Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'
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Lecture 31
II and higher order Feynman Diagrams

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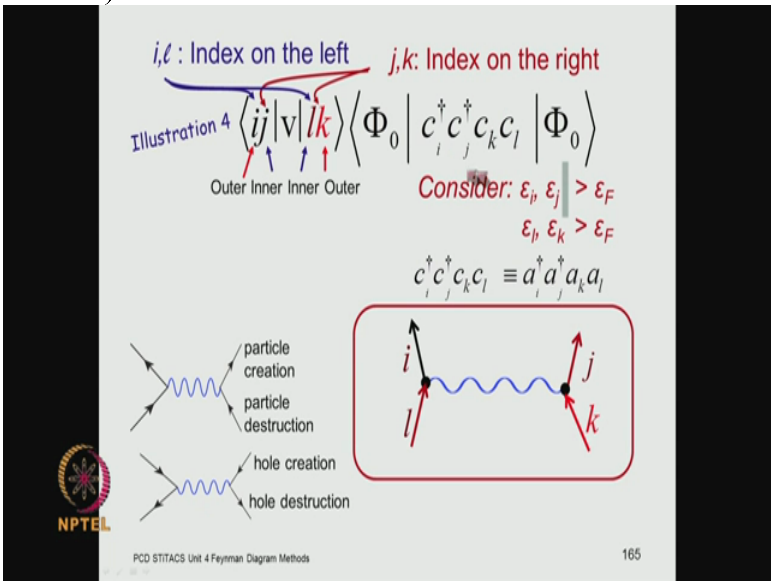

Greetings, we will discuss some more diagrams of order one then we will introduce the second ordering second order ring diagrams in today's class. So, let me quickly recapitulate this a little bit but the terms that we are focusing our attention on are these terms. So, you look at this two center integral as well as the matrix element of the creation and destruction operators in the vacuum state.

So, we have the Phi 0 which I refer to as a vacuum state and the reason it is a vacuum state because we have carried out a transformation from the electrons which we write as particles these are the Fermi particles of our interest but when we refer to the electrons where we write particles with the upright p. But then we carry out a transformation to what we write as the slanted *p* particles which I discussed in the previous classes.

And these are the electrons which are above the Fermi level or the vacant States below the Fermi level is wha t we refer to as the hole states and here these particle and hole states are what we write with a slanted *p* and a slanted *h*. So, when there is no hole state and all the electrons are in their lowest state then of course you essentially have a vacuum in terms of the slanted *p* particles and the slanted *h* holes okay.

So that is the vacuum state that I am now referring to and Phi 0 is the vacuum state. So, we are taking the expectation value of a certain set of creation and destruction operators in the vacuum state and we consider in this example the states i, j, k, l of which i and j will be above the Fermi level and l and k will also be above the Fermi level. So, all our particle states with a slanted *p*.

So, you will all have essentially represented by arrows pointing upward right. So, those are the; that is the prescription that is the convention that we are following here. So, all of these will be represented by arrows pointing upward and by creation and destruction operators which are the a operators okay. So, these operate above the Fermi level and then you identify the vertices identify what is on the left and what is on the right.

And then essentially you have four arrows flying up and you have a particle creation and another particle creation and again a particle destruction and again a particle destruction. So, that is the kind of diagram that you generate from these terms right. So, you have got the ai dagger aj daggers which are created and the al and ak which are destroyed as represented over here.

So, this term essentially indicates the result of this matrix element of the creation and destruction operators in the vacuum state. But it also you know makes a reference to this two center integral because the locations of these indices okay which one comes to the left and which one goes to the right is determined by this over here. So, you keep track of that and that is a useful thing to remember.

So, this is like a particle from l being excited into i and you know from one from k in this. So, that's the usual physical picture that you can draw however that is that is a little cumbersome when you deal with a large number of particle hole excitation, so which is why the Feynman diagrams are really of great use.

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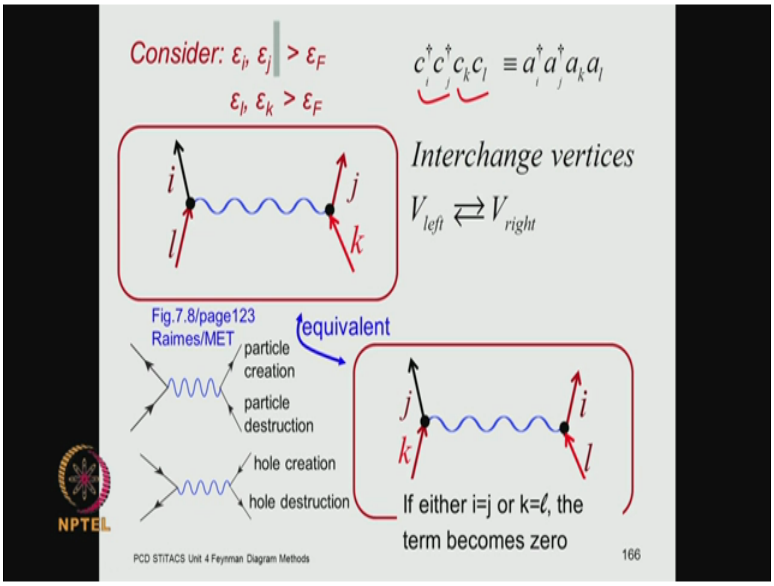

What I also pointed out and this is of importance to keep track of that when you interchange the way of vertices. So this left vertex will go to the right and right to the left, so l and i will go to the right and j and k will go to the left, so that is what an interchange of vertices will mean. And essentially as you see from these operators when you interchange i and j you will pick a minus sign over here.

Because these two creation operators anti commute likewise if you interchange k and l then you will have these annihilation operators which also anti commute, so you will have you will pick up a minus sign here and a minus sign here. And essentially the result will remain invariant okay the two minus signs -1 into -1 is +1 as we say even in quantum theory right, so you will not any have any difference.

So, this is what we get so if you interchange the vertices you will get this diagram to be completely equivalent to this diagram when you interchange vertices. Now of course if either i = j or k = l you will get 0 contribution from this term because you cannot destroy a particle from the same state twice.

Because these are Fermi particles nor can you create these particles into the same state twice. Because again for the same reason that Fermi particle occupies the state and the occupation number can only be either 1 or 0 it cannot be anything else.

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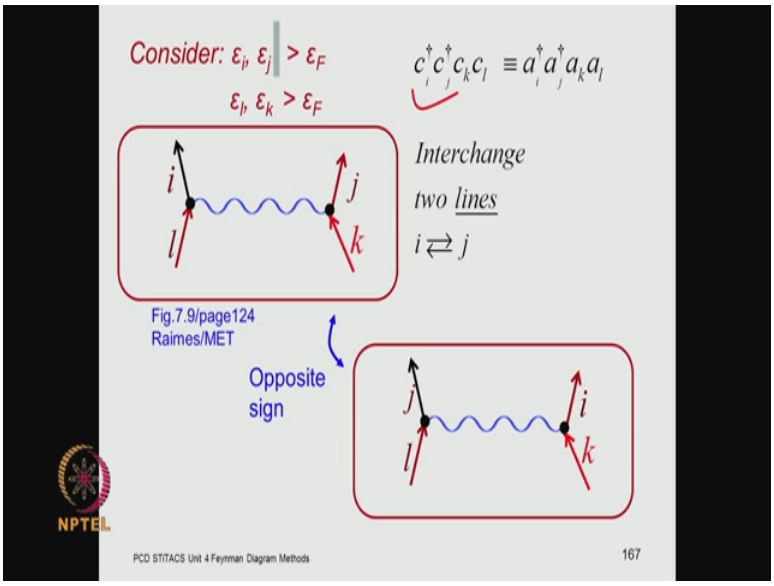

So, the other thing you should remember is that if you instead of interchanging the two vertices completely if you just seem to change two lines like i go into j and j going to i then you are going to swap the positions of these two creation operators and you will pick up a minus sign from that swapping. And you can certainly have the corresponding diagram in which i goes to j and j goes to i but then the signs will be opposite okay.

So, these are certain conventions which consequences of the fact that you have followed a certain convention of writing which index goes to which vertex left or right and then of course the overriding principle of course is the fact that the positions of these operators is important because these are fermi operators and they anti commute okay. So, let us take another example over here.

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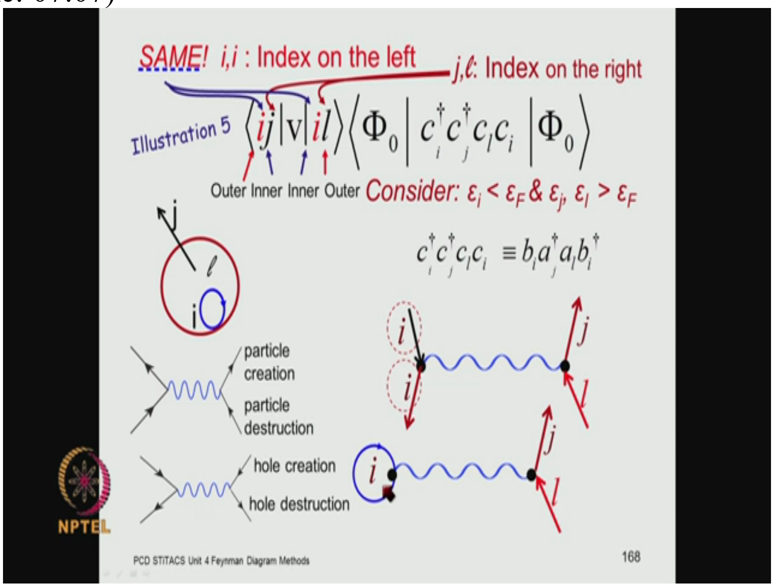

But in this case we normally deal with four indices over here but remember that you are summing over i, j, k, l okay. So, each index will take all the values that particular index can which are all the infinite values and in some of the combinations you will find that some of these indices may be the same you can also have all the indices to be the same or some of the indices to be the same and so on right.

So, here in this case I have these two indices the ci dagger and the ci these two indices are the same j and l are different now when you have this you consider a situation in which the common index which is here and here if this index is below the Fermi level. So, up Ei this energy is below the Fermi level Ef whereas the other two indices refer to electron states Ej and El which are above the Fermi level.

So, that is an example that I am considering we have now in this example you have ci dagger cj dagger cl ci and then the ci dagger is creation of an electron below the Fermi level which you are going to do when you destroy a hole in that state. So, this will this ci dagger will be Vi and this ci will be destroying a particle in a state which is below the Fermi level or when you do so you create a hole.

So, that will be represented by this bi dagger and then this cj dagger cl j and l are both above the Fermi level so you have got aj dagger here okay. Because both of these states the j and the lth state are above the Fermi level. So, now we can write these because hole creation is represented by an arrow pointing downward.

You have a hole destruction, so this is represented by an arrow pointing downward but out of the vertex this one goes into the vertex and likewise you have got aj dagger and al aj dagger is particle creation, so an arrow pointing upward but it will go out of the vertex whereas al will be a particle destruction. So, it will be an arrow pointing upward again but going into the vertex okay.

So it is just those conventions that we are playing with and you can build the Feynman diagram corresponding to it. So, you have got the bi aj dagger al bi dagger all of this processes you know are then represented by this diagram. Now I would like you to note, so that here you have the index i and here also you have the index i okay. So, notice that this is the common index over here.

And when you have a situation like this okay essentially you have got the same index. So, it is the same particle which gets scattered into the same state okay it is the same hole in this case right. These are arrows pointing downward and you have this going into the same state and this is then represented by a ring of this kind okay. So, this is a little topological you know adjustment that you make to tell you that okay.

There is only one index which is involved over here okay. It so it does not mean that the left half of this ring that you have drawn has got any particular significance okay. It is just indicating the fact that the hole state which is created is the same one corresponding to the hole state which is destroyed okay. This process is then represented by this circle over here, so that is the usual convention in drawing these diagrams.

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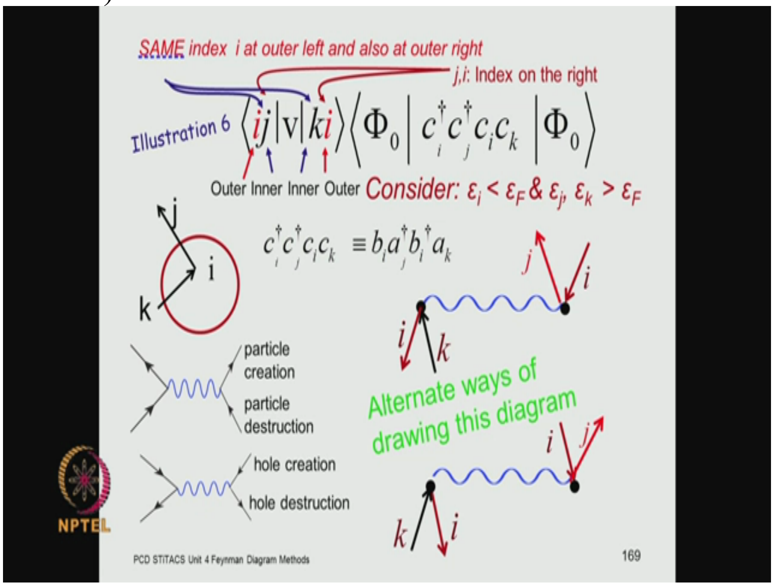

So, this is something that we will extend further by; so, let us take another example over here. In this example again I consider i less than f this is and then j and k are above the Fermi level. So, let us start building this diagram we first identify the operators using the same convention that we have defined okay. So, you write this in terms of the corresponding particle and hole operators now this is the slanted *p* particle above the Fermi level.

And the hole operators which are below the Fermi level and you have got a particle creation. So, this is this is a particle destruction in the kth state. So ak is this is an electron above the Fermi level, so it will be represented by an arrow pointing upward it is destruction, so it goes into the vertex, so k is going into the vertex and then you have got i which is a hole creation which is coming from this bi dagger here.

And then you also have a hole destruction which is coming from here okay and this is the diagram that we construct okay. So, if you just follow all the steps one by one you will be able to build this diagram. So, this is the kind of picture that of a physical picture that you can draw but now remind yourself of the fact that I had mentioned that the leanings of these arrows does not have any particular significance.

And what you can do is draw the same diagram in an alternate man because what is important about the arrows k and i is that k goes into the vertex and it is an arrow pointing upward and if it is leaning from right to left or to left to right is of no great significance okay. And you can draw this diagram equivalently as k with an arrow going upward into the vertex which is also the case over here okay.

This is also an arrow pointing upward going into the vertex but this one the first time when we have drawn this diagram you had an arrow leaning from right to left. Now I have got an arrow which means from left to right and that is not of any big difference and these are completely equivalent ways of drawing these diagrams.

Not only that the reason I have chosen this example is because here you have an index i and here also you have an index i and that is something that we are going to play with just the way we played in the previous diagram that you had an arrow with the index ai going downward.

And it was again this into the vertex and you had the same index which was going downward but out of the vertex. And then we indicated that these two states being the same both being i, we closed the loop right. So, here again we will be able to set up some conventions. So, let us do that.

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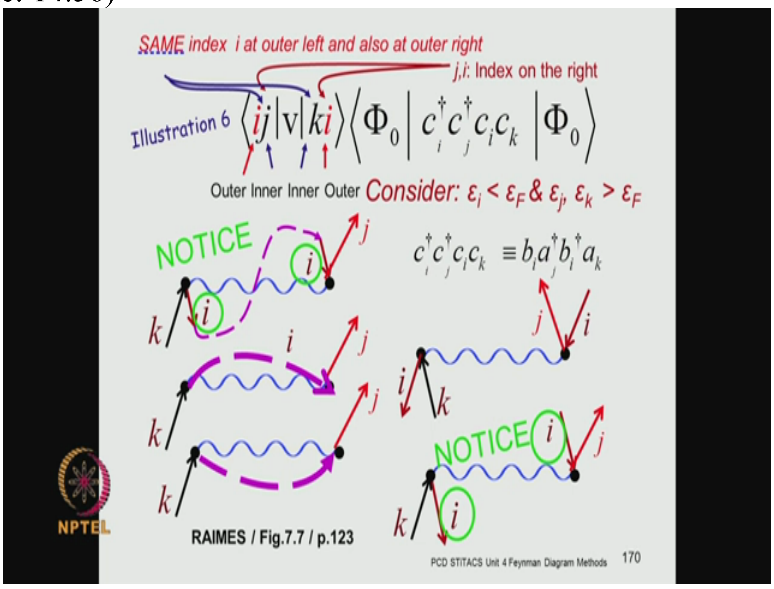

So, this is what we have these are the two equivalent diagrams which I have brought from the previous slide. So, this is the first one and this is what we have drawn again okay and now we take cognizance of the fact that these two indices are the same okay. So, you can; how do you indicate that they are the same you can draw a line between them here it goes. So, this is the line which goes down and you twist it bring it up and bring it down okay.

So, that is the diagram you get. Alternatively you can also show it like this because what you are doing is indicating this twist okay. So, these are certain conventions which are defined in terms of drawing the diagram. So, you show this twist by an arrow going like this but you can also show it equivalently by an arrow going like this okay. So, this is like a half loop which goes over here and this is an equivalent.

So, there is no mathematical difference between any of these four diagrams. So, this one is what we have drawn first this is what we have drawn second, this one third, this one the fourth time and this is the fifth time. So, we have drawn the same diagram in five different; you know which look like five different pictures to the eye but they are all essentially the same and what they are telling us is essentially this particular interaction.

That you are creating a hole and you are destroying a hole but now it is not at the same vertex. In the previous example you destroyed a hole and you created a hole but it was at the same vertex. What this picture is telling us that you are creating the hole and you are destroying a hole but this is not being done at the same vertex which is why this half semi circle that you see this purple colour arrow.

Which is going from left to right either above the wiggle or below the wiggle does not matter but essentially what it is telling us is that it is the same state and the operation is taking place at different vertices, so there is an exchange here okay. There was no exchange in the previous case.

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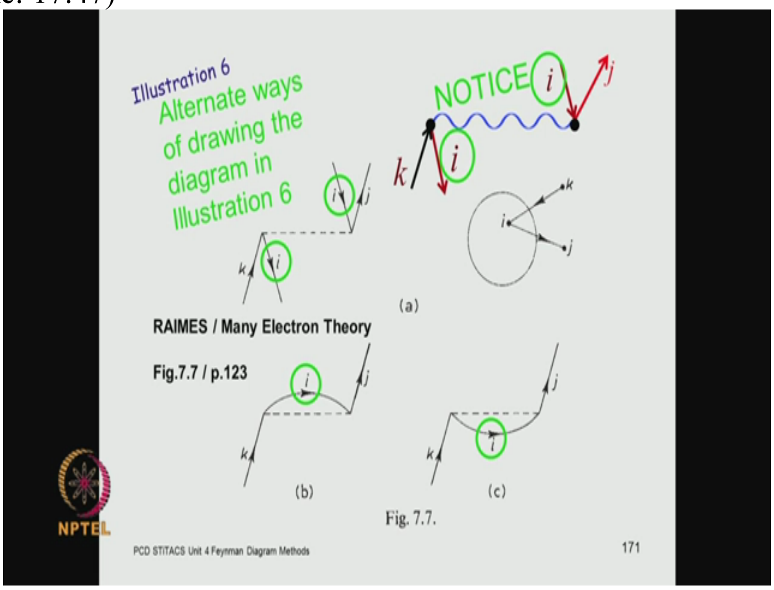

So, let us draw these diagrams in the manner in which you will find them in the book by Raimes this is figure 7.7. It is the same thing you have this half circle flying from left to right and in print it will look like a neat diagram it is exactly the same interaction okay. And this is how it is built that this is the half circle which flies from the left vertex to the right vertex it is the same one which goes from the left to the right.

But it does not matter whether you close it above this line or above or below this line okay that is not relevant. So, this is the term corresponding to exchange, so let me remind you once again what the what the previous diagram was that was this one here the creation and destruction of the hole was at the same vertex okay which is represented by this by this circle here.

But in the next example we again have a creation of a hole in the ith state and the destruction of a hole also in the ith state but not at the same vertex the vertices are exchanged. So, this is the picture that we get and these are the Feynman diagrams corresponding to this case all right.

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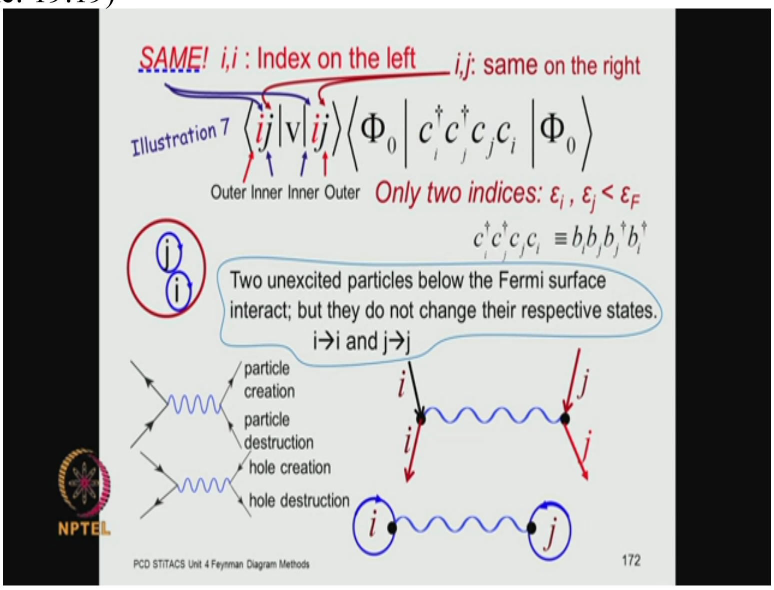

Now let me take one more example over here and now I have out of the four indices i, j, k, l. I have two indices here and here which are both i and here and here which are both j okay. So, there are actually two only, two rather than four indices to think about. And let us consider both of these indices to be below the Fermi level. So, they will all be represented by hole operators and they will all be represented by the operators b as we refer to them right.

So, you will have ci dagger will be bi cj dagger will be bj and cj and ci will be bj dagger and bi. So, these are the operators and now again you follow the same conventions, so you have got a hole creation again a hole creation at the other vertex and a hole destruction at the first vertex with the same index and again a hole destruction with the same index at the other vertex so that is the picture that is emerging.

And what you can obviously do is to show it show just the way we had closed the left side with a circle we can do so also with the right side this time around. So, you will have essentially two circles one with the index i and the other with the index j. So, this is they not only look nice and fancy they also have got fancy names. So, now this one is called as a double bubble okay.

So, that makes it so much more fun to play with these diagrams and essentially what it is telling us that you have got two unexcited particles below the Fermi surface they there is an interaction between them but they do not change their respective states they interact but stay within their own state. So that i goes to i and j goes to j without any exchange all right.

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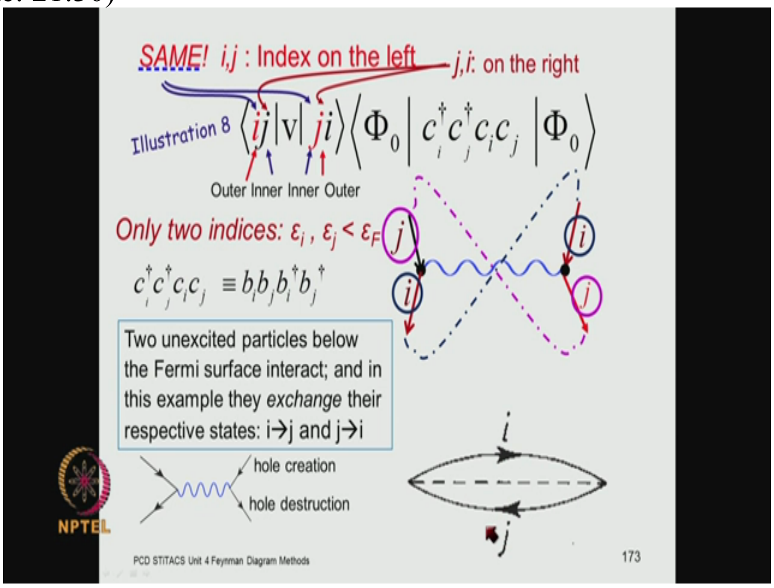

But then you can have a situation again with the same set of four indices in which two are the same so you will have ci dagger and ci in this and again you have the other indexes cj dagger and cj okay. But now we have swaped the positions both of these are below the Fermi levels. So, again you would have only the hole particles hole operators which are the operators b and you represent this using the same convention.

And you get a diagram in which you have the creation of holes in the state j and i and it also the destruction of holes in the j and i but that is at the opposite vertex now okay. So, just the way we had you know close the loop earlier you can find that these two indices are the same both are i and these two can be connected using this connected line. So, that what this line is telling us that it is the hole destruction of the same state.

And in the same state you also have a hole creation but at a different vertex okay. So, the same whole state is destroyed as is created but at a different vertex and likewise you also have the j's over here. So, which again have a similar feature, so now you draw this with these two lobes but just the way we had twisted them in the earlier case because what is important is that you are indicating that the same hole state is created as is destroyed.

But this is happening at two different vertices and we have read to show this by an arrow going from left to right or by right to left and it does not matter whether you draw it above the line or below the line. So, now you draw it like this and what does it look like I at least Ankur should be able to recognize this, this is an oyster right. So, those who are fond of seafood may be quite familiar with this.

So, then so this the previous one is called as a double bubble this is an oyster and these diagrams are then you know named as double bubbles or oysters and so on. So, what the oyster diagram is doing is it is telling us about the two hole creation and destruction but corresponding to the exchange term. So, these are the conventions that we are going to follow now.

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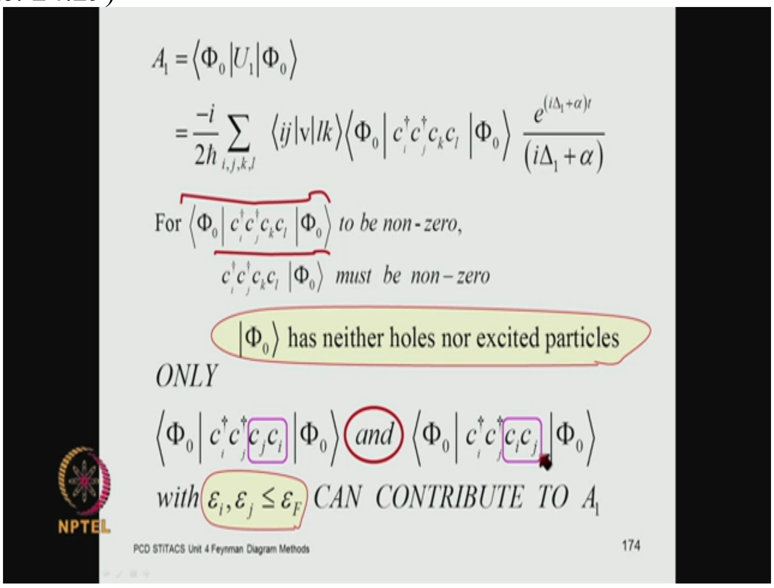

And now let us look at their contributions to the correction; the correction is coming because of the correlations okay. The correlations to what we began with an electron system which we consider to be non interacting these are represented by the Hamiltonian which is the unperturbed Hamiltonian H0. Now you introduce the interaction between them and this interaction would lead to certain correlations.

And these are the correlations that you are not able to account for in the Hartree Fock or in the Dirac Hartree Fock formalism the correlations that you do take cognizance of are only the statistical correlations which come from the anti symmetry of the wave functions. So, the residual correlations are still sitting over there and we developed this adiabatic hypothesis by which we switch on the interaction using this mathematical device.

Which is a parameter alpha and this alpha parameter shows up explicitly over here okay. Then you have these energy sum and difference of all of these i, j, k and l right. So, that is what goes into this delta 1, so we have considered these terms earlier and then of course when you evaluate this matrix element. It is obvious that for this matrix element of the creation and destruction operators in the vacuum state to be nonzero.

This result of the creation and destruction operators on the vacuum state must have a nonzero projection on the vacuum state right. Because it is you operate on the vacuum by these operators and take the result which gives you a new vector in the occupation number space and take the projection of this new occupation number vectors state on the vacuum state again. It is just a expectation value of those creation and destruction operators.

No one will display nonzero, there are certain conditions which must be satisfied for example we already saw that if you have a combination of ck cl in which ck and cl both refer to the same electron state like k = l, if both the states are the same states. So, you are trying to destroy a Fermi particle from some state and even if that state was occupied to begin with you would destroy it by the first time you operate by the annihilation operator.

And having destroyed it by that you cannot destroy it any further once again okay because it is already destroyed which is what I often say by saying marehuve ko kya marna okay. So, you cannot destroy a Fermi particle twice and you cannot destroy a Fermi particle from a vacant state that state has to be occupied then you can destroy that particle if it is already occupied and then once it is destroyed you have got a vacancy over there.

And then you can create an electron over there but you cannot then create a hole okay. So, these are just the consequences of the Fermi Dirac statistics. So, this must be nonzero and which means that you are really dealing with a vacuum state because it does not have either holes or excited particles that is why we call it as a vacuum. And in this you can only carry out certain operations.

So, all of these i, j, k, l each of which can take infinite values they will not make a nonzero contribution because whenever you do not have the right combinations of the creation and destruction of particles. You will get a contribution which is 0 from this infinite sum of i, j, k, l vector i, j, k, l indices okay. So, you have this only certain conditions and these conditions are written over here.

That i and j both must be either at or below the Fermi level okay they can be at the Fermi level because those particles are occupied. Fermi level is the level up to which all the electron states are occupied. And you can have only epsilon i and epsilon j both must be less than or equal to and they have to come in this particular order okay. So, that is the only way you can have a nonzero contribution is that clear everybody.

So, this is the only possibility you can destroy electrons c's are the electron operators these are not the particles with a slanted *p* okay. So, when it is above the Fermi level they are represented by the operators a when they are below the Fermi levels you can write the corresponding operators b. But essentially you can destroy electrons from the vacuum because that is where you have occupied electrons.

So, this is the only case that you can have ci and cj destroy two electrons from the vacuum and then you have to create them subsequently. Because now that you have holes over there you have vacancies, so you can sure enough you can have electrons created over there by destroying the corresponding holes.

So, these are the two possibilities so one is that you have; if these are you are creating two electrons in the state i and j you have to destroy them first but you can destroy them in this order cj ci or in the order ci cj does not matter but when you have when you destroy them in this order.

And when you destroy them in this order you will have contributions with opposite signs okay. Because ci and cj are Fermions operators which anti commutes. So, these are the only two possibilities which you are going to consider.

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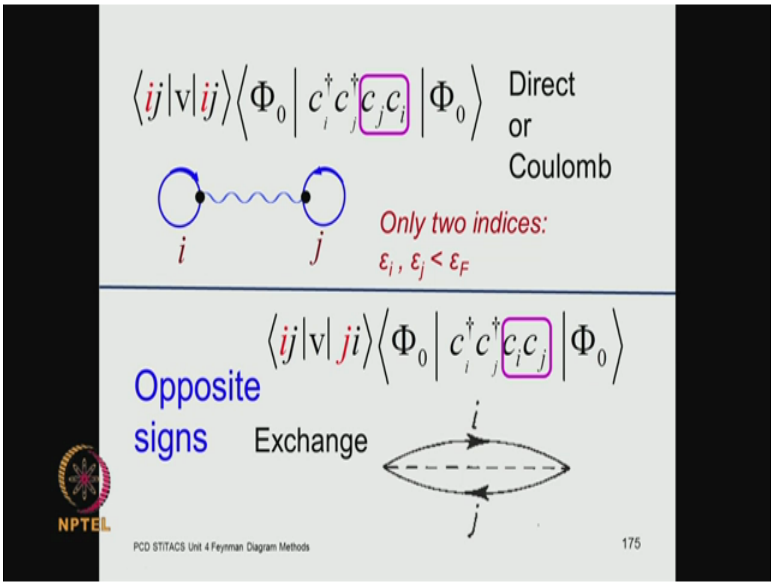

So, let us consider this further and you have only these two indices which are both below the Fermi level. So, this one we have seen we discussed this a little while ago and we have seen that we get this double bubble in this particular case. And this is coming from the direct or interaction or what is also called as the Coulomb interaction. The other is when the indices switched their positions with respect to the vertices.

That is when you have got the exchange, so that is the oyster diagram that we have drawn. So, you have got these two possibilities one corresponding to cj ci and the other corresponding to ci cj they will have opposite signs and they will be represented direct respectively by the double bubble for the direct interaction which is also called as the Coulomb interaction.

So, Coulomb and direct in this context are synonymous and the other possibility is the exchange. So, these are the first-order diagrams and these are the only ones which can really contribute to the correction, correction to what, correction to the non-interacting sea of electrons okay. So, those are like free electrons they have no interaction between each other their only energy will be the kinetic energy.

And if you now make corrections because of the electron-electron interaction and consider this in first order perturbation theory then you will get two contributions one coming from the Coulomb term and the other coming from the exchange term. And you will represent the Coulomb contribution by the double bubble and the exchange contribution by the oyster diagram.

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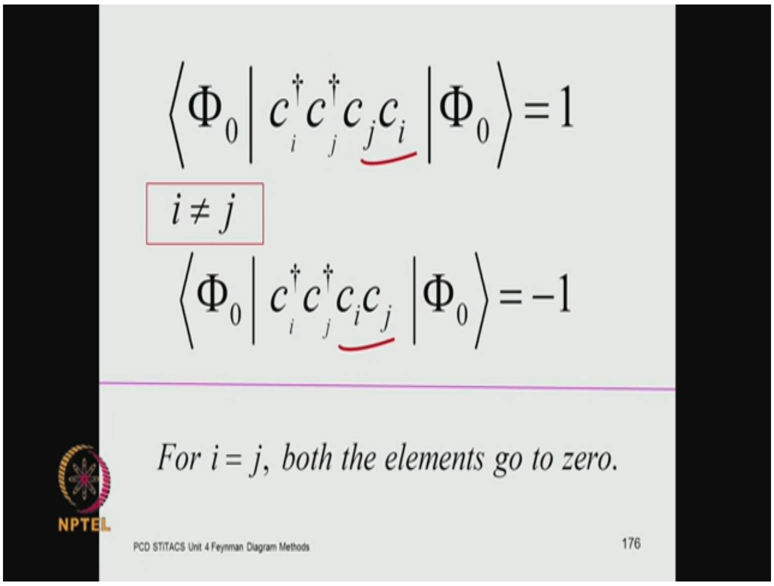

So, they contribute either +1 or -1 right because this will contribute a +1 sign right. Because the projection of cj ci on Phi 0 will be exactly it will be equal to unity when you take the scalar projection when you take the shadow this is nothing but the adjoint of this vector on if you take if you consider a mirror image over here then you have got a vector to the right of the central line and a vector to the left of the central line.

And they are just adjoints of each other, so it is like the norm which is 1. So, you get +1 from the Coulomb term and a -1 from the exchange term of course when i = j both the elements go to 0 right. So, these are the contributions from the Coulomb and exchange terms.

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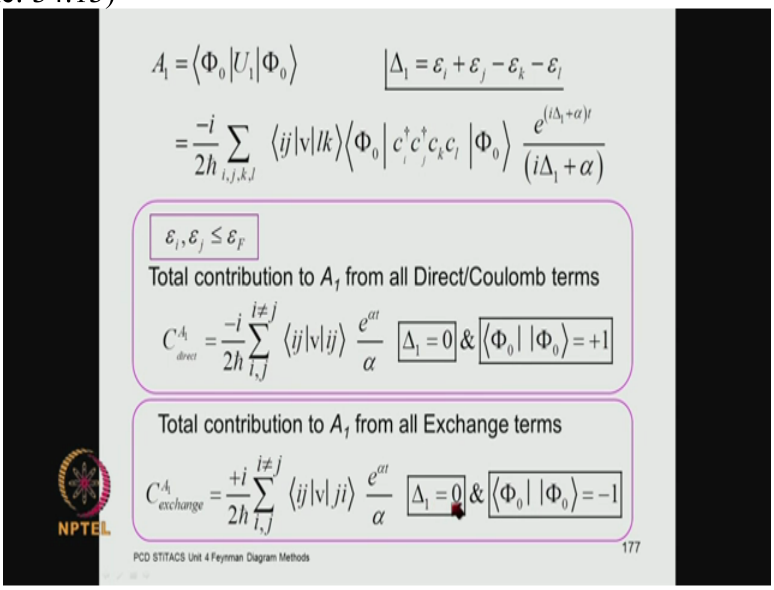

And let us evaluate their net contributions. So, we introduced this matrix elements of the time evolution operator which we indicated by the terms A's. And then you of course have to consider the contributions coming from the Coulomb term. So, this are contribution will be 1 from here delta 1 is just this energy sum and difference which is epsilon i + epsilon j because these two are creation operators and then you have ck and cl.

So, these two come with a minus sign, so delta 1 is just the energy difference between all of these. And this when k and l are respectively i and j, so delta 1 will go to 0 right because there are only two indices epsilon k = epsilon i and epsilon l = epsilon j. So, you have delta 1 = 0 this matrix element is now +1.

So, this is the net contribution you get to A1 from the direct or the Coulomb terms. And then of course you have to take the contribution from the exchange terms and from the exchange terms you have got a -1 over here delta 1 is again 0.

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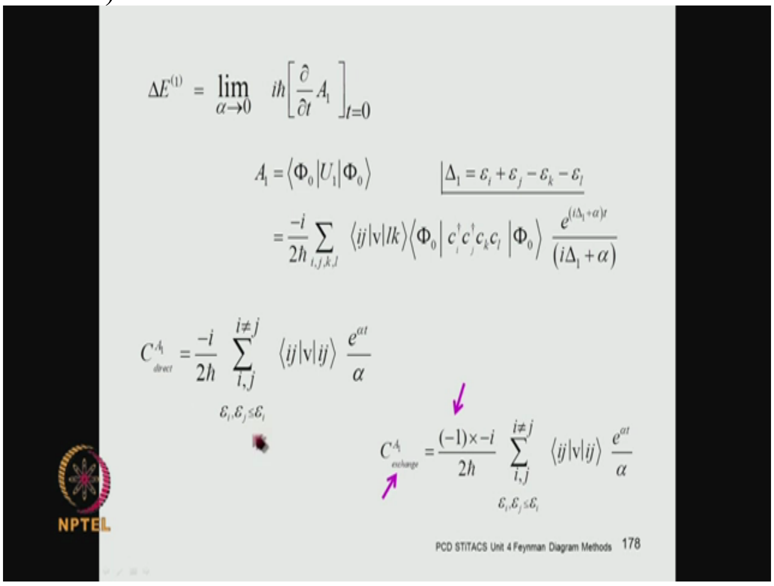

Subsequently you have to take the partial derivative of A1 with respect to time, derivative is to be taken at the value t =0. So, all this we have done in our previous classes. You have to take the derivative at t = 0 and finally take the limit alpha going to 0 because our results cannot really depend on this mathematical model switch which is the adiabatic hypothesis. What it did was to help us get into the interaction picture of the Dirac picture.

And develop a formulation to handle the electron correlations. So, now this is your contribution to A1 and contribution to A1 from the direct term contribution to A1 from the exchange term which comes with a minus sign.

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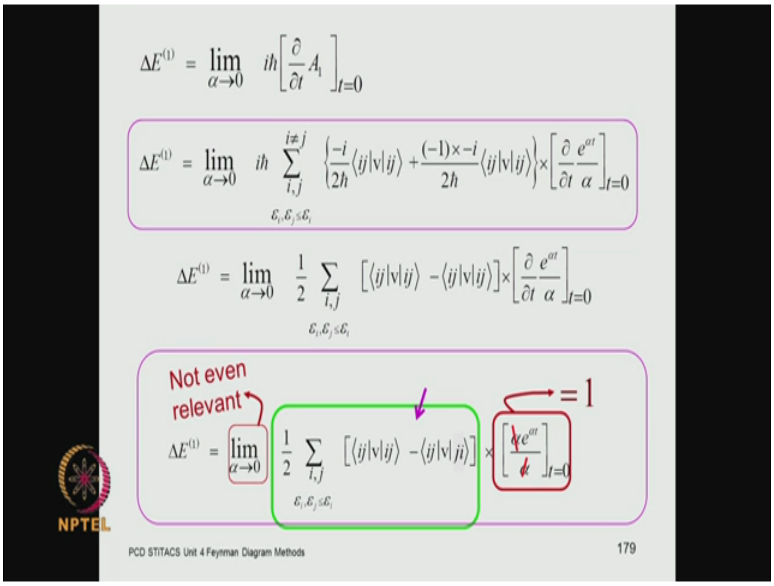

And then you take the derivative with respect to time at t = 0. So, when you take the derivative of this term this is the only time dependent term everything else is independent of time. So, you have to take the time derivative over here and it is just the time derivative del by del t of e to the alpha t which is alpha times e to the alpha t. So, here you have it, so you have alpha times e to the alpha t the alpha in the numerator and denominator will cancel.

And e to the alpha t in the limit at t = 0 goes to unity and the consequence is that this particular may limit alpha going to 0 does not even matter because your result becomes completely independent of alpha this we have discussed earlier that the first order correction for the first order correction alpha really does not matter.

So, what is the correction see what the energy of the non-interacting electrons system and then in first order because of the electron-electron Coulomb interaction given the fact that anti symmetry is taken into account you have got the Coulomb terms and the exchange terms and this is nothing but the Hartree Fock result which we did not only earlier in this course but also in our earlier course.

Essential results here is that alpha going to 0 this limit does not matter in this case and this is a result of the Hartree Fock theory all it is doing is taking into account the anti symmetry of the wave functions. And the Coulomb correlations really are yet to be taken into account and they will come from second and higher order corrections to the free electron system. So, this is a result that we have seen earlier not only the Hartree Fock.

If you remember when we did the random phase approximation unit there again we considered certain corrections from first order terms and we found in that was the previous unit, unit 3 and in that unit also we found that when we you carry out the Bohm and Pines kind of treatment what corresponds to first order corrections gives you essentially the same results as the Hartree Fock.

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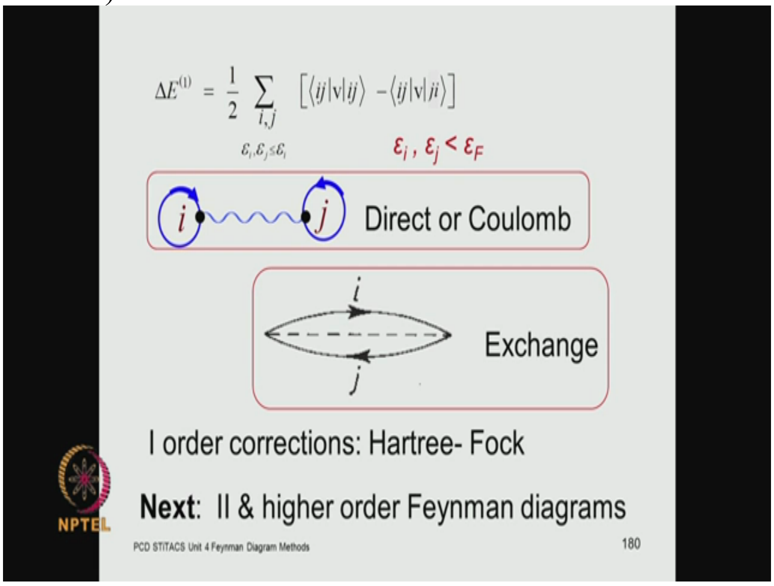

So, everything falls in place and these are the direct and the exchanged terms and essentially you have the Hartree Fock result is represented by a combination of this double bubble and the oyster okay. So, these two diagrams represent the Hartree Fock correction to the free electron gas to the non interacting N electron system okay.

So, these are the first-order diagrams they correspond to the Hartree Fock approximation and now we consider second-order diagrams. So, second and of course higher order.

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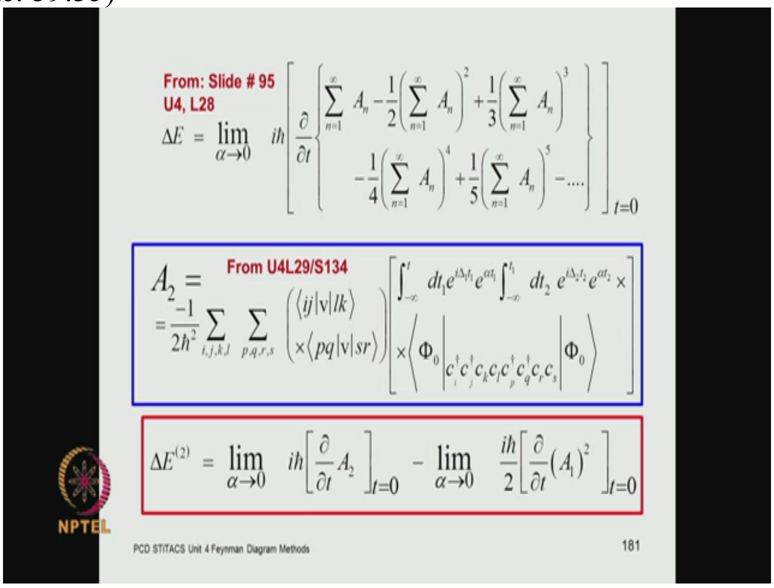

So, we will do it step by step now of course to take into account all the correlations you have infinite order terms and you have a fairly complicated relation to work with. We have developed this formalism in some of our earlier classes. So, we pick up the term corresponding to the second order correction in which the time evolution operator will be dealt with appropriately to second order okay.

And then you will have these two time integrals this one with respect to t1 this one with respect to t2 you will have these delta's twice 1 as delta 1, 1 as delta 2 you will have the e to the alpha t again twice once with the index t1 and the other with the index t2 and we have dealt with these time integrals very carefully. So, that these integrations are carry out within appropriate limits.

Notice that the limit of integration for t2 is from minus infinity to t1 but then t1 gets integrated from minus infinity to t. So, all of this is nicely taken into account when we use the chronological time operator or we have this alternate formulation of the time evolution operator like the Dyson chronological you know which we have written in two different equivalent ways.

Then in the second order you will have a product of these two integrals. So, there will be two center integrals one is this and the other is this, so one comes with indices i, j, l, k okay. The other comes with indices p, q, s, r and again some of these i, j, l, k and p,q, s, r will happen to be the same or not because each is going to run over all the possible values.

So, i, j, k, l so there is a summation which is a double summation, summation over i, j, l, k now this is actually summation over four indices okay. Each index is a set of four quantum numbers, so there are multiple summations okay. So, what comes as a single index is already a set of four quantum numbers, so all that of course we remember.

But this is the compact way of writing all that but you certainly have to carry all that information at the back of your mind and then the matrix element of the creation and destruction operators in the vacuum state which is here. So, this is the matrix element of the creation and destruction operators in the vacuum Phi 0. And now you have got the ci dagger cj dagger ck cl.

But then you also have the cp dagger cq dagger cr cs. So, now you have got each of these operators four and four okay. Subsequently you evaluate the contribution by taking the partial derivative of A2 with respect to time take the value of the derivative at t = 0 and then take the limit alpha going to 0 this is what gives you one of the two contributions to the second order correction.

The other correction to second order comes from this term and we have worked with both of these terms in our previous classes right. So, you will remember those discussions so you had two terms contributing to the second order corrections. One was coming from A2 and the other from the square of A1.

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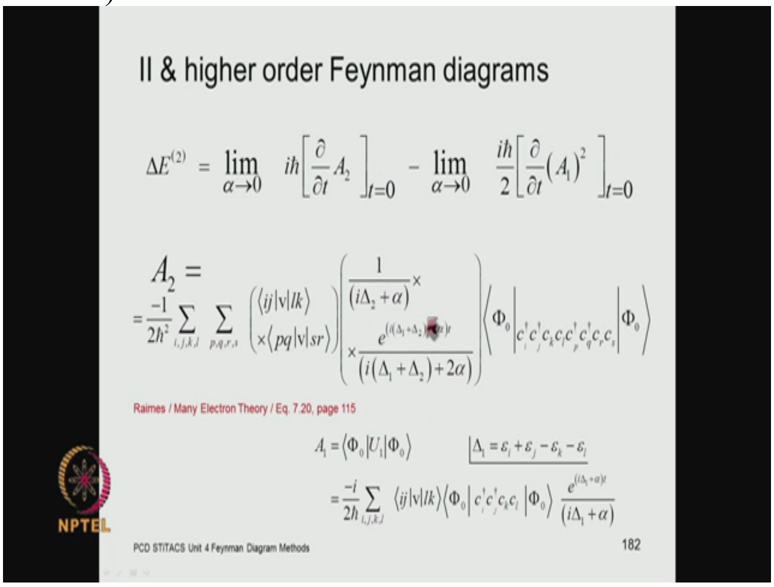

So, both of these terms have to be kept track off, so this is the first term and this is the second and then you take evaluate the time integrals these time integrals we have seen earlier in the context of the first order terms. So, they have been evaluated and we can use those results in determining these time integrals. So, now they can be written by a simple extension of what we did in our previous classes.

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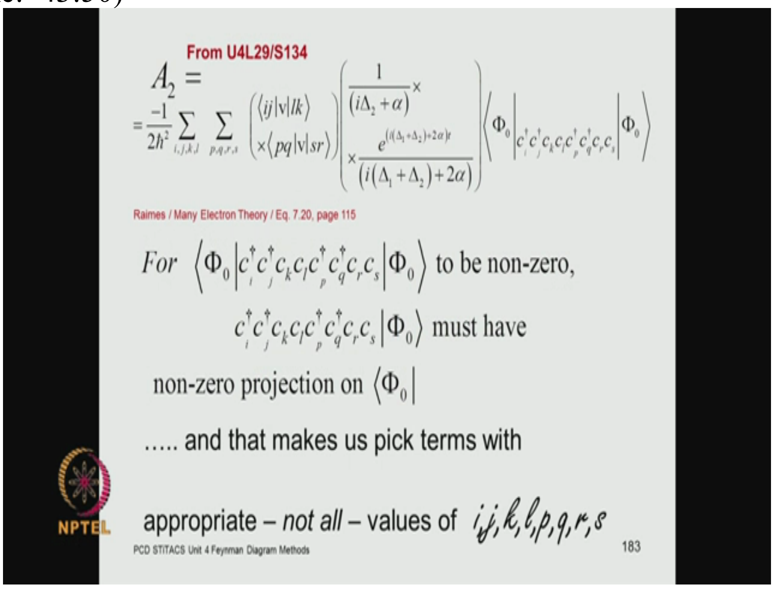

So, let us put all the terms it looks messy but we have done each of these terms carefully and independently in considerable detail in our earlier classes. So, if you do not recognize any of those terms just go back to one of our earlier classes maybe two or three classes prior to this one and you will find a detailed discussion on these terms. Now once again you have to remember that for this to be nonzero.

The result of this operator on Phi 0 must have a non projection on Phi 0 right. And what does it mean that i, j, k, l, p, q, r, s these indices cannot be arbitrary. They take each can case infinite values but they cannot be arbitrary for example if cr and cs are the same you will get 0 contribution.

If two of these creation operators are the same or two of these destruction operators are the same you will get 0 or if you try to destroy a particle which is not there or if you destroy try to destroy a particle from a state which is above the Fermi level when it has not been excited yet in the free electron state then you will get a zero contribution.

So i, j, k,l and p, q, r, s, cannot be arbitrary indices they can only need some chosen sets and not arbitrary now that puts some restrictions and this restriction will manifest as admitting only certain second order diagrams and not any arbitrary diagram okay. Because how these arrows go in and out is just a statement of the creation and destruction of particles and holes okay. So, not all diagrams will contribute to the ground state.

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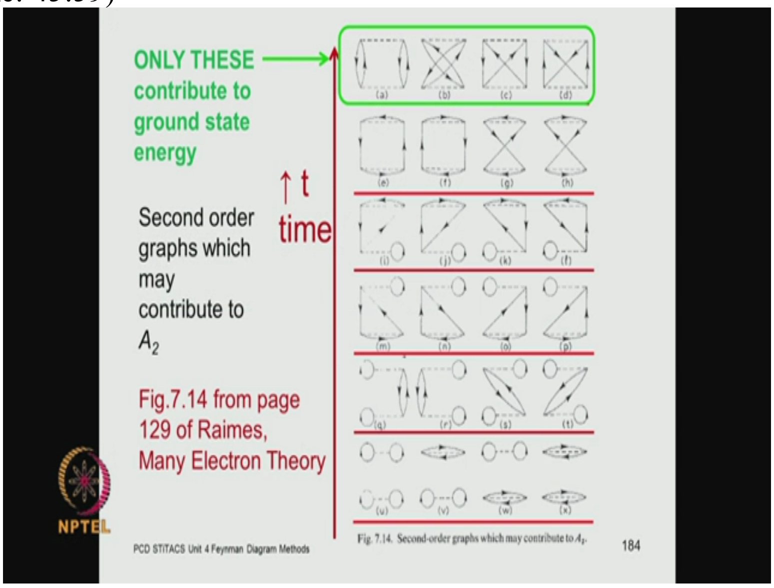

Only some diagrams will and some will not so you can draw a number of second order diagrams okay. When you consider all kinds of possibilities you can get various second order diagrams however not all of them will be possible, so now there are two times that you are considering in second order diagrams, so if you take the lowest block, so what is between the lowest redline and the next maroon line.

So, you have time going from the bottom to the top, so you have time t1 here and this is time t2 okay. So, this is just one set of second order diagrams, this is another set okay, this is another set, this is a fourth set, this is a fifth set. So, there are a number of second order diagrams on this picture.

And they come as you can very easily imagine and I think it is too much work and too much time to discuss all the terms which contribute to these but I think you now have essentially the idea. Because depending on what values the i, j, k,l and p, q, r, s take you can have you can certainly draw diagrams of all kinds.

But not all of them will contribute to the correction to the ground state energy in the second order. What will only contribute are the diagrams which are in the top row in this okay. So, these are second order diagrams there is a time t1 here and this is the time t2 here okay. So, this is a time t1 at the lower edge and this is the upper edge.

So, these are the two t1 and t2 time parameters and only these contribute to second order diagrams. You have many of other pictures but they do not contribute to the term which is going into the term A2 which is what we will have to plug in to get the second order corrections.

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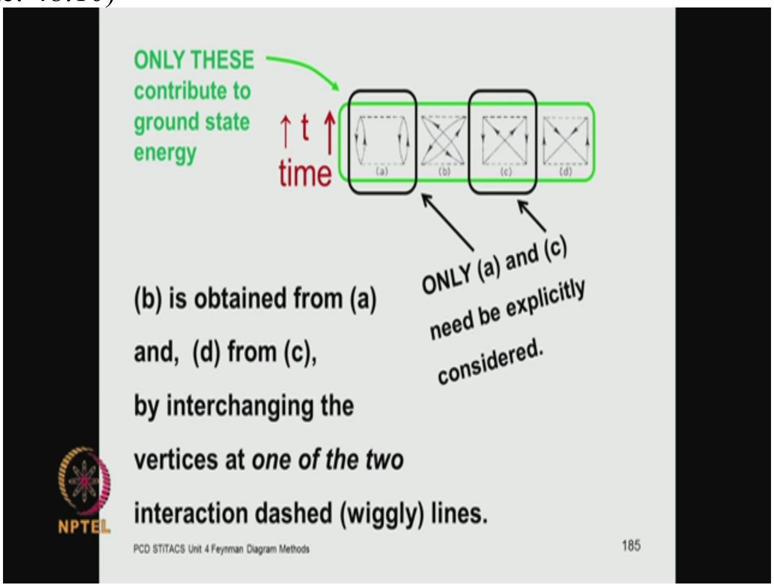

So these are the only ones to be considered and that offers a lot of simplification not only that it turns out that only these two a and c you have four diagrams over there a b c and d only a and c need to be explicitly considered. So, out of these four only a and c need to be explicitly considered because you can get b and d from the previous ones all you do is to interchange the vertices and at one of the two interactions.

If you just do that you get the diagrams b and d, so they come simply by swapping the vertices as one of the two interactions dash line okay. So, you do not have a lot of diagrams to work with and essentially you have to work with only the diagrams a and c.

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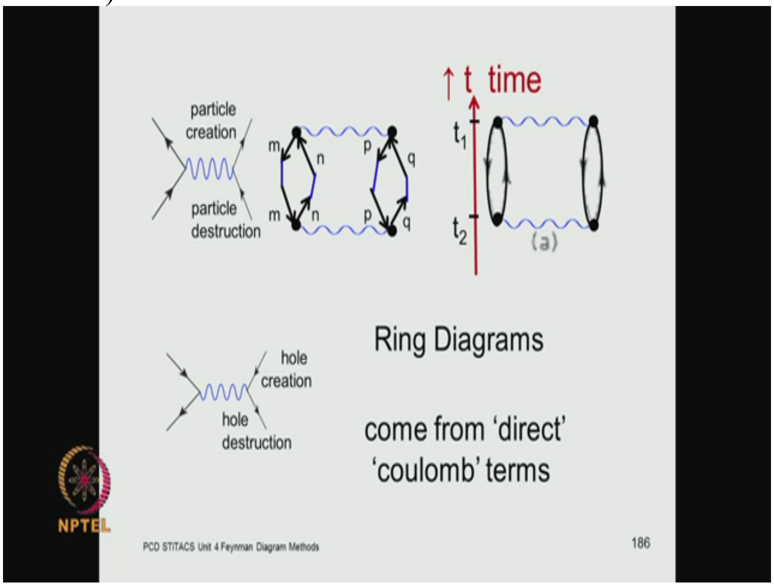

So, let us get the diagrams a and c we will focus our attention on a and c. Now you are just following the same prescription which is; these pictures I have run through every slide to remind us that particles are represented by arrows pointing upward holes by arrows pointing downward particle creation by an arrow pointing upward but out of the vortex and particle destruction by arrows pointing upward but into the vertex.

And a similar convention for the hole operator. So, this is a picture which I keep in the margin just, so that you can always refer back to that. And now consider the time axis going from bottom to the top I mentioned that you had those six different sets of second order diagrams each set refer to one value of time and another value of time. So, I will consider t1 and t2, t1 greater than t2 it does not matter one of which is greater than the other.

So, let us consider the diagrams which matter, so you have t1 and t2 and let us consider a situation in which at each instant of time we have considered first order diagrams okay. So, just think of a first order diagram at time t2 and another first order diagram at time t1 in which the diagram is represented by these arrows and now you know what these arrows are telling you okay.

The arrows pointing upward are particle operators the arrows pointing downward are the hole operators right. If it is an arrow pointing upward and into the vertex it is a particle destruction and if it is an arrow pointing upward and out of the vertex it is a particle creation okay. So, now this is the kind of picture that we are now considering this is a kind of diagram that we are considering at two time intervals.

At two time instants one is t1 the other is t2 but what are these states these days can be anything i, j, k,l can take various different values and we already know that they cannot take arbitrary different values okay they can be only certain value. So, let us consider a situation in which these states are 1 in electron 1 states which is indexed by m which is a set of four quantum numbers okay.

And then this is n so I am just making some choices and I consider those situations in which this is m and n and the indices at the upper time at time t1 are also m and n okay. Likewise on the other vertex I consider pq and I consider the indices at the later time at t1 to be also p and q. Now when you have a diagram of this kind it makes sense to join the m's and the n's okay right.

Because when you join it tells you that the same state same hole state which is destroyed at t1 is the one which is created at the previous time t2 that is the information which is contained in the fact that both of these are represented by the state m and that information is then included in simply joining this. Likewise you join the indices n as well but it now you do the same with the labels p and now again with the label q okay.

What do you get you get a ring diagram okay this is the second order ring diagram okay and it is giving you a particular information about what kind of hole destruction and creation and electron destruction and electron creation essentially it is telling you what kind of correlation which configurations are now being referred to by this diagram.

Because all of these occupations number states they translate to different configurations okay. There is a one-to-one correspondence between an occupation number state and the Slater determinant which you write for a given configuration. So, essentially it amounts to doing a multi configuration Hartree Fock or a multi configuration Dirac Hartree Fock if you are doing relativistic.

So, this is what you get from this particular type of interaction you can consider another example over here let me take it over here. So, these are the ring diagrams which come from the direct interactions which are also referred to as the Coulomb terms.
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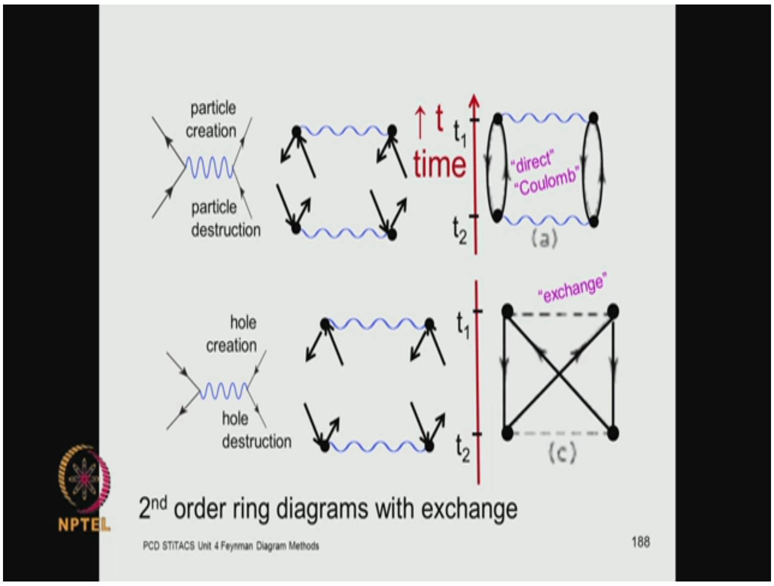

Let us draw another second order diagram, so here again you have got two time interval, two time instants t1 and t2 and here again you have got to first order diagrams to begin with. But now consider the indices to be pm over here and one of the two indices at the top is the same as the one at the bottom p is the same. But the other index is not m now it is n, so it is different from the previous case notice that right.

And then if you go to the other vertex let us have n and q over here and m and q over here. Now what this will suggest to you is that you can connect the m right and you can connect the n right. Because those are the same single particle states or single hole states right and then you can connect the p's okay. So, you have got the p at the top connect to the p at the time t2 and you do the same for the label q.

Now what is the picture that you get because you already know that whether these arrows lean to the left or right really does not matter okay? It is only how they are topologically placed that is the only point of interest in these diagrams. So, the picture that you get instead of drawing this diagram in such a clumsy way you can draw it neatly and essentially what comes out of it is the exchange diagram.

This is the second order exchange diagram okay, now this is the one which corresponds to the same ring diagram as such but this is the exchange part the previous one is the Coulomb term. So, you can get second order direct effects and second order exchange effects and when you do all calculation you are any study. You, if you are taking corrections to second order then you must of course include all the Coulomb terms.
And it is automatic that you also include the exchange terms. So, sometimes you can refer to this as terms with exchange but that goes really without saying because there is no point in

including one type of second order term but not another type of second order term okay. Because all second order corrections should be taken into account on the same footing.

So this term automatically goes in, so this is the exchange term corresponding to the ring diagram. So, these are the second-order diagrams, so you have got the direct or the Coulomb contributions and then you have got the exchange contributions. So, these are the second order direct and exchange terms corresponding to the ring diagram.

You very often in literature you refer to this only as the ring diagram because the default implication is that you will of course take into account the corresponding exchange. So, when you talk about the direct diagrams or the ring diagrams okay the terminology already includes the consideration of the corresponding exchange.

Because nobody going to do a second order Coulomb correction without doing the corresponding exchange correction because after all the statistical correct correlations are the most important ones those are the ones that we first do those are the ones that we discussed in the Hartree Fock approximation, so they are already taken into account.

So, you may or may not explicitly mention the term exchange but it is implied that it is always taken cognizance off okay.
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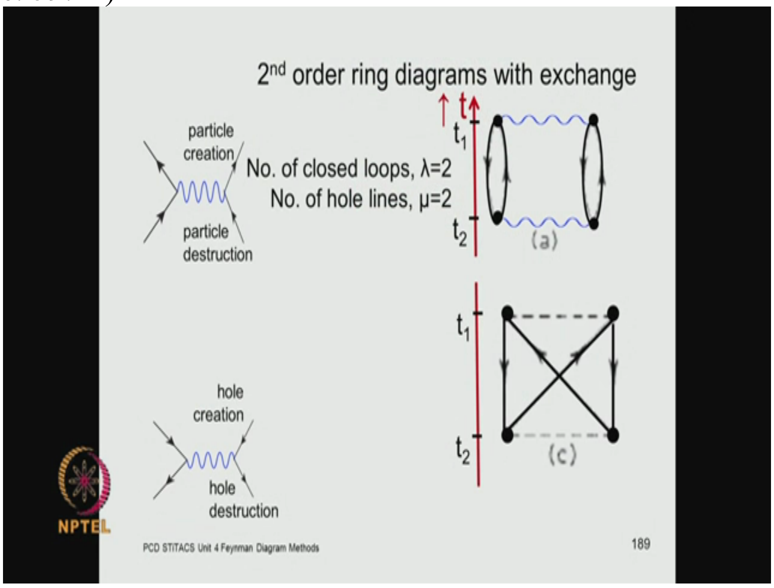

So, these are the second order diagrams and now notice that here you can actually count the number of loops and this is represented by the letter lambda you can choose any letter but I am using the notation in the book by Raimes okay. So, if you look at the number of closed loops you have lambda = 2 and the number of hole lines is also 2.

The number of hole lines which are the arrows pointing downward is 2 there are two arrows pointing downward and there are two closed loops. So, it is now important for the analysis of higher order terms it becomes very useful to keep track of how many loops do you have and how many hole lines do you have.

Now if you look at the Coulomb term which is the one at the top lambda = 2 and mu = 2 however if you look at this diagram over here the closed loop and the hole lines. So, here again you have lambda = 1 and mu = 2 okay. So, you have got two hole lines one loop over here but they come with opposite signs.

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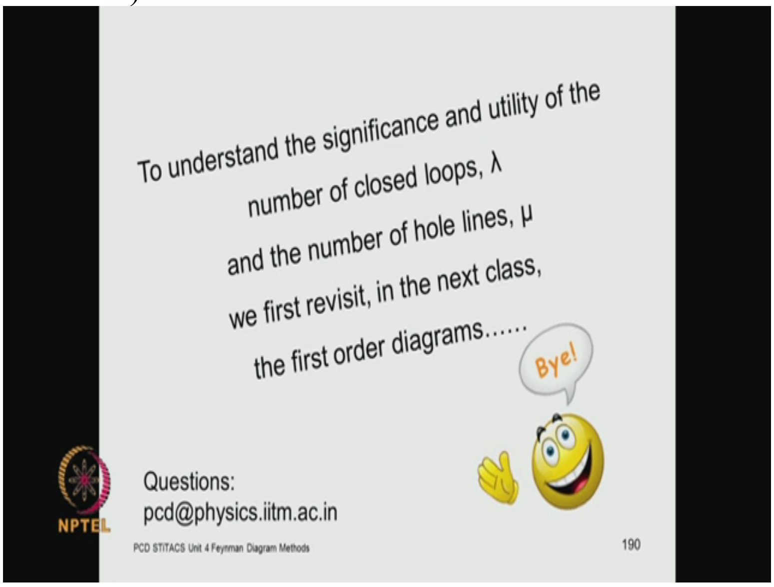

So, to understand how these are used we will go back a little bit to the first order terms and then discuss how these are used so that is something that I will do in the next class if there is any question I will be happy to take yes Jobin (Question time: 1:00:50-not audible) so you said that pattern b can be obtained from a explicit the diagram b where it is sir you so what does that mean so you pinch this vertex here okay.

If this were made of strings you pinch it over here and drag it to this point and likewise you pinch this and drag it over here when you do that you will get b. So, it is topologically the same so essentially if you just pinch that the combination of that hole and particle interaction line at a given vertex and drag it to the other vertex you get a corresponding equivalent diagram okay. So we will take a short break here.