Electronic Theory of Solids
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Lecture – 54
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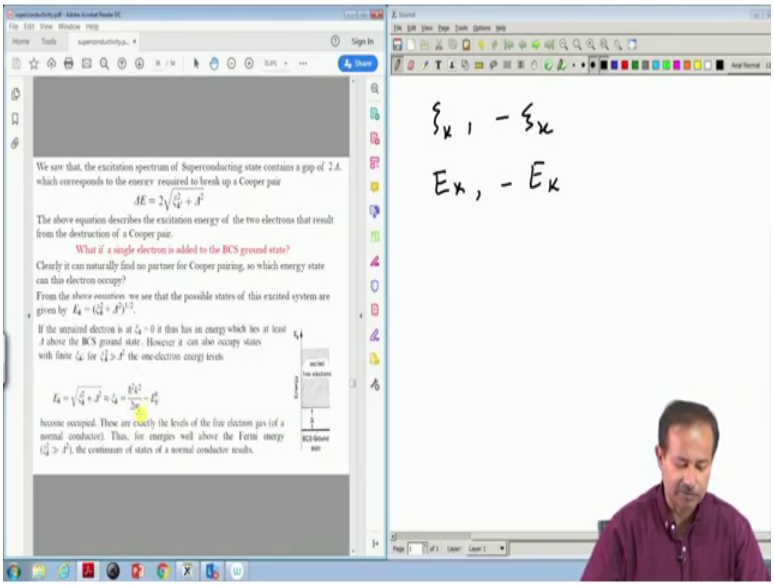

Welcome back. We have been discussing Superconductivity, in particular BCS theory of superconductivity and we found out that there is an excitation spectrum with energy E of k and this is that E of k that we discussed where we found that it is it has a gap in the spectrum. So, what is this E of k; whose spectrum is it, I mean that is a question one can ask. First of all, these are fermionic excitations, single particle excitations.

Secondly, these are actually is very strange mix of both an electron and a hole. These are very special about superconducting ground state that the excitations above it are have a character of both it is mixture of both hole and electron. So, it has a character of both hole and electron and that is interesting because you have now a mixed particle in the sense that you have mixed holes and electrons to form a new ground, new excitation spectrum and the excitation is gapped and the gap is delta. The gap is actually two delta spectrum has a gap of delta above 0.

So,. So, this is what this excitation is all about. So, this is like for example, if you had a normal metal like a degenerate Fermi sea, then to add an electron you have to give this energy right; E of k. To add a hole you have to give energy minus k. Here similarly, you have to add you want to add a quasi particle; these new excitations, they are called quasi particles, these particles which are a mix of holes and electrons.

If you want to add, then you have to give this energy; if you want to add at the corresponding to this, then you have to give an energy minus E k. So, the spectrum for example, if you look at the spectrum, then for example, if E k is far greater than delta k delta, then it will go back to our original spectrum; right h cross k square by twice m minus E F naught which is a c of k.

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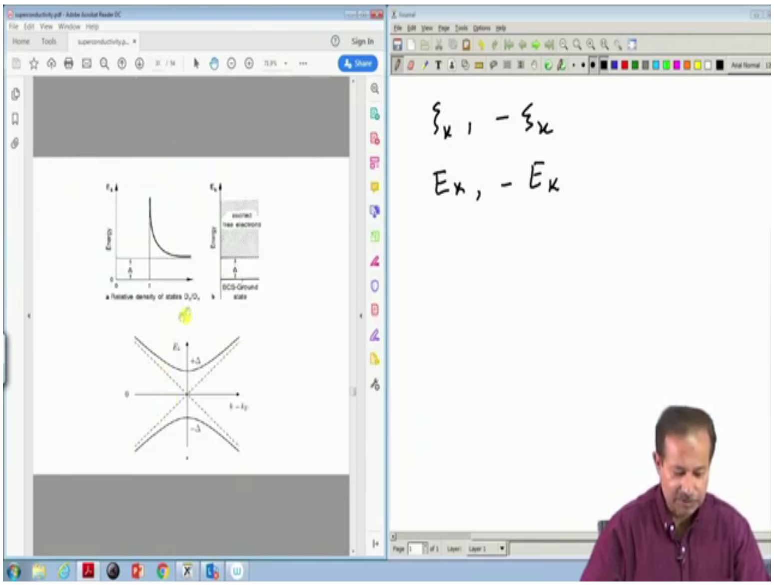

The interesting thing is when it is close to the delta is much larger and delta and epsilon k is small delta compared to delta, in that case you can see that the spectrum is like this. The dashed one is the original fermionic spectrum which is the free the metallic conduction band spectrum of the degenerate fermi gas; whereas, these solid lines tell you that the new spectrum of the excitations E of k has a gap.

The minimum is the this 2 delta right and as a k becomes larger and larger, epsilon k becomes large compared to delta; then, you asymptotically again go back to the original gap, original spectrum. Now, the this is like because what happened is that the particle and hole states hybridized and they form this new excitation so that this original dash spectrum has now changed to this kind of a spectrum, the solid line. Now, one can actually calculate the density of states of this new excitations. This new these quasi particles over the BCS ground state and that is very simple.

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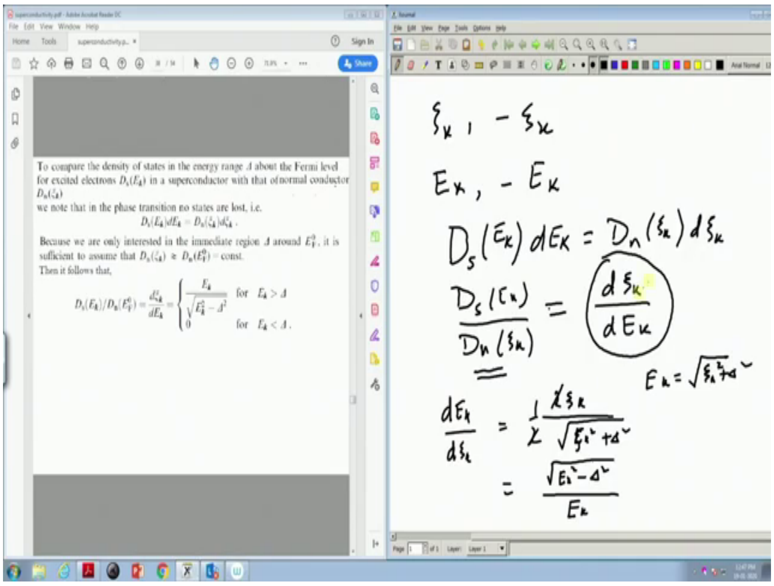

What you do is that you use the fact that you do not lose any of the density of states. So, the Ds the if I write in terms of D s of E of k is the density of states between E and E plus D k D d E, then the number of states must remain the same as the original density of states.

So, number the density of states is not eaten up; but they can pile up and that is what we will see immediately that D s E k by D D n E k. This is the same as the g that we were writing for free electrons. So, D n of E of epsilon c of k is D c k D E k and this is easily calculated and the two things are done here. One replaces this by it is fermi level value because that is for all practical purposes, in three-dimensions in particular this is more or less constant at the end in two-dimension of course the density of states is a constant.

And so, the you can replace the this by it is fermi level value that without any loss of generality. So, all you need to calculate is this one ok and so, let us just find out what it is. So, D E k E k D c k is half c k by twice c k by root over E k square c k square plus delta square right because E k is root over c k square plus delta square.

Now, what you do is that this 2 cancels and c k you write in terms of E k. So, it has to be entirely written in terms of E k. So, this is a E k square minus delta square divided by E of k.

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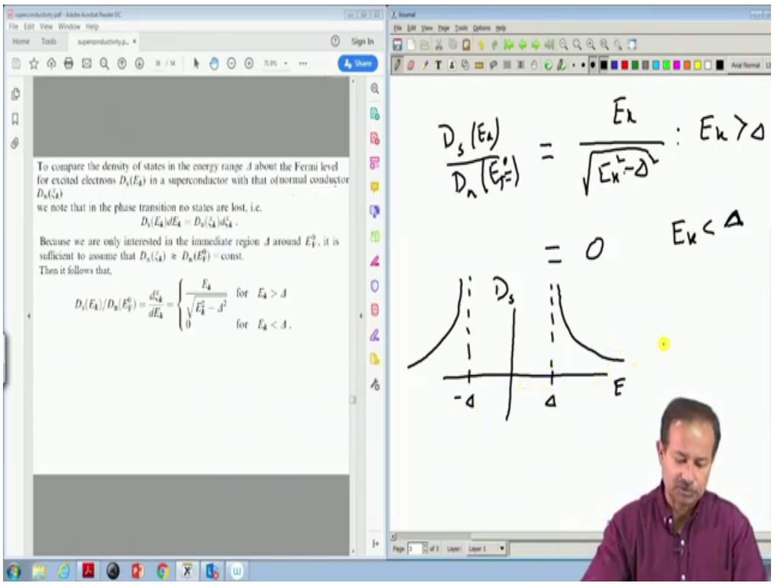

And so that means, the density of states is just the just the inverse of that and that is D of s E k by D n at the fermi level which is what you do is equal to E k by root over E k square minus delta square ok. Now, for example, you can easily see that this is ill-defined. It is it has to imply that E k has to be greater than equal to delta, greater than delta and it has to be 0 for E k less than equal to delta.

So, there at delta it is the it diverges. So, this delta. So, that is the result that you have from the density of states. How does it look like? Well, it looks; you can immediately see how it looks like, it has a huge pile up at minus delta and plus delta and that means, the density of states is like this. D s versus E and that is the density of states. You have not lost any states of course, that is how we calculated it. But what you have is that you do not you of course, do not have any density of states here which you had originally right. You had originally density of states here; whereas, now the in the gap there are no states.

So, those states have all been pushed up or down and you have this huge pile up of density of states at close to delta. At large distances of course, it again goes back to the original density of states large energies ok.

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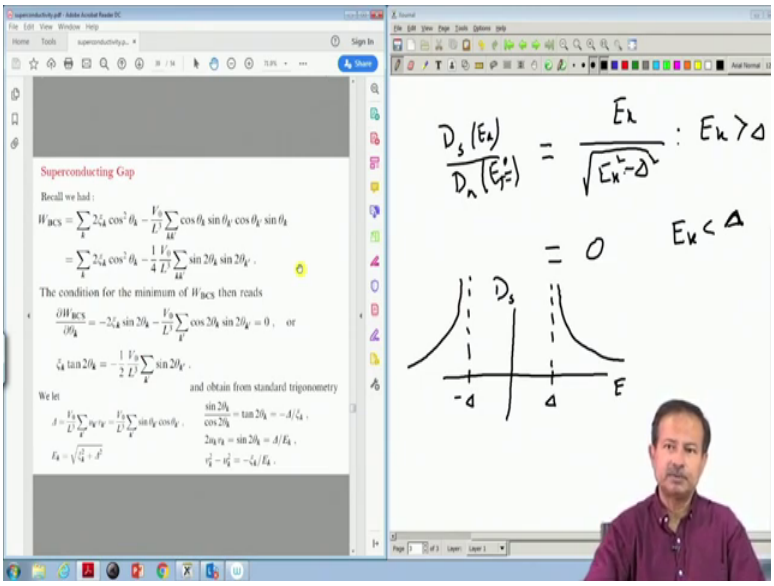

So, this is this such pileup of density of states has fundamental consequences in the superconductivity and these are these have been found out and these are extremely important as far as superconducting ground state is concerned and particularly, their physical properties. So, let us now go to calculate something which is we had to calculate and we decide we wanted to calculate right from the beginning which is the gap.

Now, that we found that the excitation spectrum has a gap, we need to find it. So, let us just go back to our original calculations. Remember this equation, this is all that you require. These equations were obtained originally.

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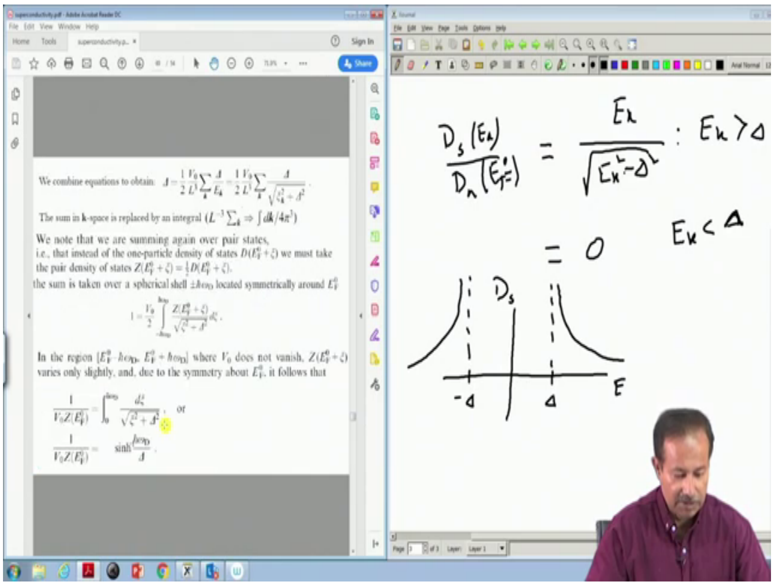

And from that, we showed that this is the equation for the gap. So, basically you see that delta will get cancelled from the numerator in on the both sides; but then delta remains in the denominator. So, this is like you have to invert this equation to get the delta. So, how does one do it? So, this is how one does it. So, convert this case sum to a to an integral as we have done so long and then, to a density of states integral and then, replace the density of states by s, by it is fermi surface fermi level value which is a trick we have been doing all the time.

If a function is if. So, remember if a function is only if a quantity is a function; the integrand is a function or the one you are summing is a function only of epsilon k, the non interacting energies. Then, you can convert it into a integral involving the density of states. This we have done in the past and I am sure you know how to do it. So, that is what we are doing. So, this c of k, see there is no explicit k dependence except through c of k. So, you can convert it into a first to an integral and that integral to a integral over the energy.

So, life becomes much simpler because this is a three-dimensional integral over k. Now, this is an energy integral and this is what we did all through ok. So, now look at where delta appears? Delta appears in this denominator right in the this integrand and so, you have to do the integral and then invert this to get the value of delta and that is exactly what is done. This integral again remember that V 0 being active only in a narrow energy range above the fermi level, then you can only integrate from 0 to h cross omega Debye.

Below fermi level, all states are blocked. So, so what you do is you just do this integral and this is the result. So, remember this is a ground state calculation. So, we are doing this calculation at 0 temperature. These are were obtained at 0 temperature ground for the for the ground state ok. So, here is the result and now sin inverse sin hyperbolic inverse, h plus omega D by delta is this quantity.

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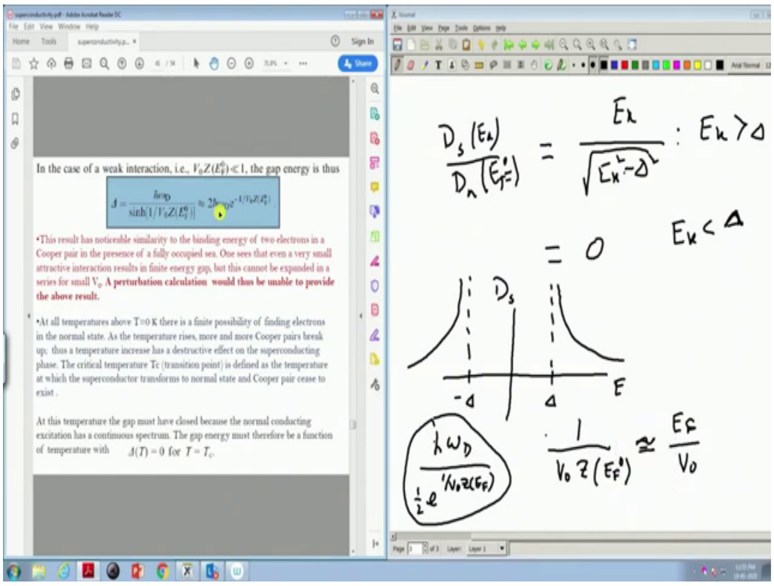

So, I just go one more step. Write the delta equal to h cross omega D by sin hyperbolic of this quantity. Now again, this quantity 1 by V 0 density of states which is written here as Z, we can write it as the original g also, it does not matter.

So, this is basically the density of states and as I said many times, Z or g or density of states in the in the in the normal state can be written as 1 over E F. I mean it is more or less, the ballpark figure is correct; I mean that is the typical scale of the density of states at the fermi level and so, this becomes of the order of this. And now you see this is very large. So, and sin hyperbolic has E to the power x plus E to the power minus E to the power minus x and so, out of which we just pick, take the one which is larger and that means, sin x E to the power plus x because this is very large; the argument inside is very large.

So, in the denominator, then you have h cross omega D divided by E to the power 1 by V 0 Z E F and that when you convert you will get this. So, this is half and the 2 goes at the top. So, that is the result that is given here. Now, if you look at this result; this result is very similar to the one, we obtained for cooper problem.

So, this is a verification or sort of a justification of cooper problem even in the many body situation. Remember cooper problem was for only two particles that they were blocked by the fermi sea or fermi surface was very important in that calculation and that same argument, now leads to a many body ground state and similar argument.

I should not say same, but it is similar argument, where the many body ground state is was written down and in that many body ground state, we find that there is a this is a gap which is this and this gap actually corresponds to breaking a cooper pair and that is exactly what we got I mean here as we did in the cooper problem.

So, the physics more or less survives, but the physics is very different in the sense that this is a many body situation that was just a two particle problem. So, that different distinction you should make. There is a another important thing that you should notice here is that this kind of a state for example, this kind of energy if you look at it is not perturbative in V 0. V 0 being small one could be tempted to do a perturbation theory, but look at this expression, it has all orders. If I expand it, it will have all orders in 1 by V 0 and V 0 being small, 1 by V 0 is large.

So, you should not be able to actually V 0 going to 0 limit is ill-defined in that expansion. So, if you I mean take any order of expansion, it will not work. So, a perturbation calculation would thus be unable to provide this result. So, that is one important issue you should remember and that is actually one of the reasons many of the perturbative calculations had failed to account for this theory, the correct theory for the superconductors ok.

Now, the question is we have to find out what happens above T equal to 0. So, above T equal to 0 there will be some electrons in the in the normal state and also some cooper pairs will start breaking up and so, as temperature increases, the phase the remember this cooper this wave function that BCS wrote down as I said has a fixed phase throughout the entire system, it has a fixed phase. So, and that now starts breaking up and that is a strong phase fluctuation starts and so, the superconducting phase bricks up at some places.

So, it fluctuates and then, cooper pairs are breaking up therefore, and you get this excitations normal electrons and so on and what will happen is that if you keep on raising the temperature, at some point this effect will just kill the superconductivity and that is what T c is. The value at which superconductivity disappears. What does that mean in terms of this theory? It means delta, the gap will become 0 in at that temperature.

So,. So, delta will become a function of temperature, has to become and delta is has to has to be such a function of temperature that it disappears become 0 at T equal to T c.

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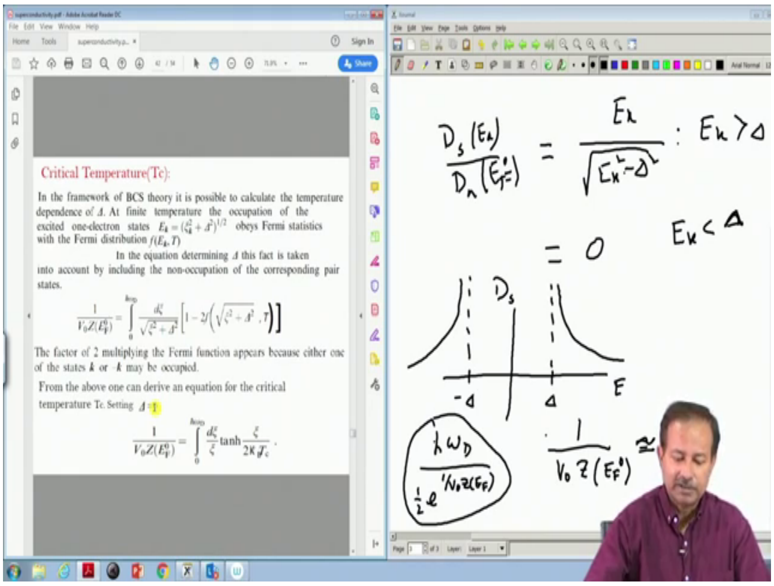

And so, let us find that out and to find that out, what you do is that in that equation for delta, all you do is the add the probability of non occupation of the paired states. So, that is why the factor two comes 1 minus suppose you do not you want to find out the probability of an of the absence of an electron at a particular energy E at a state epsilon k or c of k, then or any energy E of E. then, there will be 1 minus f of E; 1 minus the fermi function of E. Here, it will be 1 minus twice f the fermi function of this energy E of k.

And so, that is what you have to multiply this quantity right. The only extra piece at finite temperature is this 1 minus 2f of E E at a temperature T that is all. So, temperature enters in this integrand through this integral through the fermi function and that one has to remember. Now, this part this 1 minus 2f E can be written down as a tan hyperbolic quantity and then again, you do the integral. Remember, we are looking now for T c. Now, at T c as I said delta has to go to 0 that is how T c is defined, where the gap vanishes.

So, in this equation two things you have done here; one is set delta equal to 0 and the other thing is written this thing 1 minus 2f whatever in terms of a tan hyperbolic which is just a simple algebra you can check. Well, that integral is doable.

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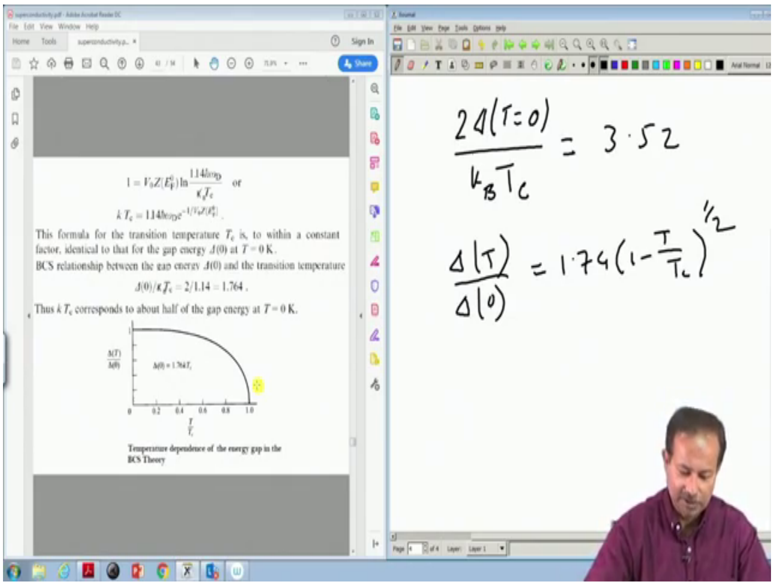

And again, the integral goes from 0 to h cross omega D and if the result is known, it is this. This is the result is and therefore, the this is the temperature, where delta was 0 remember. So, this is written as k B T c now and that k B T c turns out to be 1.14 h cross omega D by E to the power minus again that factor; 1 by V 0 Z E f ok.

So that means, that. So, the expression the exponential factor remains identical except that there are numerical factors that change from delta 0. Remember the delta 0 calculation, we did delta at 0 temperature had had 2 h cross omega D and the exponential factor remained the same.

So, usually one writes this in terms of a famous quantity which is 2 delta 0 by k B T; 2 delta T equal to 0 by k B T c and that turns out to be this 1.746 into 2 to about 3.52 and that quantity is a something that experimentally verified and that was a that was one of the successes of BCS theory that immediately they predicted this value of three point close to 3.5 2 delta 0 by k B T c.

Historically, these 2 delta being the gap that is why 2 delta by k B T c was the measurement done experimentally and that turned out to be 3.52 and this exactly is reproduced by this theory. And you can also find out the how delta move goes as a function of T c from this if you just do this integral keeping the delta and you can you could do it and you will find out that this will be a function of T minus T c as. So, it is given. So, this will be a function of 1 minus T minus 1.

So, delta T by delta 0, if you do this integral in the previous page, you will find this relation from here, from here ok. If you if you can do this integral and invert it, then you can find delta as a function of T and that relation is what I am writing now is 1.74 into 1 minus T by T c to the power half. So, this is the temperature dependence of the energy gap in the BCS theory. So, it is a calculation that can be experimentally now checked and that was checked of course.

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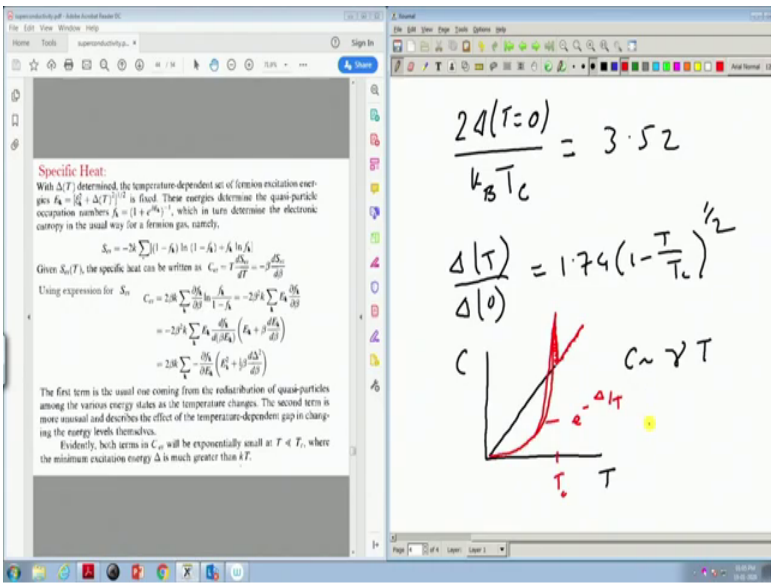

So, one can now go ahead and calculate several physical quantities. These quantities like specific heat for example, for a normal state we remember you know that for a normal metal degenerate fermi gas; the specific heat versus temperature is a linear curve c goes as gamma T ok. Now, what will happen here? Now, you also know that D is a what does specific heat tell us? Specific heat is a measure of the entropy right; c by T integral over D T integral over T is a measure of the entropy.

So,; that means, we should be able to find out from the entropy as to what this specific heat is and we can even guess it. What will happen? Till T c it will be like just the it will follow the normal state because at T c; so, suppose this is T c, so at T c till T c it is a normal state normal metal and then, of course, below the T c, there is a gap opening in the spectrum. So, there will be an exponential decay of excitations.

So that means, it will get depressed below the usual value; somewhere it has to come down below the usual value and then, but you cannot lose your entropy. So, entropy has to come up and peak somewhere here; whatever you lost here, should be gained somewhere here. So, so this should be the nature of the entropy curve and this should be exponentially down. So, it will be minus delta by T or some such thing. I mean that is a guess one can immediately make.

So, let us see what happens. So, this is the calculation that is a standard calculation for any fermionic, see the entropy comes from the excitation. So, so. So, you have to excite. When you supply thermal energy, you have to excite and so, the specific the entropy has to come from this and the standard formula for a fermionic system for the entropy is this 2 k sum over k 1 minus f k log 1 minus f k plus f k log f k ok.

This is a standard in statistical mechanics, you have done it. If you have not, just check any book in stat-mech, you will find this formula; how it is derived is also, it is a straightforward derivation. These are basically non interacting fermions and they are their entropy is this; I mean this; there is no other choice. Actually, we will see that this is the only way you can you can write it off straight away. So, then what you do is that you calculate T d S d T ok. So, that is since s since the we prefer to do it in terms of beta which is 1 by k B T fine.

So, one calculates this. So, this is the basically this is this algebra can be easily done, you can do it and this has two pieces which is in important. This has this piece first piece and then, there is a second piece. The first piece actually this E k square term into minus del f del E k gives you the.

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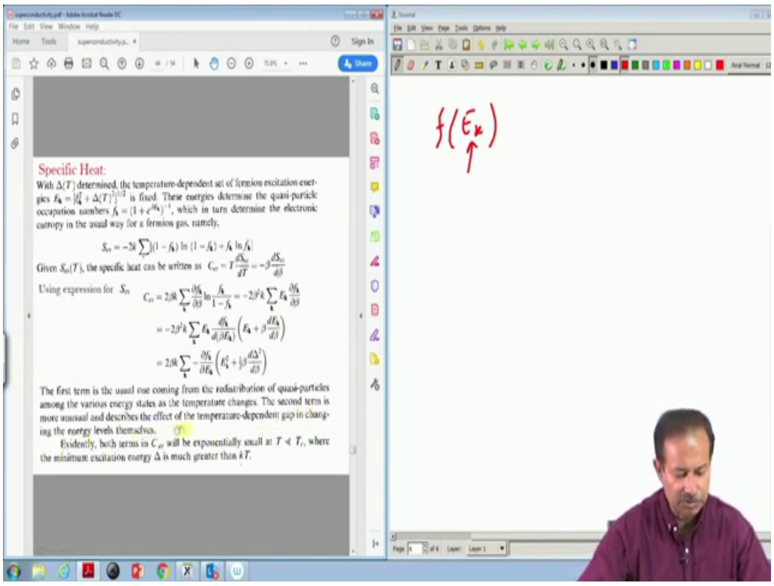

Remember that f of k f has a f is a is E of k. So, that is what you are using here the because that is the excitation spectrum for the for the superconductor, for BCS superconductor. So, you take this derivative we will get up to here it is straightforward to get here. Now, the in the last line this term, the first term gives you the original entropy, if you do not have a gap. If your gap was 0 that means, beyond T c this term, first term will recover your original entropy of the normal metal, normal state.

So, second term is the unusual term and it describes the effect of temperature dependent gap. So, as I said the gap had a temperature dependence. So, the second term will reflect this temperature dependence of this gap; 1.74 1 minus T by T c to the power half.

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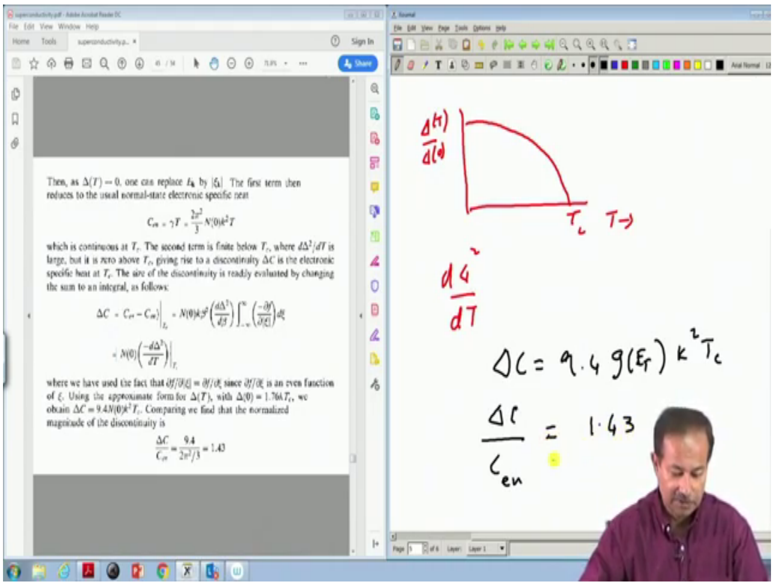

So,. So, that gap structure that we wrote down is now coming to play a role in this. So, delta versus T; remember delta T by delta 0 had the structure T by T right. At T c, it goes to 0 and this is the one that is now going to contribute to the second term. So, you can go ahead as delta T goes to 0 which is close to T c. As I said, you can replace E k by the original electronic spectrum, normal state spectrum and you will get this c e n which is the normal electronic state as gamma T which is 2 pi by square 2 pi square by 3, the original density of states of the original fermi 1 at the fermi level times k square T.

So, this was a result we already calculated long back. That is what is reproduced here also, fine. The interesting thing is the second term second term is finite below T c and is 0 above T c, so this will give a discontinuity at T c right. So, that is the discontinuity one can calculate and that is one thing that is done here. So, this calculation is very straightforward. d f d mod E at T c, they are calculating into at T c. So, delta was set to 0 and then, you get this formula and of course, the d delta square by d beta is there; I mean that temperature dependence is already there.

So, you can do this. This of course, we know how to use this derivative of a Fermi function is a Fermi function is an even function. So, you can just calculate this thing and this is peaked only around the Fermi level and then, it just gives you n at Fermi level the density of states at

Fermi level and that is exactly what we did in many other cases; this use this as a delta function and.

So, all you have to do is now basically calculate this from here you have to calculate d delta square by d T and that calculation is said simple and that is what gives this delta c equal to 9.4. See in our original notation it is g of E F; here it they call it n of 0 k square T c and this then is delta c by c e n, you can take the ratio is 1.43 and this can be checked and this is what is checked experimentally.

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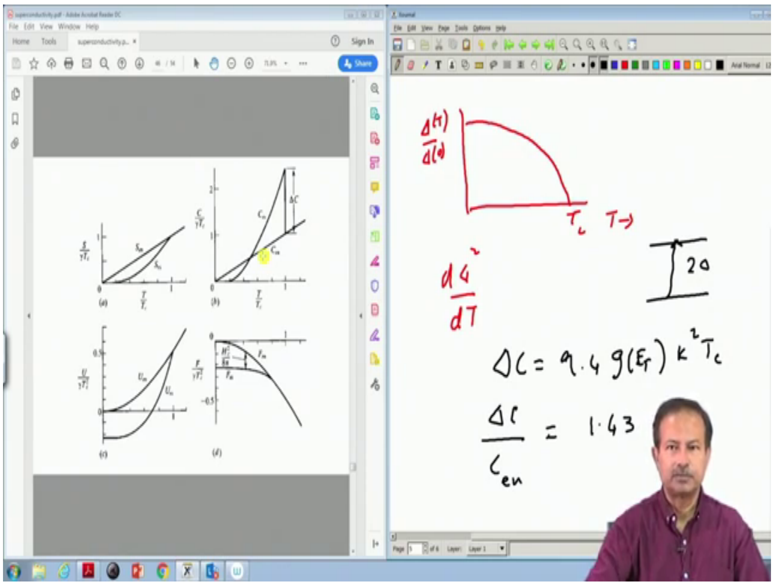

So, let me show you the experimental result. Llook at the entropy as I said, entropy has to drop below the these free electron entropy and specific heat of course, has this jump here. So, whatever you lose here, you have to gain here and that is what is I mean if you lose it you have to gain it somewhere, the entropy cannot be cannot just vanish and. So, this is the. So, ok. So, the way it I one sees it that this part the part below the below the normal intra normal specific heat comes from the fact that there is a gap.

So, that gap reflects in this entropy going exponentially up at low temperatures and then, it cuts it goes above the normal state at finite at some temperature and then, you basically has have a jump at this point in the entropy. So, the entropy of course, has to go to 0 at 0 temperature. So, that happens in both cases. So, that is not a problem. Specific heat has this exponential behavior below the below this as I said the below because there is a gap, it has this. So, it comes down below the normal state as a function of temperature and that had to happen because there is a gap in the spectrum ok.

So,. the idea is that you since you have a gap, you have to excite the quasiparticles across the gap and that has a temperature dependence and that gives rise to this coming down of the specific heat as a function of temperature. So, in the next class, what we will do is we will discuss electron tunneling and that is for the next class and that is another experiment that one does to find out the verification for a superconducting theory of superconductivity, BCS theory of superconductivity.