Electronic Theory of Solids
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Lecture – 53
BCS Theory, Excitation Spectrum

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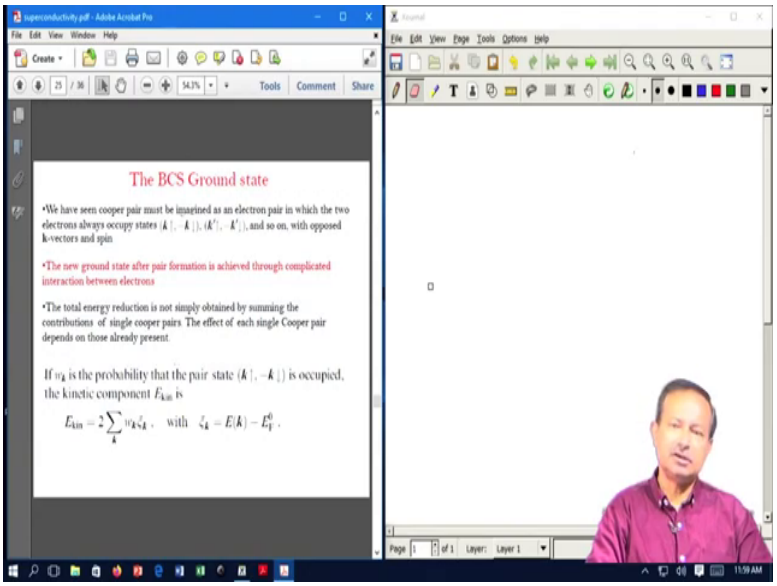

Hello, we have been start working on BCS Theory, which we motivated from a first from a physical point of view and second from the famous calculation of Leon Cooper; where, he showed that a 2 electrons placed at the top of the Fermi level, just above the Fermi level and allowed to interact by a weak attractive interaction.

No matter how weak that interaction is that will form a bound state and that bound state has a negative energy of course, and that problem was solved we showed how to solve that problem. And the results are really remarkable that in such cases you will have 2 electrons forming a bound state and these bound states are in having a negative energy as all bound states too, negative energy bound state.

So, that led to the idea that the Fermi surface therefore, becomes unstable of against such pair formation and these pairs are called Cooper pairs. Nowadays, they are charged 2 E pairs and they conduct electricity because they have a charge. So, the actually that is a and as an aside

is that superfluid is a very similar state, but the super fluids do not have charge; whereas, superconductors the cooper pairs have a charge so that they carry current.

The way BCS theory was set up was a interesting because unlike in many cases, where 1 start nowadays does many body perturbation theory. In this case, what a Bardeen Cooper and Schrieffer did was that they just wrote down a wave function for the many body states which is a remarkable achievement, which is very rarely done that you are writing down an eigenstate for a problem, a many body wave function for a problem which constitutes 10 to the power 23 particles interacting with each other.

And that this worked beautifully was partly due to the reason that the coulomb interaction repulsive part was screened off and the attractive interaction worked at a large distance and in a very narrow range in frequency which is retarded interaction and it is very weak. So, that leads us to this theory of BCS and the so called BCS ground state.

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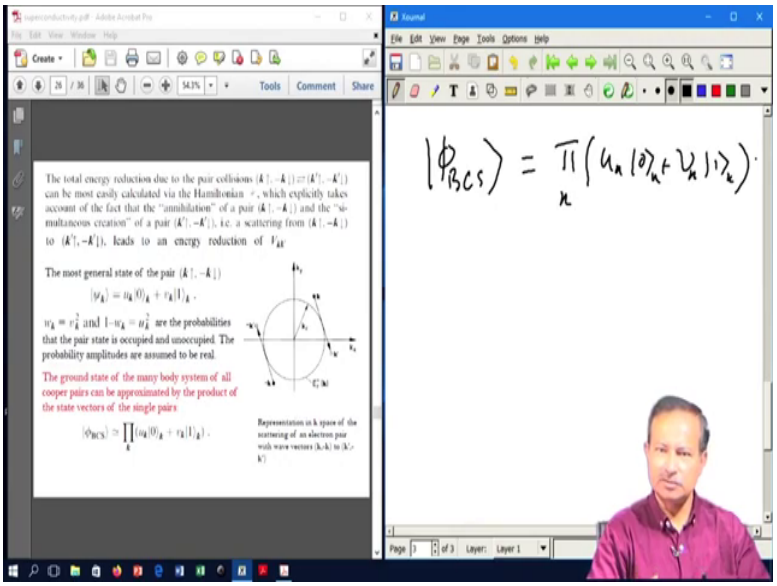

I have also mentioned that the BCS ground state as written here for example, this one is basically it is like a two level system which is you have a pair state which is either occupied or unoccupied. So, a pair state means 2 electrons occupying the minus k down plus k up kind of state simultaneously and forming a bound state and you can either occupy it or not occupy it with probabilities v k v k square and u k square.

So, this is a typical wave function that you write down for a two level system with two states and then of course, you can take a product of such states and that is what these people did. So, this product state as I mentioned just taking just take 2 values of k say 1 and 2 and you will see that this state is not a state with fixed number of particles. So, it is not an eigenstate of the number operator.

In fact, the Hamiltonian which BCS wrote down does not commute with the number operator. So that means, this state has all even number of electrons and that is what I showed. So, this state is basically 0 pair, 1 pair, 2 pair, 3 pair and so on and so forth. It contains all possible pair n by 2 possible pairs in it; n is the total number of electrons in the system. So, it is not a number eigen state.

If that has fundamental consequences which if we get time, we will mention and that is that what Anderson showed was that this wave function is actually a wave function for a it is a eigenstate for phase operator. So, phase is the phase of the function is the right quantum number is the well, the number is not a good quantum number; where, phase is the is the good quantum remember n and phi if you remember your Heisenberg uncertainty n and phi are the conjugate variables.

So, if n fluctuates enormously, then phi becomes fixed and that is exactly what happens here ok.

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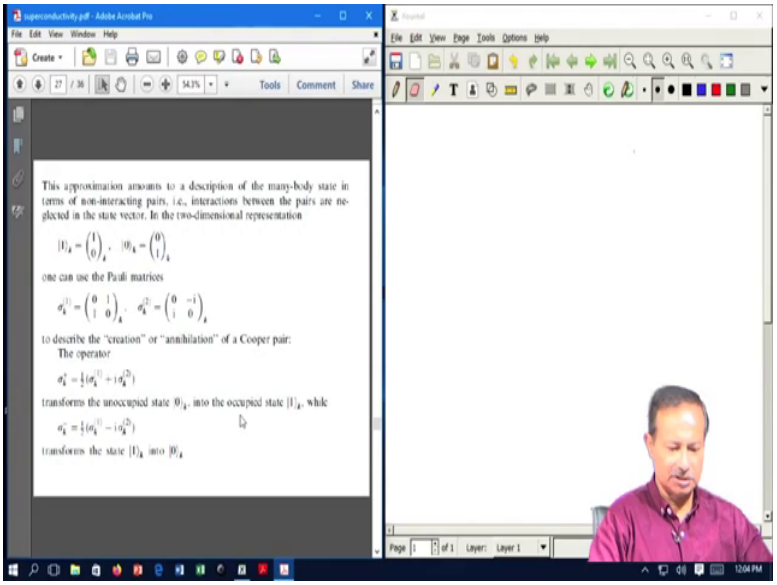

So, that is an aside. So, let us just go ahead and do the calculation that BCS did. So, they wrote down the I mean you can write down, they did not do it in this way, but you can write down a kind of spin algebra for excuse me for this kind of a system for two level systems that we mentioned earlier also and you write down in terms of say sigma x and sigma y which is sigma 1 and sigma 2 written here and you can define raising and lowering operator and these.

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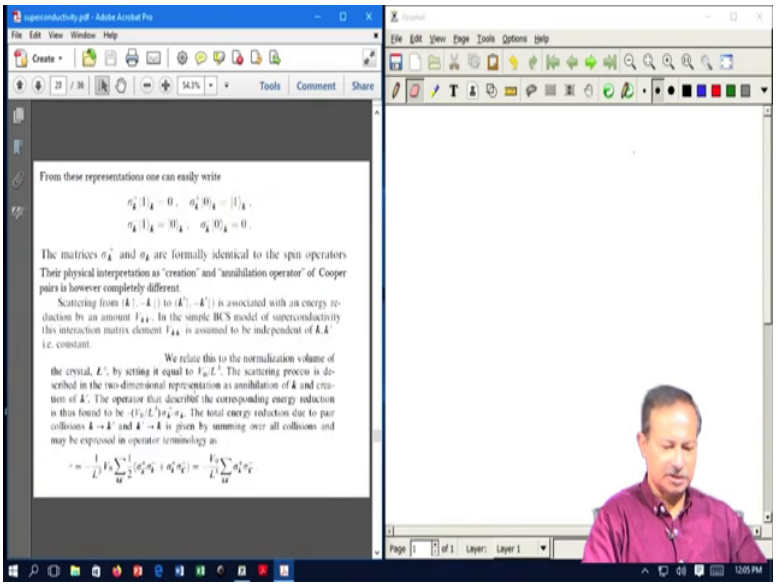

So, this is just straightforward algebra and then of course, you know that 1 is the highest occupied state. So, you cannot raise beyond 1. So, you will get 0. Similarly, if you raise from 0, you will get 1 and so on and so forth and you can choose a basis which is this and then, correspondingly the sigmas are the power 2 by 2 poly matrices.

Now, as we saw in the problem of cooper scattering from a one occupied k state which means a pair state to another k prime state is associated with an energy reduction. So, that is why the scattering takes place and that is what finally, reduces the energy and that is the V k k prime.

So, in the BCS model one then just writes down a Hamiltonian of this kind. I mean this is the energy reduction due to pair collision is then given by all such collisions all such scattering processes involving this V k k prime and involving all possible pairs k and k prime and that is exactly what this Hamiltonian does ok. And since, k and k prime are different you can commute them and you can write it in this fashion.

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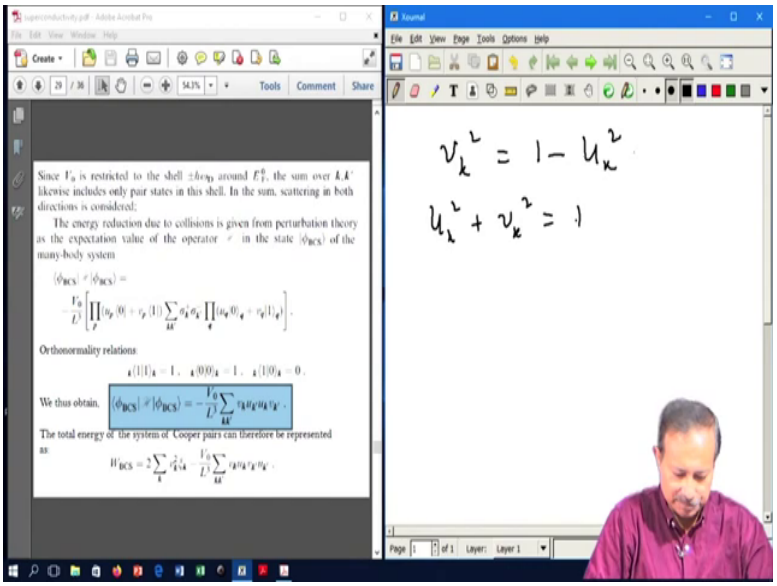

So, then we went ahead and we said that you now because the energies are so small compared to the other energy scales, just the you are allowed to do this calculation that you are trying to figure out the expectation value of. So, the scheme of things is just is to calculate this expectation value, which is the ground state energy. If you can find it out, of the Hamiltonian, in this basis in the psi BCS.

So, one basically finds out this energy and these remember these energies are very very small. So, you have to be careful and you have to do everything correctly ok. In this of course, this basis is interesting because it is very easy to calculate expectation values in this wave function. So, then use these orthonormality relations and you can immediately find out the expectation value of the Hamiltonian in this BCS state.

This is the scattering part the part that is in that involves V, so that is what you are doing. Now, the kinetic energy part is trivial, I mean it is just that to every pair has 2 electrons. So, it is the original 2 electron energies and the multiplied by the probability of v k square and that the pair is occupied.

So, psi k into 2 multiplied by the probability of occupancy of the state and summed over all k in. So, this is all that one has to do here. But now of course, you have to remember these u k's and v k's are variational parameters. So, this is how all variational theories go as we did in several cases even that remember that hydrogen atom hydrogen molecule problem, we did the variational calculation. So, exactly same way.

The variational parameters here are of course, these probabilities u k square and v k square. So, u k, v k are the variational parameters that you have to minimize with width and this W BCS is the energy that you will minimize with respect to u k and v k. But what is interesting is that remember we had this relation that v k square equal to 1 minus u k square.

So that means, u k square plus v k square equal to 1 which is which we basically is a statement of the fact that there the pair has to be either occupied or unoccupied. That means u k and v k are not 2 independent variables, there is only 1 variable that you need to minimize with respect to.

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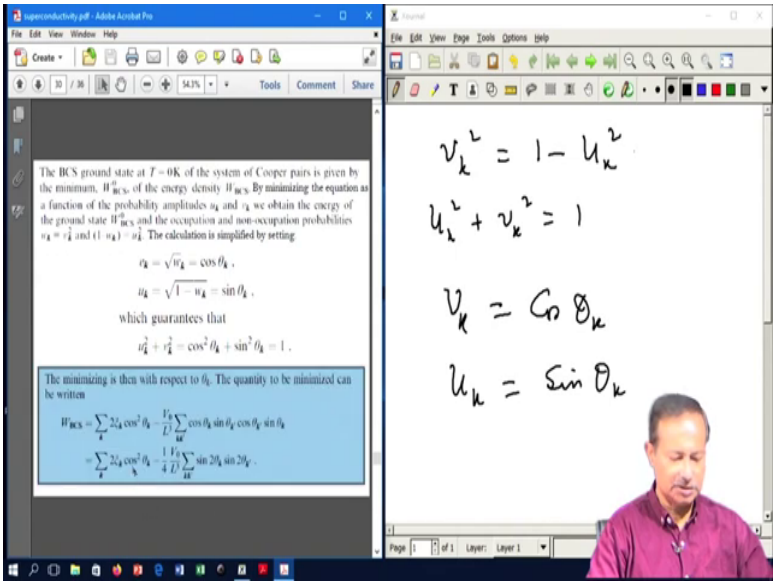

So, a convenient representation to do that is to convert in this kind of situations is to write down this as a cos theta and sine theta. So, write v k as cosine of sum theta k and then u k has to be sin of theta k and then, you have only 1 variable to minimize width which is theta of k and that is exactly what we are doing here.

So, we write this as psi BCS; W BCS in terms of these variables right cos theta k and sine theta k ok. So, once you do that, this is the result it is absolutely trivial to do. So, you can do it.

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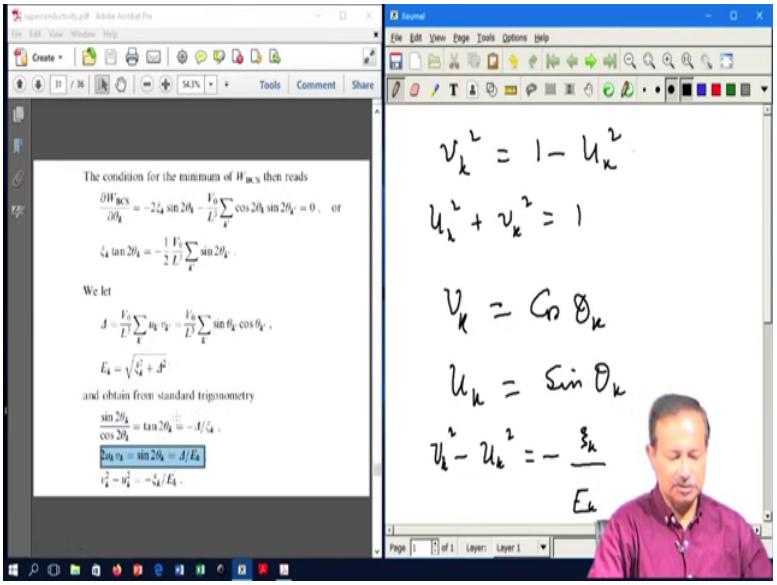

So, then, there is just one more step which is to minimize with respect to theta k and that gives you this relation and set it to 0. So, this gives me c k tan 2 theta k equal to minus half V 0 by L cube sum over all k prime sine 2 theta k prime. Then, you define delta. This is just the definition at the moment that this variable, we called this quantity which is k independent of course, because all k's are k's are summed here is called a delta.

Then, E k is a basically c k square plus delta square right. And from standard trigonometry, so let us just go back one more page. So, using this and of course, this is another definition you are using ok. So, you are going to calculate the W BCS finally, after finding out what the right theta k is. So, let us use these two definitions.

This is very standard definition; delta k and E k and then, just go ahead the go ahead and do the calculations. See this is tan 2 theta k is then minus delta by epsilon k and this to u k v k is sin 2 theta k is delta by E k and then, this relation is very important. The last one v k square minus u k square equal to minus c k by E k. This is what you will get. So, in terms of delta and E, capital E k you can write down your u k and v k from these two relations ok, the last two relations.

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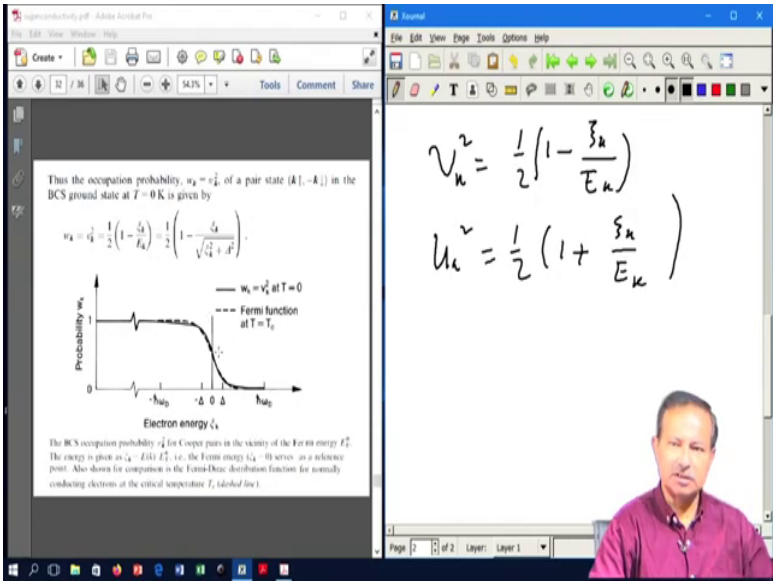

And that is exactly what is done v k square is so that gives me v k square equal to half 1 minus c k by E k and immediately I know what u k square will be because they have to sum up to give me 1. So, u k square equal to half into 1 plus c k by E k so, that is the these are the 2 values. Here, the v k square is plotted at T equal to 0. It almost mimics the Fermi function at T equal to T c and it is deviates from this vertical fall within a region of minus delta 2 plus delta.

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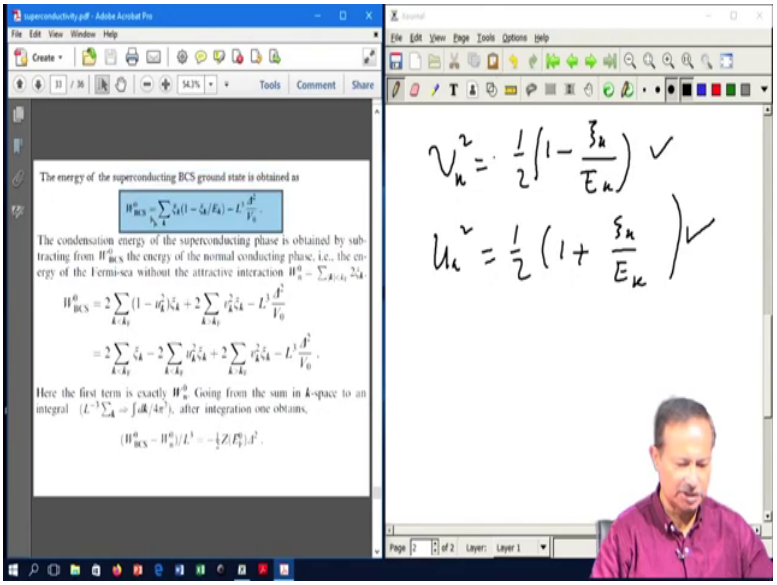

So, now that we have we found out this these variables u k and v k parameters the psi BCS you can calculate in the ground state. So, we have found out u k and v k and the right hand side as I wrote down and of course, it is written here also v k square is this one and then of course, u k square is this one.

And now, we of course, showed that v k square is follows the Fermi function more or less we and there is a drop within the region minus delta 2 plus delta ok. So, now what we have is the W BCS and in the ground state. So, energy of the BCS ground states ground state for that Hamiltonian that we wrote down and that energy can be now written down and one can do all kinds of things that one does this is very standard.

So, let me not get into it. See the first term here 2 into epsilon k k less than k F, this term if you remember, this is just the energy of the electron, the Fermi sea up to the Fermi sea the electron gas that we started with. So, and these 2 is taking care of the spin; the 2 spins per momentum per state k.

So, and then c k is the energy sum over all k's below k F is the original the energy which is the energy of the Fermi sea without the attractive interaction; without that V term at all. So, this was the original energy. So, whatever gain you have is you have to have over this. So, the total energy has to be less than this sum. So, that is what one finds out and you can see that this is negative.

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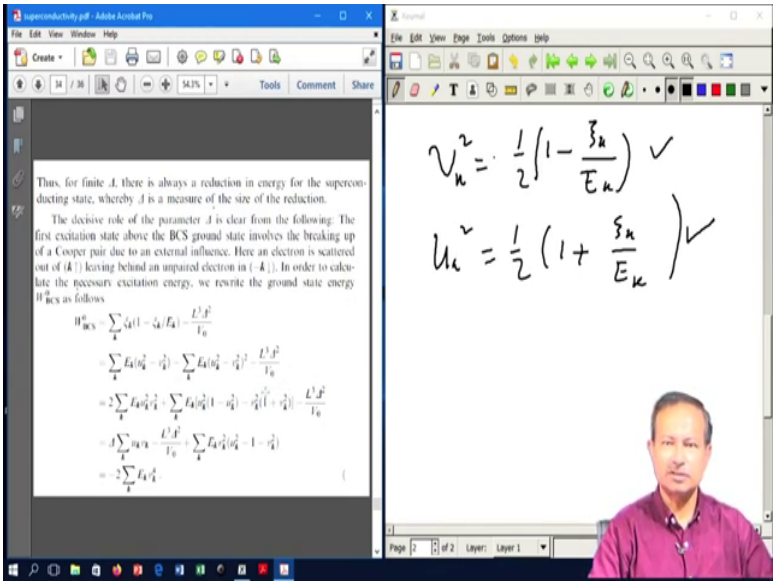

And so that is about it that you need to know. These algebra you can do at home and this is not difficult, but this is not something that you have to remember, in the sense that you know how to calculate it and you know now that there is a gain in energy. So, that is about it.

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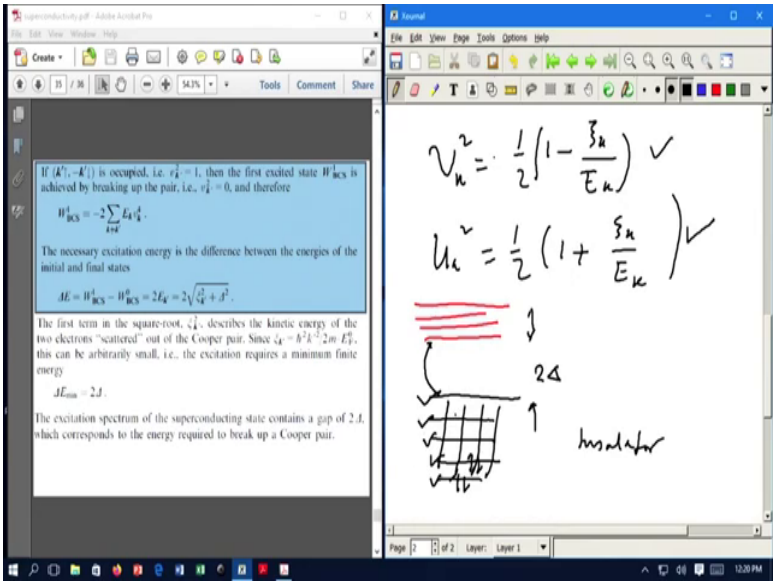

So, let us try to find out the BCS energy which is basically the this and therefore, this is the first excited state in BCS; excitation of the energy. This is the BCS ground state and this is the first excited state energy and you just subtract these two and you will get the energy of the

first excited state. And we will I will show you in a few slides, how the density of states is now arranged and then, you will see that there is a gap in the density of states.

So, this energy actually this delta E tells you that there is a gap because c k minimum of c k can be 0; whereas, even then you will still have a gap which is 2 delta and that is exactly what it shows. So, the excitation requires a minimum finite energy of 2 delta. So that means, the spectrum is such the density of states are such that you have these 2 sets of states and there is a gap of a 2 delta; this is 2 delta.

So, it is very different from the Fermi sea. So, a gap has now opened up where there was originally a Fermi surface Fermi level where there was the Fermi level. So, basically that means, that there is no Fermi surface anymore. So, this gap is basically the energy that we have to supply to break a cooper pair and that is the; that is the consequence of the BCS theory and remember, I mentioned that the essential picture that BCS wanted to get was that there has to be a gap in the spectrum.

Because there are already experimental evidences there from thermal conductivity and so on that there exists a gap in the spectrum. There must be a gap in the spectrum. But then, the difference from a semiconductor for example, or an insulator is just enormous because this is not a picture of a semiconductor or an insulator, where these states are single particle states and these are the states, where you fill in like this in semiconductors.

In insulator, what you do is that you just keep on filling these states. Here, you of course, fill these states, but these states are not the semiconducting states. I mean these are not a single particle states which are just obtained by a single particle calculation.

So, these are many body states and this picture here is very very different from the picture of a semiconductor. Because here, all the states are filled up that is it; whereas, you want to excite of course, you have to break a pair and the pair goes here. So, these this is like this these are single particle excitations of course, but the nature of this states is very very different from the picture that we give when we did band structure calculation.

There we had obtained we just had a rigid band bands were there, we form the bands irrespective of the number of electrons. We always did it for 1 electron actually and then, we

calculated the bands available, the states available for the single electrons and then filled them up. Here, it is very different. Here the these those states that you had in the Fermi sea that you had is no longer stable. So, you have completely obliterated those states, but the number of states counts have to be the same.

So, that has to be the same and that is what leads to this excitation leads to the density of states for a BCS superconductor.

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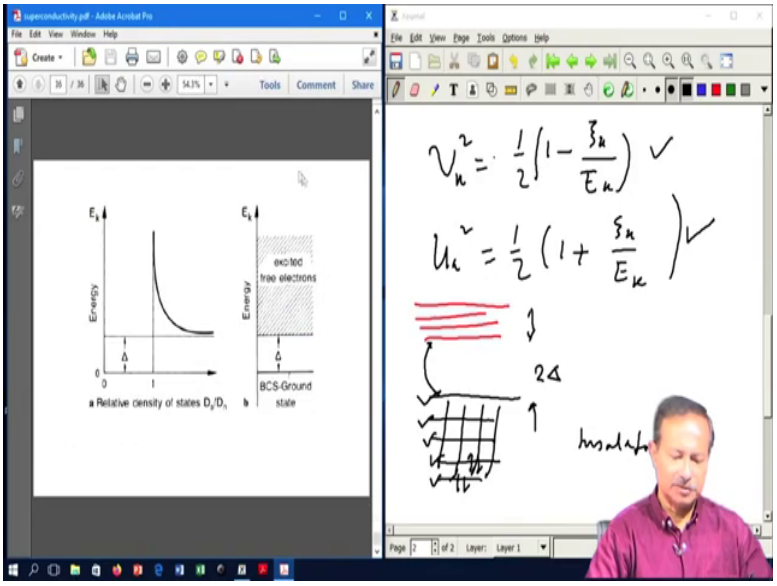

So, what we did so far let me just recap a bit we have done something very very different from what we have so far done in our all our calculations. This is the first time, we are encountering in a free electron gas in an electron gas interacting via a very weak coulomb interaction, the weak attractive interaction, we found out a many body ground state. By many body ground state, I mean that if you take this ground state psi BCS equal to pi over k u k 0 k plus v k 1 k.

Then you can see that this state contains all the particles, I mean it has all the it is a superposition of 0, 1, 2, 3 up to n by 2 pairs and that means, that this is a you in one shot you are writing down the ground state. And that that was the assumption of BCS that we do have a ground state and we know what it is and this represents the ground state and that is what it is.

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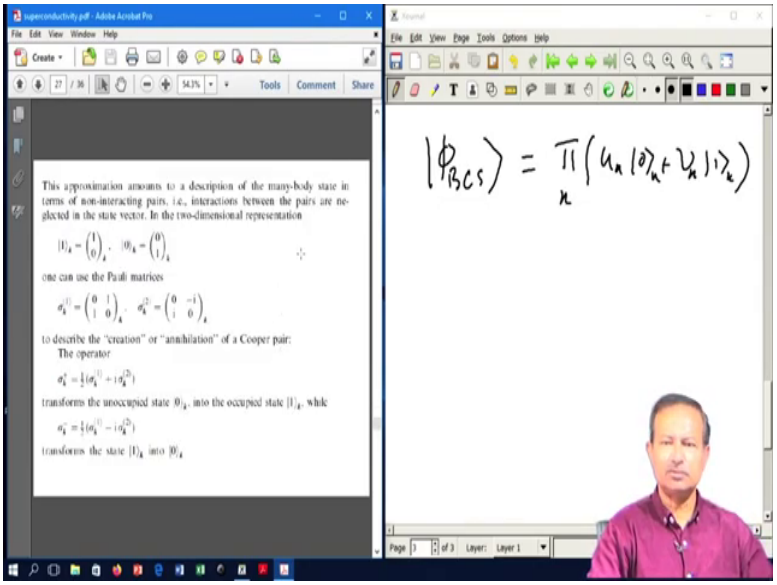

And then, the question was how do I find its energy and we sort of did a trick in the sense that because it is a there are only 2 levels a for every k value either it is occupied or it is unoccupied. So, 2 energy states. Then, we can write down the whole thing in terms of spin operators. These are pseudo spin operators in some sense and we can create and annihilate a cooper pair and that representation is a this right. It is exactly like s plus and s minus for each k state and that is what we did.

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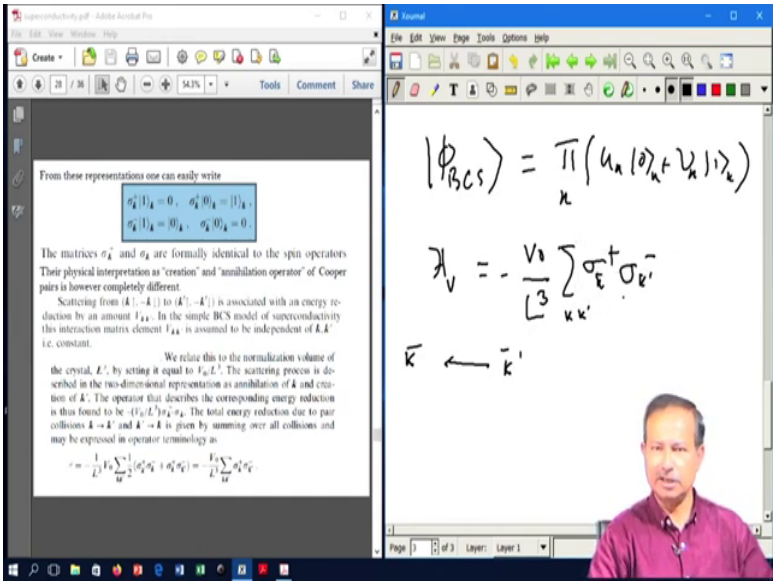

And then, what we did was that we just carried on and we just completed the algebra here, just wrote down what the algebra is and using that what we tried to do was to calculate. First, we wrote down the interaction part of the Hamiltonian which is the V part which is V 0 by L cube sigma k plus sigma k prime minus. So, what it does is that it destroys a pair at k prime and creates a pair at k.

So, that is all it does. So, this term right. So, it takes a pair from k prime to k ok. So, and of course, there is a Hermitian conjugate because that is ensured by this sum over k k prime, that term is also there. So, with this because you are summing over all that term will already be there.

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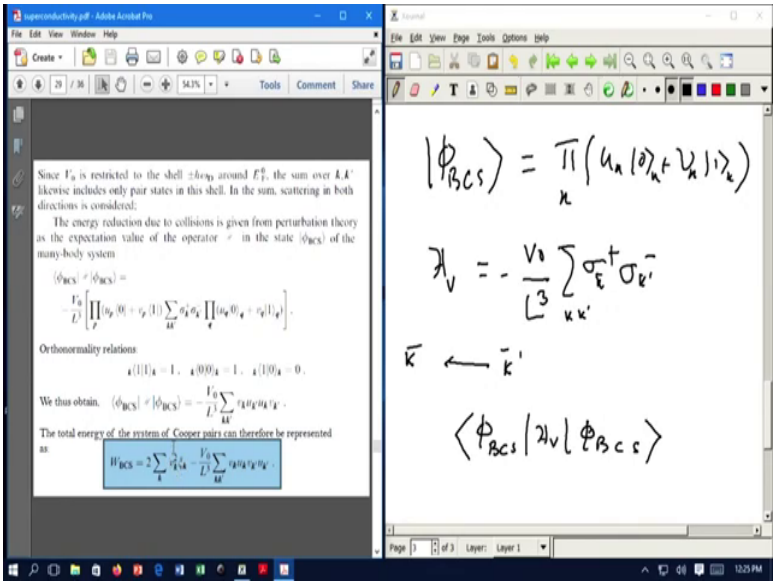

And then, what we did is that we just calculated the expectation value. We calculated psi ok. So, what we calculated is this thing psi BCS in this H, in this H V psi BCS and then, we just added the energy for the number of pairs. So, energy twice epsilon k is the energy of the pair times v k square is it is probability of being there ok.

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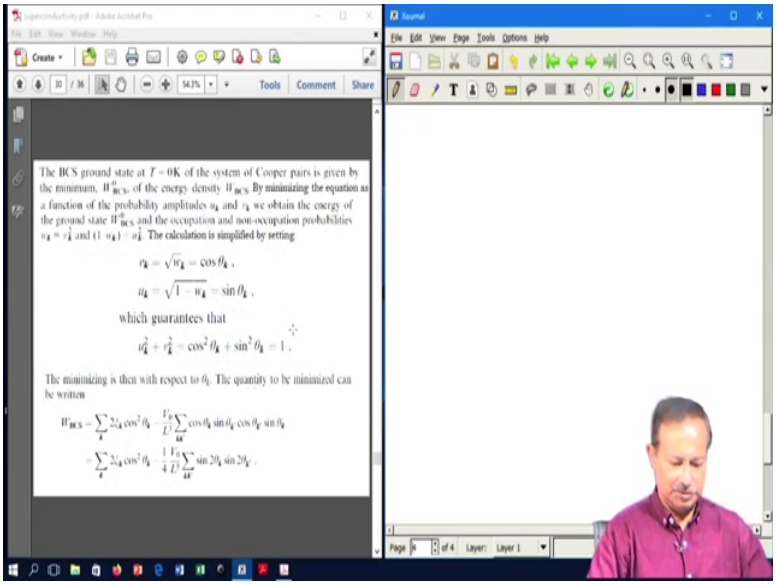

So, that gives us a the total energy and then of course, since only 1 variable is relevant because u k and v k are connected. So, we converted into a 1 variable minimization by writing this. So, it is like a rotation so, in the u k, v k space and. So, basically a rotation in the you can look at it in the rotation of the pair and not pair 0 and 1 in this space, in the bases between the bases.

So, you choose the right direction of the linear combination between 0 and 1. So, that is what we do I mean when we want to diagonalize a Hamiltonian. So, that is what we did we basically found out the right combination of 0 and 1 k states and the correspondingly, we defined something called delta and E k and so on and we finally, found out the values of u k and v k which is given here.

This is v k square and u k square is just 1 minus v k square. So then, we actually found out that the there is a condensation energy, in the sense that the energy has now become less than the original Fermi sea energy and that means, there is a new ground state.

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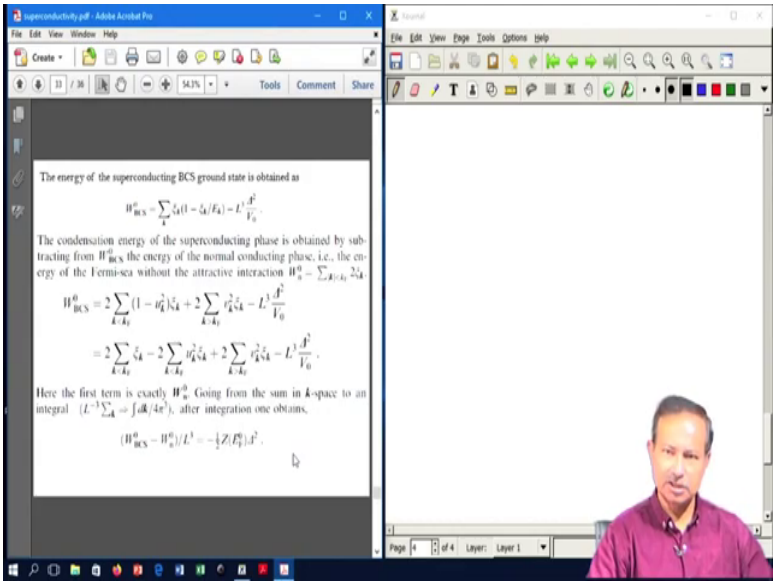

And this ground state is lower in energy than the original Fermi sea ground state ok. So, far so good and then, what we found that we found the excitation energy of the first excited state over the ground state energy and that has this form and there is a difference between the two which gives us the first the gap in the excitation and that is this excitation.

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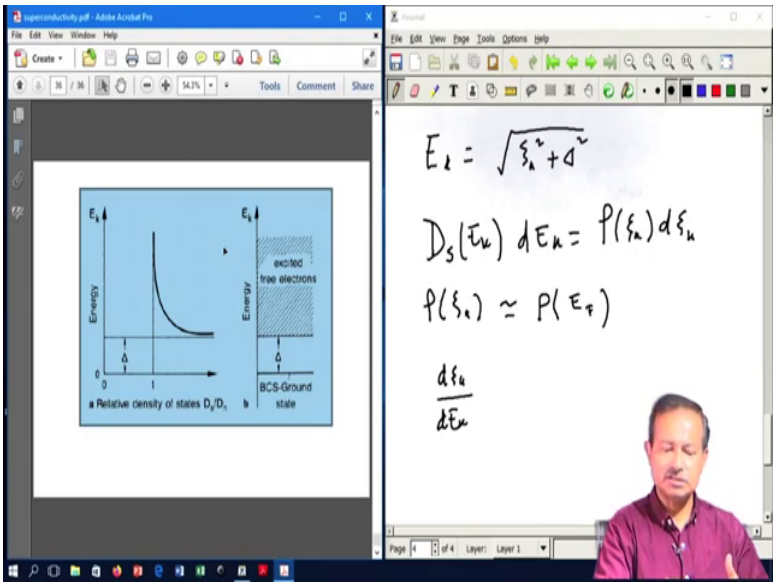

What is interesting is that now you can actually calculate the. So, this is the new spectrum E k equal to c k square plus delta square. Delta has no k dependence in this theory. There are

theories where delta is also k dependent. We will mention them when if you have time. Now, what you can do is that you can just calculate the density of states which is I will show in detail, which is which basically comes from this relation that D s E k d E k must be equal to must be preserved.

So, the density of states cannot be eaten up, number of states cannot be eaten up. So, that should be equal to the original rho E k d E k. So, this relation and then, what you do is that you just replace this rho E k by it is Fermi level value. This generally written as rho 0 or rho E F whatever you want here we are using rho E f. So, let me use that E F and you can do it yourself to find out.

So, all you have to do sorry rho, I am sorry this. So, all you have to do is to find this derivative d epsilon k d E k and you will find that you have a density of states of this kind which is divergent and which there is no state between in the gap in this region from minus delta 2 plus delta. So, that is the gap, that is the excitation.

All the states in the negative energy are filled up the positive energy states states are empty and there is a gap the in the density of states and that. So, these are single particle density of states that we are talking about. So, these are excitations and then, the excitation has a gap which is 2 delta and that density of states is divergent at E equal to delta. So, so there is a pile-up of density of states.

So, you move density of states away from a Fermi level and pile them up at a plus delta and minus delta. Of course, that is like a this old Fermi old Fermi sea states are not there. These are new excitations. These excitations are excitations over the BCS ground state and their spectrum has this pile up at plus delta and minus delta and that has fundamental consequences.

Two things; one is this gap and the other is there is a pileup. There is a divergence at plus delta and minus. So, these things are very important and these have experimental ramifications which we will discuss in the next class.