



gk\* is just the guy in the wavefunction ansatz above:



When λ = 0, we should find them to be zero because then |υk|2 = θ(k<kF) and so |ψ>GS would be a state of *definite* particle number, NF. For non-zero λ, we should expect a non-zero value for the g’s, and moreover a value which increases with λ, as then the occupation number |υk|2 increasingly deviates from 1 or 0, and so the ground state wavefunction increasingly becomes a state with non-definite particle number (but with expectation still pretty close to NF as we saw above), and so there is an increasing likelihood ψGS comprising a superposition state of say N-2 and N (vis a vis gk), or N+2 and N (vis a vis gk†) particles. As such, g should function as a sort of order parameter (0 in the normal state, and non-zero in the super-conducting state) Okay, so:



We can slide k ≠ ±q, and k´ ≠ ±q terms to the front or back, as we saw above. And so we’ll have:



The result of the last product is 1, as we saw above. Then we’re left with:



We can slide all the k terms right past ( ). And when k´ = -q, we can slide it left past ( ). So we can combine the k = k´ = -q terms and slide them to <0| and to |0> to get 1. Then we have:



So we have:



We can fill in our results for these guys,



So we do get 0 when λ = 0 at least. Might observe that since:



we have:



which will be useful to know in a bit.

**Reformulation of BCS theory in terms of constant particle number ψ**

Doesn’t seem as much of a necessity as it did a while ago, but we can circumvent the non-particle number conserving feature of our wavefunction. So note that H is invariant under the transformation ckσ → e-iθckσ. And this is related to particle conservation (see QFT folder maybe). But our wavefunction does not possess this symmetry, as it would go to:



This would mean that different values of θ give us different ground states (but with same energy because of the aforementioned H invariance). So I think that instead of having a wavefunction where number of particles, N, is arbitrary but fixed, we have a wavefunction where θ is arbitrary but fixed. These two d.o.f. are sort of complementary, and we can sort of think of θ as akin to the chemical potential. We could construct a superposition of these |ψ(θ)> that gives us a fairly definite number of particles via:



And so can see that this would pick out the term in |ψ(θ)> which has N/2 of the c†k↑c-k↓ operators (cause this term would have phase (e2iθ)N/2 = eNiθ and would therefore cancel the phase in the integrand – all other terms in |ψ(θ)> would ‘wash out’). Conversely we can say,



where,



It so happens that aN(θ) is highly peaked about a particular N for a particular θ, and in fact stdev(N)/N → 0. Therefore in the thermodynamic limit, the N’s and θ’s are in 1-1 correspondance, and we may work with wavefunctions that are defined in terms of either. But so happens that working with θ wavefunctions is easier, analytically.