**Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'**

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**Lecture 30**
**I Order Feynman Diagrams**

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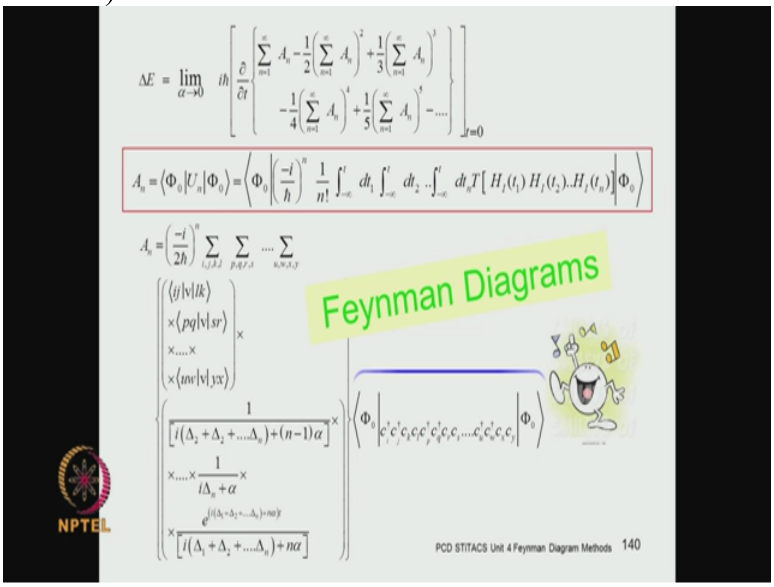


Greetings today we will introduce first order Feynman diagrams and essentially our aim is to handle this correction that we have to make because we could not take into account all the correlations and it is only the unperturbed part of the Hamiltonian that we could handle. The corrections are of infinite order first order, second order and so on.

And the in nth order term has got these n times appearance of the interaction term which is to be taken into account. So, you have got the chronological operators here and this is the difficult term we got a general expression for the nth order term. And we found that it really, really has an extremely complicated pattern. So, we did we got this by generalizing the first; we got the first order term explicitly.

We got the second order term explicitly and then we generalize this to the nth order term and it has got a number of these two central integrals number of these terms which come from integration over time and then we have a lot of this creation and annihilation of electrons which are responsible for the configuration interactions.

And these are the ones we generate the electron correlations. So, these are the terms which we are having difficulty in addressing and to represent these terms the diagrams known as the Feynman diagrams they provide us with a very convenient and a very powerful tool which is what we will discuss today.

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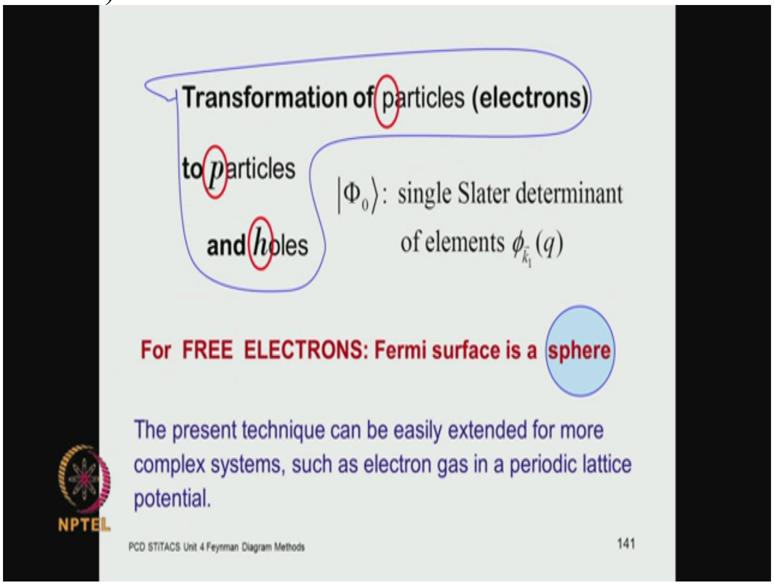


So, the first thing we will do is carry out the transformation from particles which are our electrons we are in atomic physics we are basically concerned with the electron number of it is an N electron problem to what we will call as particles and holes but written differently and they mean different things. So, this is particles as we normally write it which are the electrons these are the normal particles that we work with.

And then we will deal with these particles which are written with a slanted *p* okay. So, this first letter p is written in italics, so the font is different. And then there are these holes that we will be talking about and the *h* is also written in italics, so this is a font change which I want you to notice. I am following a notation which you will find in the book by Raimes which we have been referring to for this discussion okay.

So, the first thing we will do is to carry out the transformation of particles to these slanted *p* particles and the slanted *h* holes. And this font is what I want you to notice this is the upright p and this is a slanted *p* or in italicized *p* and this is an italicized *h*. Now our basic unperturbed Hamiltonian has got an Eigen state Phi 0 which is known which is an N particle Slater determinant made up of these unperturbed single particle wave functions.

And this is the part of the problem that has been solved and we have the solution completely with us now the unperturbed part is just the H0 that has no electron-electron interaction. So, they are like free electrons okay and this is a free electron system and it will typically occupy the lowest possible states. Everything will be filled up to the Fermi level and in the momentum space you will have the Fermi surface which will be spherical okay.

So, that is the picture you have for a free electron gas. Now we can very easily extend this to more complex systems like when the electrons are in a molecule in some other symmetry or in a periodic potential as in a solid okay in bulk matter. And we can extend the same techniques to other N electron systems very comfortably using essentially the foundations that we are laying down over here.

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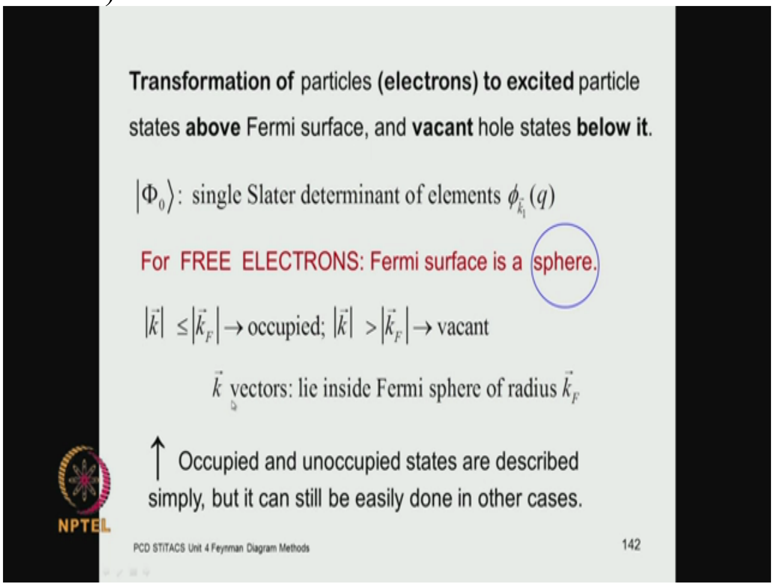


So the first thing we do is to transform from particles electrons to excited particle states above the Fermi surface and vacant hole states below it. So, let me explain what I mean by this. So, up to the Fermi level, so if the Fermi level momentum is indicated by kf then all the momentum states with a modulus of k which is less than or equal to kf will be occupied and everything above it is vacant for a free electron gas in the lowest ground state okay.

So that is the usual picture that we have. Now these are the wave vectors which whose magnitudes we are considering here. So, the momentum space is actually a three dimensional space it is the reciprocal space actually not the real three dimensional physical space but the inverse which is the momentum space. And essentially what we have done is to classify the occupied states up to the Fermi level and unoccupied states above the Fermi level.

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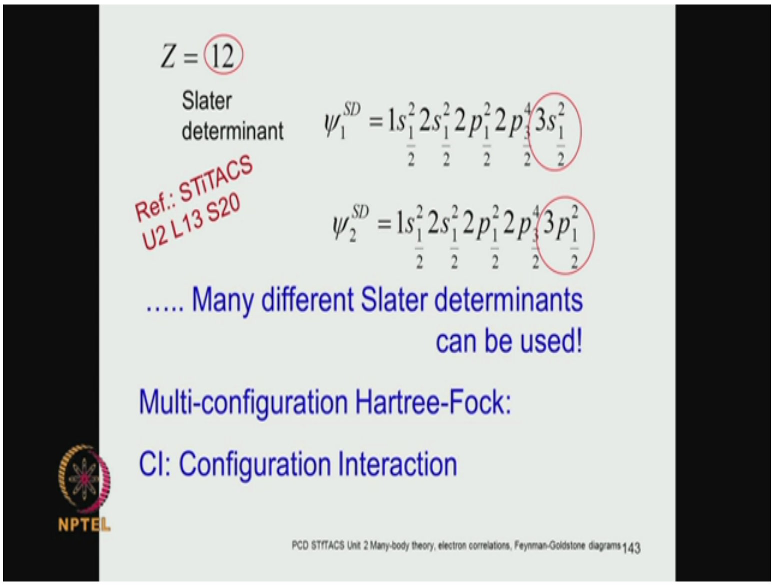


And I would like to remind you a small discussion we had from this course in unit 2 and I will refer you to the 13 lecture slide number 20 which all of you will have a reference to and I gave the example of configuration interactions in this lecture. And that is the residual problem which we had not solved in the Hartree Fock or Dirac Fock formalism. But which required the treatment of electron Coulomb correlations.

So, what was that problem let me remind you what it was and I gave you the example of atomic magnesia okay. Atomic magnesium has got 12 electrons and the normal configuration is 1s2 2s2 2p6 2 into p 1 half + 4 into 2p 3 half in the relativistic formulation and then 2 in the 3s2.

So, this is the normal singlet s naught state which we consider as the Hartree Fock ground state or the Dirac Fock Hartree Fock ground state for ground state of the magnesium atom. What I had brought to your notice was that in this in writing a single Slater determinant we have ignored certain correlations which are the Coulomb correlation.

So, the statistical correlations the exchange Fermi core, exchange correlations were taken into account but the Coulomb correlations were not taken into account in this. And what do the Coulomb correlations do they tell you that this Slater determinants may not be the only component of the N electron system.

There may be additional components and one of those which we considered at that time was the promotion of these two electrons in the 3s state to the 3p state. So, this is one possible additional configuration what have we changed we have changed occupation numbers. So, 3s which was occupied in configuration 1 is now vacant in configuration 2.

And 3p which was vacant in configuration 1 is now occupied in the configuration number 2. So, there are two different Slater determinants Psi1 and Psi2 and both are possible Eigen states of the N electron system which you should now express as a linear superposition of Psi1 and Psi2 what is generating this possibility.

The configuration interaction which was ignored in the Dirac Hartree Fock okay, so that configuration interaction which is coming from what we call it the Coulomb correlation, so this is what we want to address. So, you can in fact have not just these two Slater determinants but even with many more okay.

And the complete set of bases if it were to be used you might actually need infinite only, although only some of them will come with some weight factors with some coefficients which are significant. You may not really have to deal with more than maybe half a dozen Slater determinants.

But sometimes you have to deal with even more maybe 10, 20 and sometimes you do calculations with as many as 50 or 100 Slater determinants. So, depending on what kind of configuration interaction you are really working with. So, the important thing is that what the correlations do is to generate a different occupation number state.

And there is a one-to-one correspondence between how you write a Slater determinant and how you write the occupation numbers which is why the second quantized notation comes in handy. Because the Eigen state of the occupation number gives you the number of occupied states and when you change this occupancy you can represent this change using creation and annihilation operators.

So, this is what you are looking at on this slide you have got two determinants and effectively you can represent this by saying that okay you have destroyed the two electrons in the 2's states. And you have created two electrons in the 3p state because that is exactly what you have done which is to change the configuration.

And this is what you would do if you were to do a multi configuration Hartree Fock or a multi configurational Dirac Hartree Fock are effectively some sort of configuration interaction resulting from correlations. So, let us work with this picture essentially we are now addressing the many-body correlations.

We are going beyond the Hartree Fock going beyond the Dirac Hartree Fock using second quantized methods and the Feynman diagram methods. So, everything will come in together in this discussion.

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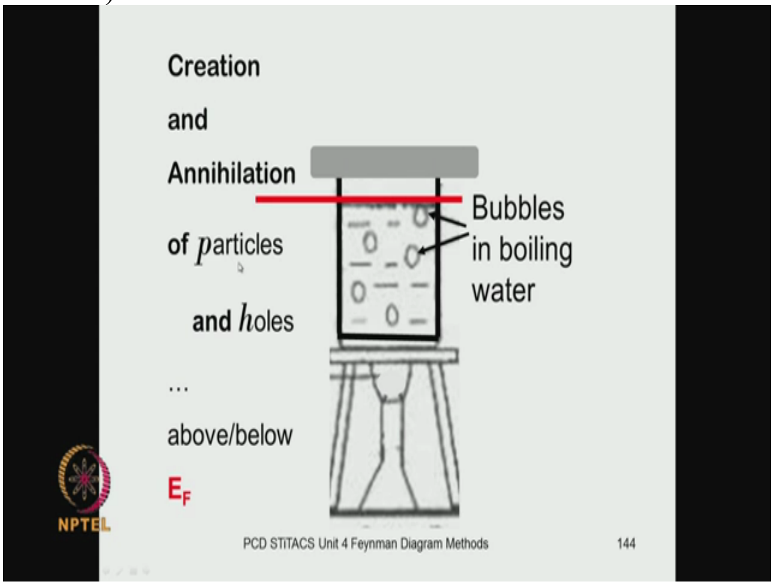


And you can think about this just as if you are boiling water, so you if you have water in a beaker and you heat up okay, now what is going to happen is that as water turns into steam some of the molecules of water will escape from the surface they will go into the atmosphere right. Now if you put a lid on this okay, they are not going to escape they are going to be there. And we need this because we are not really in atomic physics.

We are not creating or destroying particles with the real sense of going above the energies is where particle creation and destruction is possible we are only changing the occupation numbers of various one electron states okay. So, the total number of electrons is conserved they may go from below the Fermi level to above the Fermi level but then they are trapped, the total number of electrons is conserved in the processes that we are working with.

So, that is a picture I would like to bring to your mind and what you have is some sort of a Fermi level and then electrons you know go from below the Fermi level to above the Fermi level it is like a molecule of water which jumps out from below the surface of the water to the region above it. But then it leaves some sort of a cavity okay that cavity is like a hole okay.

But at the same time because this molecule which has gone above this level has not really escaped into some infinite space it is trapped over there it could in principle go back into the beaker and become a part of the rest of the bulk water right. And when it does that whatever cavity was there will now be filled by this molecule of water which has jumped from above the surface level into the cavity.

Now that is the kind of thing which changes in occupation numbers are resulting it. It is a very similar situation because when you have two electrons in the three s state of magnesium, so you have got the 1s2 2s2 2p6 3s2 configuration of electrons these two electrons go into the 3p2 state but then they can also go back into this. So, you have got these two electron processes, two electron two hole processes.

And these are coming because of some interaction or some something that you are left out of the Dirac Hartree Fock formalism. Because Dirac Hartree Fock would give you only a single Slater determinant but now you need at least two maybe more at least several maybe even infinite okay. So, this is the picture that you have in the consideration of the creation and annihilation of particles and holes.

And these particles which are above the Fermi level are the ones that we will write with a slanted $p$ with italics $p$ and then the cavities below the Fermi level are what you will write with a slanted $h$. Now what this allows you to do is whatever other electron states single particle electron states are there and which are not involved in any change in a particular particle hole excitation.

You do not have to worry about them you can just focus on those which are really involved in the change in the configuration. So, if you go back to the previous slide like the occupancy of 1s remains the same in both the configurations the occupancy of 2s remains the same in both the configurations. So is the occupancy of 2$p$ half + 2 $p$3 half. So, these are not changing when you go from Slater determinant 1 to the Slater determinant 2.

And you can focus attention on the occupation only of those single particle states which are affected by the configuration interaction. So, that offers you a lot of simplification because when you are working with an N electron system the less you have to deal with the better it is. So, that is the advantage you get in carry on carrying out this transformation to these particles with a slanted $p$.

Because these are then the electrons above the Fermi level okay and these are the vacant states below the Fermi level which are the whole state. So, this is our picture of particles and holes above and below the Fermi level okay.
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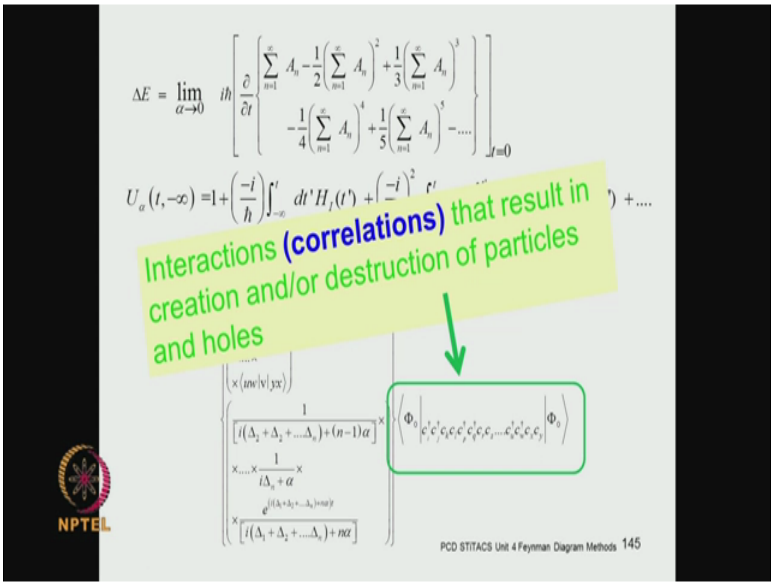


So, we will work with this and what is responsible for this particle hole picture why are we having these cavities which we did not have in the single Slater determinant. The reason we have them is because there are correlations which we had left out in the Dirac Hartree Fock and these are called the correlations which are causing the changes in the occupation numbers and how do they appear in our expressions for the energy correction.

Due to the correlations here it is this is the delta E and it has got all of these terms and the change in the occupation numbers is coming from the result of these creation and destruction operators. These are the ones which operate now on them what we can call as a vacuum state okay. And in this you can either create particles or destroy particles.

And this is the term which is really a very complicated thing the rest of the things we can handle using some techniques. So, these are the time integrals we know how to manage them right. But this is where you have the challenge and to represent these terms the Feynman diagrams come in very handy.

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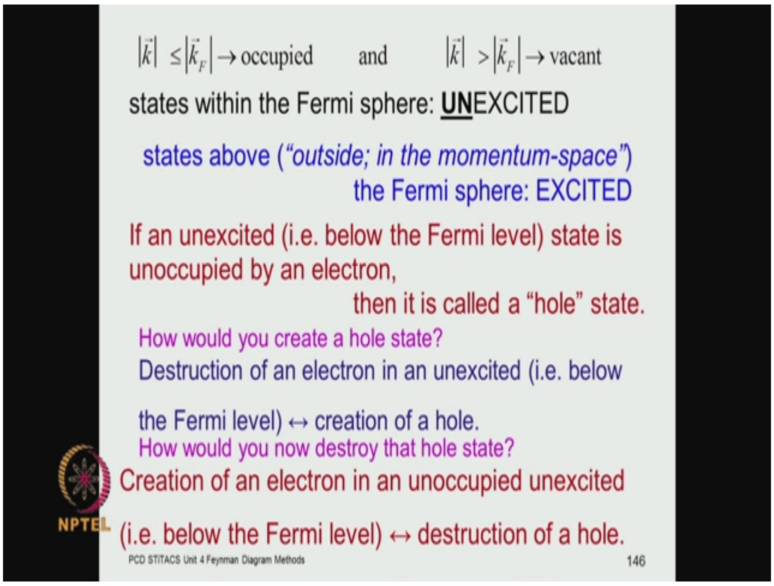


So, we will work with this now, so here again we have the occupied states up to the Fermi level. Above the Fermi level you have got vacant states and states which are within the Fermi sphere these are the normally unexcited state. These are like what you will say are the particles which have occupied the lowest possible states and these are therefore the ground states or the unexcited states.

So, that is the reason I have underlined the unpart of the unexcited. So these are the unexcited states then there are states above the Fermi level now above actually means outside because the Fermi level has got three dimensions and there is nothing like above and below there are all sides although this is in the reciprocal momentum space. So, these are outside the Fermi sphere and these are the excited states.

So, we classify the states between unoccupied states and occupied states which are by this we mean which are normally unoccupied and normally occupied okay. So, that is our reference point. So, now if you have an unexcited state now where do these unexcited states reside they are below the Fermi level and if this unexcited state is vacant if it is unoccupied if it is vacant then it is referred to as a hole state okay.

So, the terminology is almost obvious but it is good to have our definitions in place okay. So this is a hole state and how would you generate a hole state, you will need to generate a hole state, you can generate a hole state by destroying an electron in what is a normally occupied state right. So, you will have to destroy an electron okay you will have annihilate, so you will need a particle destruction operator there.

At that particle destruction operator when it operates on a state below the Fermi level you could create a hole. So, the creation of a hole is effectively the same as destruction of an electron in an unexpired state. Now if you have created a hole state, so it is if you go back to your picture of the boiling water then you have got these cavities okay below the water level and how would you now destroy this cavity.

One of the molecules of water from the top from above the Fermi level will go and fill in this cavity right. So, that is what you will need to do, so the way you can destroy your hole state is by creating an electron in what is normally an unoccupied state okay. So, this would be effectively the same as destruction of a hole but below the Fermi level you will have to create that particle. So, these are the two processes that we will now be working with.

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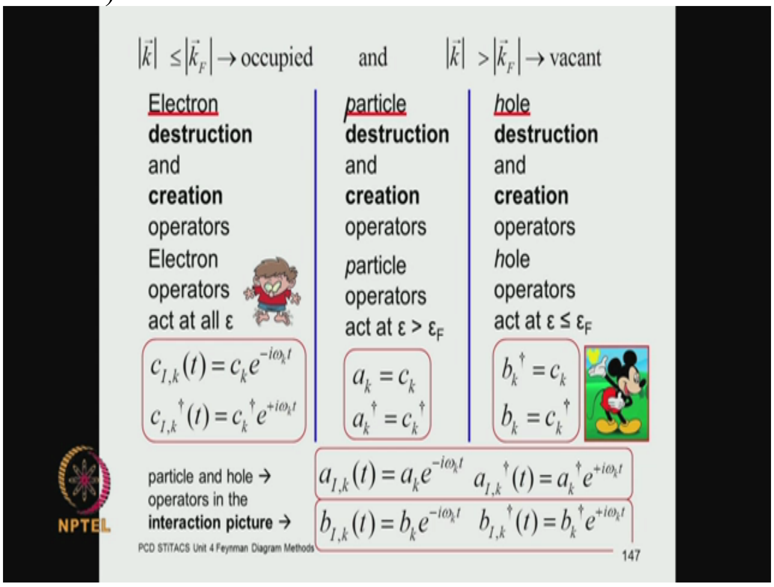


So, you now have the electron destruction and creation operators and these are the operators that we have used okay c ck and ck dagger these are hermitian adjoints of each other ck is the destruction operator in the Schrodinger picture, ck dagger is the creation operator for the kth single particle state in the Schrodinger picture. You can transform it to the interaction picture using this exponential time dependent term okay.

We have worked with this earlier and these are the electron operators, these are the particle operators this is the p that we will write as an upright p these are the normal particles the normal electrons that we have been working with okay. And these states exist above the Fermi level and also below the Fermi level at all energies. So, these are the ck's which are applicable at every possible energy.

But then we carried out transformation to the slanted *p* particles okay. Now where do these slanted *p* particles exist they are only above the Fermi level okay. Those are the ones that we want to focus attention on. So, these are the particle operators with a slanted *p* or p written in italics and these operators would act only above the Fermi level.

And we will write the creation and destruction operators for these particles using the letter a instead of c okay. So, actually ak is the same as ck, ak dagger is the same as ck dagger with the difference that we know that when we are talking about talking about ak and ak dagger. We are talking about the destruction or the creation of an electron above the Fermi level.

Because now our focus with reference to the slanted *p* particles is only on those 1 electron states which are above the Fermi level okay. Now you also have the hole destruction and creation operators and what are these? These are relevant below the Fermi level okay and what it really means is that you can you can create a hole by destroying an electron below the Fermi level.

So, the hole creation is equivalent to a destruction of an electron below the Fermi level and the hole destruction would be the creation of an electron below the Fermi level. It would amount to what in our analogy was a molecule from above the water level to jump back and fill up the cavity. So, that is the picture we have with us. So it is a fairly straightforward picture.

But you here after it will be more convenient to work with the operators a and b rather than with c you are doing the same creation and destruction but you are interpreting it in terms of only those 1 electron states which are directly relevant and then you can forget about everything else which remains unaffected in a particular configuration interaction okay.

So, here you have got these creation and destruction operators for the particle operators above the Fermi level and for the hole operators below the Fermi level. You can write these corresponding operators in the interaction picture okay. And you can write the ai dagger the destruction operator, the particle destruction operator.

And the particle creation operator ai dagger and here you have got the whole destruction and the whole creation over here right. So, these are the particle and hole creation destruction operators in the Schrodinger picture and you can carry out the transformation to the interaction picture using exactly the same analysis as we did earlier.
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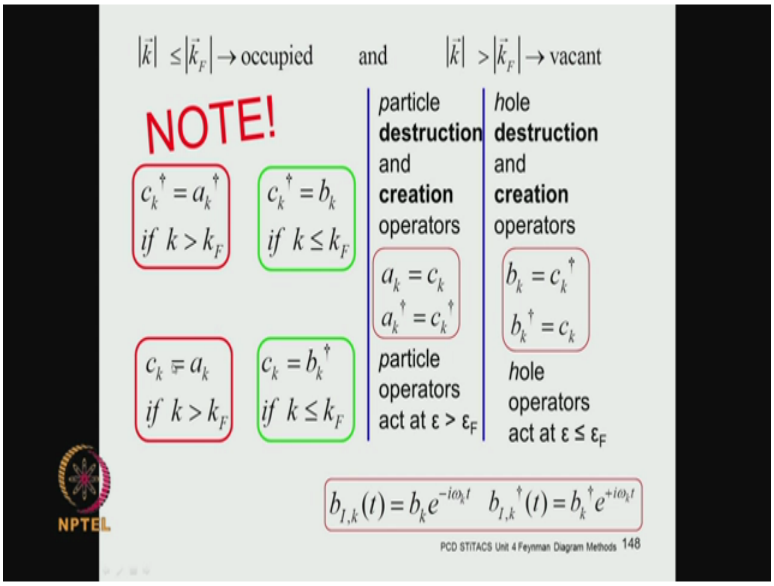


So now there is something that I would like you to note that what was the creation of an electron is represented as ak dagger as long as you are working above the Fermi level. However if you are working below the Fermi level what is what was being referred to as a creation operator would now be referred to as a destruction operator. But it is a destruction of a hole rather than creation of a particle okay.

So, we will carry out this transformation from the electrons to the slanted *p* particles and the slanted *h* holes. So, what was ck dagger above the Fermi level is written as a creation operator here but over here it is written as a destruction operator b here it was a creation operator a.

So, this is something that you should certainly remember what was a destruction operator above the Fermi level is the destruction operator above the Fermi level with the letter a but what was a destruction operator below the Fermi level is now written as a creation operator but the letter now is b rather than a or c okay. So, that is the picture we have.

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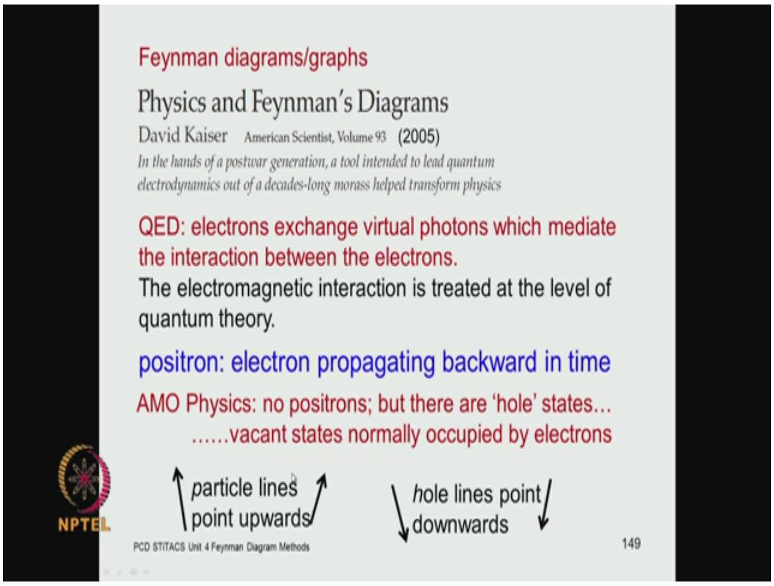

Now these Feynman diagrams they were introduced by Richard Feynman in 1948 and this is a very nice article which I would like to refer you to an article by David Kaiser an American scientist in the year 2005 you will enjoy reading this article and he points out in this article that in the hands of a post war generation of quantum theorists.

This was a very powerful tool which was intended to lead quantum electro dynamics out of decades long morass helped transform physics. Because it really became such a powerful tool that many problems which could not be done until then could be addressed because of the introduction of the diagrammatic techniques which were basically introduced by Feynman to address some problems in quantum electro dynamics.

In which the electromagnetic interaction itself is treated at the level of quantum theory and what the interaction between electrons is perceived as an exchange of a virtual photon which predates the interaction between the two electrons. So, that was a picture in QED, now what was also involved was the particle, was the positron antiparticle and it was represented as an electron propagating backward in time.

But in atomic physics which is our interest in this course we really do not work with you know high energies, so high energies that you create or destroy you know there is a positron electron annihilation or the creation of that because you will have to go well above million electron volts right. So, I think the the rest mass is about 0.5 mev 0.51 or something.

And then if you want to create an electron-positron pair you have to go well above 1 million electron volts but in atomic physics you are dealing with you know the atomic spectra and they are in the domain of a few electron volts or hundreds of electron volts thousands of electron volts or if you go to deeper inner shell processes you know several tens of thousands of electron volts but you do not get into the mev range in atomic physics.

So, you are really not dealing with positrons but what you have is what you do have in atomic physics which we just discussed were these vacant states below the Fermi level these are the cavities. And you do not have these anti particles, you do not have the positrons but we do have these hole states.

And which is why the techniques which were developed in particle physics and in quantum electrodynamics come in very handy even in atomic molecular and optical physics and these are the advantages that we will fully exploit. So what we will do in our representation of Feynman diagrams to express the configuration interaction in the atomic molecular domain is to represent particles by lines which are pointed upwards okay.

So, this is the particle with a slanted $p$ and all of these particles in our pictures in our diagrams will be represented by arrows which are pointed upwards there will also be these cavities which are the hole states which are the vacant states. These are the vacant states vacant in what are normally occupied okay.

So, there are vacant states in the excited states also like in the for a hydrogen atom in the ground state that 10P state is of course a vacant state right. But that is not our reference here what is normally occupied if that turns out to be vacant like the 3's estates in magnesium in the example that we just refer to that, that is normally occupied.

But when you go to the second configuration the seconds Slater determinant this state becomes unoccupied in the normally, in the normal Slater determinant. So, you have got the hole state and these hole states are represented by arrows which are pointed downwards. So, this is our first you know;

So, that we have to set up certain conventions how are you going to represent the particle states. And how are you going to represent the hole state. So, this is our prescription for particle states and for hole states.
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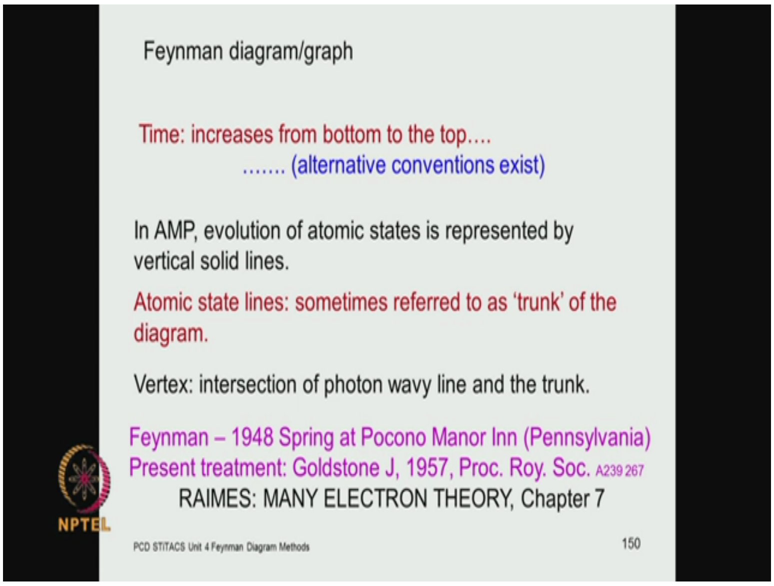


And now with reference to this we will now develop the diagrams and we will have the time axis in our convention going from bottom to the top. So, in the diagrams that we will draw the time axis will go from bottom to the top. Now this is by no means a standard convention you can have other conventions, you can have the time flowing from left to right if you like or from right to left or from some diagonal to some other diagonals.

So, you can have any convention that you like there is nothing very secret about it. But you need to follow some convention and stick to it but if you see some other Feynman diagrams in which some other convention is used usually it is either from bottom to the top which is the one that we use or else you have time going from left to right.

So at the most you may have to rotate our diagram through 90 degrees to correspond to the diagrams that you may see in some other literature. So, you have in atomic physics the system evolution will be represented by vertical lines these will be vertical solid lines and these are sometimes called as the trunk of the diagram. So, that is just a nomenclature which is sometimes used.

And then you will also be talking about vertices and the vertex represents where the photon wavy line because photon is the mediator between two electrons. So, that is a virtual photon which is exchanged between two electrons resulting in the electron-electron interaction. So, this vertex will be the intersection of a photon line which is normally indicated as a wiggle as a wavy line okay or sometimes as a dashed line.

So, you can again use different conventions we will use the wiggly line and then it is the intersection of the photon wiggle wiggly line with the trunk which are the atomic state lines.

So, these are the conventions and this was introduced by Feynman in when he was at the Pocono Manor Inn these it is a lovely mountain range in the state of Pennsylvania.

And we will follow the notation and the diagrams as discussed in the book by Raimes many electron theory in chapter 7 okay. So, you can refer to this source for further reading.
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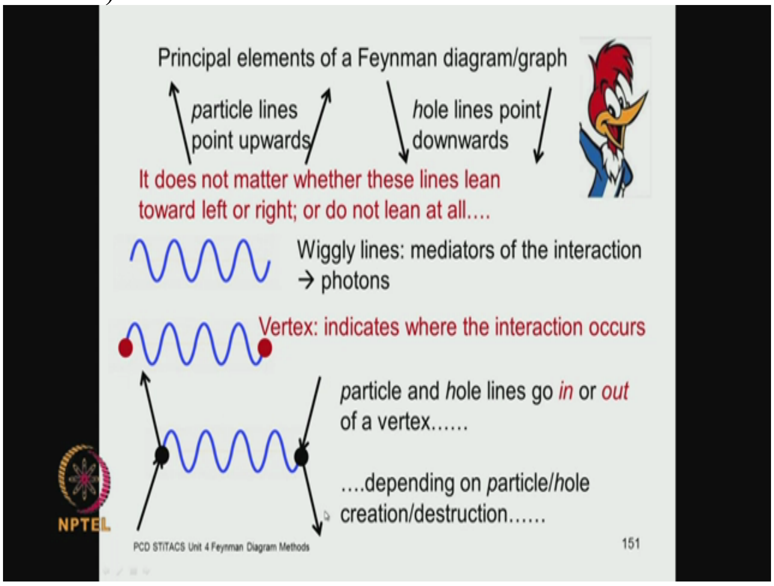


So what are the principal elements of the Feynman diagrams first of all you have got the particle lines which are pointed, arrows pointed upwards. Then you have got the hole line which are arrows pointed downward okay. Then it really does not matter if these arrows are leaning either to the left or to the right or they are just up right okay.

There is no politics over your means moving to you know you have these people who have leftward tendency or rightward tendency right of center and left of times center, so over here it really does not matter. If you have an arrow pointing up or down that is all that matters it does not matter whether it is leaning to the left or leaning to the right. So, that is completely irrelevant in our diagrammatic representation.

Then you have these wiggly lines which are sometimes as I mentioned also drawn like dashed lines or dotted lines, so you can have different conventions for that. We will be using the wiggly lines, so these represent the mediators you know this will correspond to the photon exchange between the two electrons.

And then you will have these word choices so you will have what a vertex here and vertex here. And this is where the wiggle meets the atomic state lines okay that is the intersection of the photon wiggle and the atomic state lines. So, these are the principal elements and the diagrams are made up of these elements.

So, this is the kind of diagram that you are going to see you will have arrows pointing up which you know our particle states you have arrows pointing down which you know our hole states okay. And then they either go into the vertex as this arrow or they go out of the vertex like this arrow okay.

Likewise the whole states also go into the vertex or out of the vertex and whether they go in or out depends again on some conventions which are defined for particles and holes. And the particles and holes that we are talking about are the holes, hole states which we are going to represent which we are going to operate upon by the operators b and b daggers.
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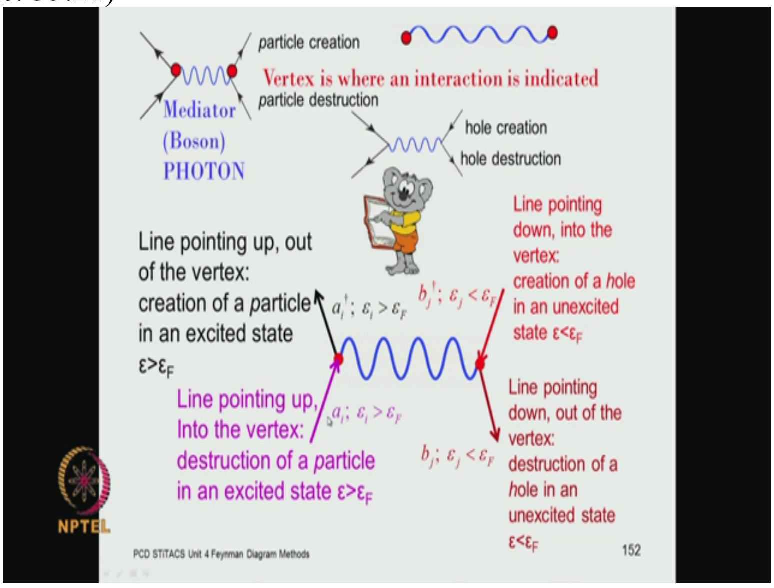


So, those are the hole destruction and creation operators b and b dagger and the particle creation and destruction operators will be a dagger and a okay. So, you have got the whole creation represented by an arrow pointed downward which goes into the vertex okay. So, that is the convention that you will use.

So, you have the mediator which is the wiggle and if you look at these pictures then if you have a line pointed up out of the vertex then you have you are talking about the creation of a particle which you will represent by the result of an operation by ai dagger because you are generating their particle you are creating a particle in the state i if the energy of the ith state is above the Fermi level okay.

So, there is a lot of referencing to be done. So, you are referencing to the Fermi level you are categorizing your single particle states by those which are above or below the Fermi level. And those states which are above the Fermi level are the slanted *p* particles and if you are creating a particle in the state.

If you are creating an electron, if you are boiling out, boiling off a molecule of water from the container into a space which is above the level of the water in the example that we worked with. Then this will be represented by a line pointing up because it is a particle state by an arrow which is coming out of the vertex because it corresponds to a creation of a particle above the Fermi level okay.

So, that is the convention you are going to use likewise if you have an arrow pointing up you know it is a particle state but if it is getting into the vertex it is the destruction of a particle. So, it will correspond to a destruction of a particle in the ith state which is above the Fermi level okay. Because operators which operate above the Fermi level are the ai okay, ai is the one which destroys a particle.

So, you are destroying a particle in an excited state, so it is this is what would happen if a molecule from above the water jumps back and fills in to the one of the cavities because then you will be destroying a particle from a state which is occupied in the normally unoccupied space okay of the momentum space. So, then you have the hole states, the hole states are represented by arrows pointing downward.

And if it is an arrow which is going into the vertex you are creating a hole okay. So, you would create a whole state in a single particle state which is below the Fermi level this is what would happen if you boil up one of the molecules from the water beaker. And likewise you could also have the destruction of a hole which is what would happen when the cavity gets filled right.

So, that is represented by a line which is pointed downward but it will be out of the vortex. So, it is important whether it is an arrow pointing upward or downward and it is important whether it gets into the vertex or it gets out of the vortex. And different single particle excitations are represented by these arrows having different meaning and they all refer to particle creation and destruction and nothing else.

And that is exactly what the electron correlation is doing what it is doing is it is generating new configurations and every new configuration is represented by a different occupation number state in the occupation number space. So, we found that there was a one-to-one correspondence between a Slater determinants and how you write the occupation numbers in the occupation number space.

So, a particular choice of writing the occupation numbers as 1 0 0 0 1 1 1 and so on as we did when we dealt with the second quantization methods in unit 2. So, there was a one-to-one correspondence between a Slater determinant and an occupation number state and that is being represented here through the process of;

You know these different Slater determinants is what you can express by writing different occupation numbers represented by these creation and destruction of particles and more simply by writing or by drawing these lovely diagrams which is what makes physics not just beautiful but actually tractable.

And that is the most important part because many problems which could not be dealt with earlier could then be dealt with as we find in this article by David Kaiser that many of these problems could actually be solved because of the introduction of this technique.

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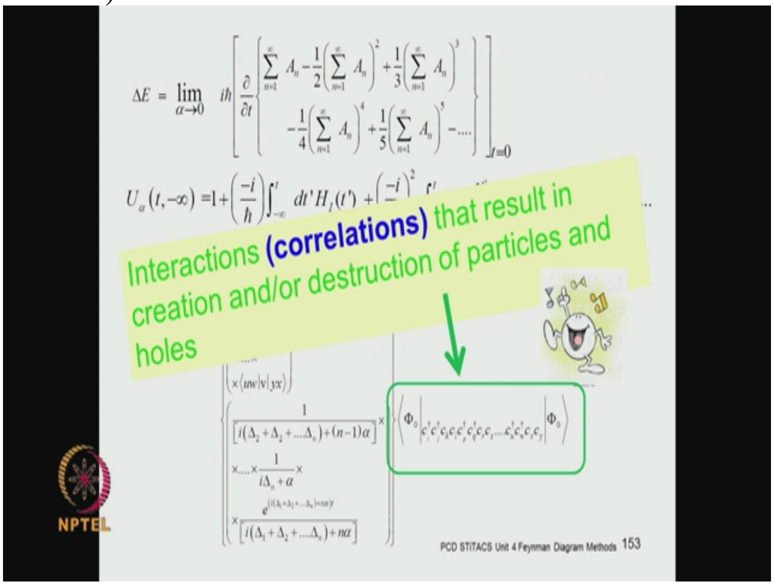


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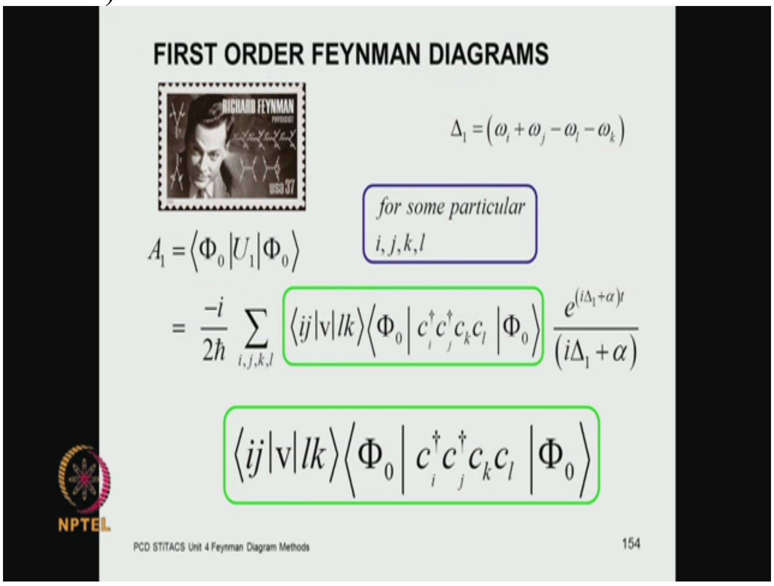


So, it is a very powerful technique and it is in our context it helps us deal with electron correlations in the atomic physics domain. So, these are the, let us acquaint ourselves with some of the first-order diagrams okay. So, we already have an explicit expression for the first-order term right.

We have discussed this term earlier in our previous classes and let us consider a typical term here because here you are destroying two particles one in the state k and one in the state l and you are creating two particles one in the state i and one in the state j and of course you are going to sum over i, j, k, l over everything you have got an infinite sum over there.

But we will deal with you know some particular choice of these four quantum numbers i, j, k, l each of course is a set of four quantum numbers each like i will stand for four so there are actually 16 quantum numbers over there okay. Each subscript denotes a set of four quantum numbers. So, we will consider a particular choice of i, j, k, l and focus our attention on this term here okay.

Now what do you have here, these are the terms that we are going to have to address when we deal with these configuration interactions. These are the ones which are which come into play because of the electron correlations which we had left out in the Dirac Hartree Fock formalism. So, here you have these terms and focus your attention on the product of this two electron integral okay.

This is the two electron integral and these are the matrix elements of creation and destruction operators in what is otherwise a vacuum state. So, vacuum state is the one in which everything is as it should be like all the occupied states are occupied and none of the normally unoccupied states are occupied which means that the water that we were talking about is at rest there is no heat being supplied.

And that is when the correlations of our N electron system are switched off okay. As if there is nothing so there are no slanted *p* particles above the Fermi level and there are no holes below the Fermi level. So, what do you have is vacuum okay nothing, so that is our vacuum state represented by this Phi 0 now.

So, this is the normal picture of course you have to remember that we are focusing our attention on what is inside this green rectangle but there are other terms which implicitly exist and we have to when you do an actual calculation and get numbers out of it you will of course have to put all those terms in and carry out the full integration over time space everything to get the final results.

But to deal with the configuration interaction, so focus our attention on what are the terms which we want, what are the kind of configuration interactions, what are the kind of correlations that we are working with. You can focus your attention on what is inside this green loop in this picture.

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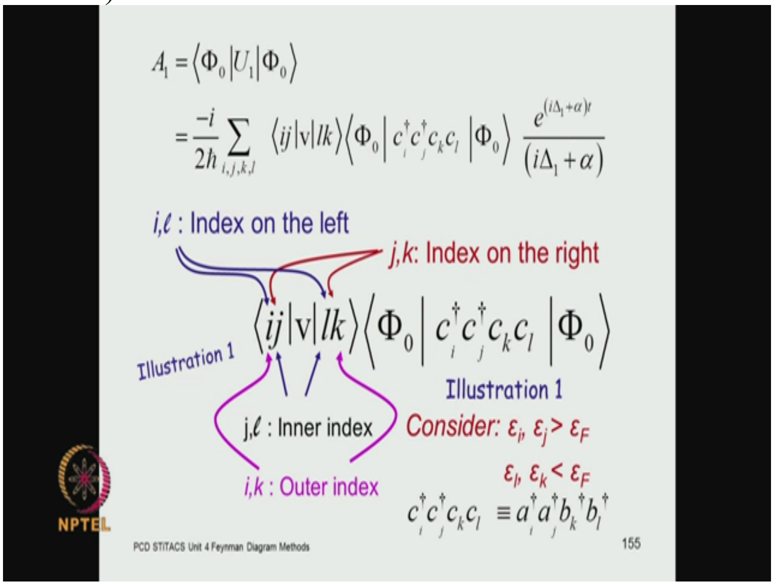


So, here you are, so this is what you are going to focus your attention on. Let me consider this first illustration here and for this first illustration I have chosen these two states the ith the jth state to be above the Fermi level and the kth and the lth state to be below the Fermi level. So, in this matrix element of the creation and destruction operator in the vacuum state okay that is the matrix element that we are considering here.

Essentially this ci dagger, cj dagger ck cl is what I write over here, so it is the same set of four operators written in exactly the same order as I want to consider for this illustration one. But now I take cognizance of the fact that in the specific example that we are discussing the ith and the jth state are above the Fermi level.

So, when you are creating a particle, when you are creating an electron above the Fermi level these, this process will be represented by the operator a with the index i. And again instead of cj dagger I will have aj dagger. Likewise this ck is an electron destruction operator this is the real electron, this is the natural electron that we began with.

But now we take cognizance of the fact that the state c, that the kth state is below the Fermi level. So, when do you destroy a form an electron below the Fermi level when you do that you effectively create a hole in that state. So, you are creating a hole in the kth state which will be represented by the creation operator for the hole which is b dagger for the kth state. And now for the last operator which is cl over here.

You have; you are destroying an electron in the lth one particle state and this one particle state is it has l for its index which is below the Fermi level and when you destroy an electron below the Fermi level you can do so by creating a hole in that state. So, the operator will be b dagger with the index l okay.

So, these are the four operators. So, instead of those operators c I will now work with the operators a and b and whether they will be creation or destruction will depend on what process is involved in the example that we are working with. Then we have to take a note of some other thing the other factor that you have to take cognizance of is the two electron integral.

Now what is that that is i, j, v, l, k and in this you have got indices on the left, so between l and k, l is on the left and between i and j, i is on the left okay. So, you have got pairs of indices ij of which i is on the left j is on the right the other pair of indices you have to work with are lk of which l is on the left and k is on the right okay.

So, you have to keep track of what is on the left and what is on the right. Then there is something else you have to keep track of, the way you look at this two center integral you have the indices j and l which are inner indices and i and k are outer indices. So, keep track of what is inner what is outer what is on the left, what is on the right.

What is creation, what is destruction, what is the particle state, what is a whole state okay? So, all of this has to be kept trackers of. Again there are a number of parameters and all of this comes together in a very neat diagram which is a very simple diagram which you will see very shortly. So, keep track of these things.
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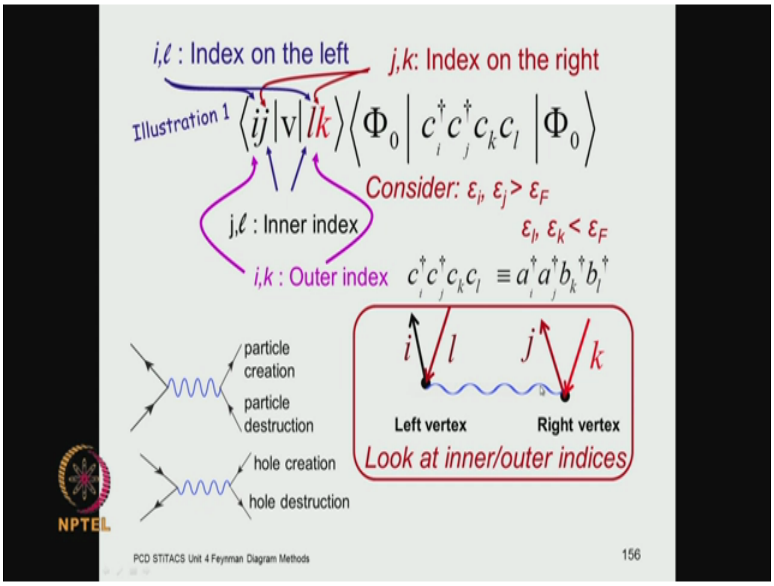


So, this is what we have got so I have got every information from the previous slide over here there is nothing new over here except for a reminder that if you are talking about a particle creation it will be represented by an arrow pointed upward and getting out of the vertex. If it is a particle destruction it will be an arrow pointed upward but into the vertex.

And if it is a hole creation a hole operators are arrows pointed downward. But if it is a hole creation it has to get into the vertex whereas a hole destruction will also be an arrow pointed downward but it will be getting out of the vortex. Now use these conventions and generate a diagram to represent this particular in your interaction how would you do that?

So, begin with the wiggle okay then identify the left vertex on the right vertex and what is on the left will go to the left what is on the right will go to the right what is inside will go to the inside what is outside will go to the outside. It cannot be simpler than that right, it just cannot be simpler than that.

So, what is on the left you have got let us look at one of the left indices. So, i and l are indices on the left what are you doing with the index i you have ci dagger what does it mean it is ai dagger right, ci dagger in our context is ai dagger. So, that will be an arrow pointed upward right and that is particle creation. So, it has to be an arrow out of the vertex got it, add you have it on the left.

And likewise you can follow the same logic and generate the other parts of this diagram. So, you have got j which is on the right between i and j, i's to the left j's to the right okay. So, j will go to the right but what are you doing with j you have a cj dagger in the original element but cj dagger in our context is aj dagger because you are dealing with a state j which is above the Fermi level right.

So, you will have an aj dagger which is a particle creation, so it is again represented by an arrow pointed upward and out of the vertex because arrows pointed upward are the particle creation operators that is the convention we have set up. So, you just follow that convention strictly and it takes a little while to get used to it but I will give you a number of examples so that you will be quite comfortable with this.

Then what about l and k, so l is over here, l is appearing on the left because between l and k this pair of indices k's to the right l's is to the left, so l will be at the left vertex okay what is happening with l you have an electron destruction in a state which is below the Fermi level and this is represented by bl dagger by the creation of a hole in the lth state. So hole state means arrow pointed downward.

Creation of a hole means that it should be an arrow pointed downward but getting into the vertex like over here. So, this is a convention the whole creation is an arrow pointed downward into the vortex. So, you have got the state l over here and now you have got the state k which is very similar okay.

So, this diagram represents this entire term together okay it has brought information from this two center integral and it has brought information from this matrix element in the vacuum state with reference to the Fermi level because the Fermi level separates the occupied the normally occupied state and the normally unoccupied state.

So, this is the Feynman diagram which represents this particular term. And what is such a complicated term even in our first order correction is now a simple diagram over here right. So, we can represent this diagram alternatively by some other pictures because essentially you are removing of an electron from this state and knocking it into a state i.

So, this gives a little more physical picture but these are not the pictures which are normally used because these pictures will become extremely complicated when you start talking about N electrons from below the Fermi level going to electrons above the Fermi level. That will become terribly messy but these diagrams are quite neat so okay.

So, you have to keep track of what is and inner index and what is an outer index and you have to keep track of what is the left and what is it the right and what are particle and hole operators.

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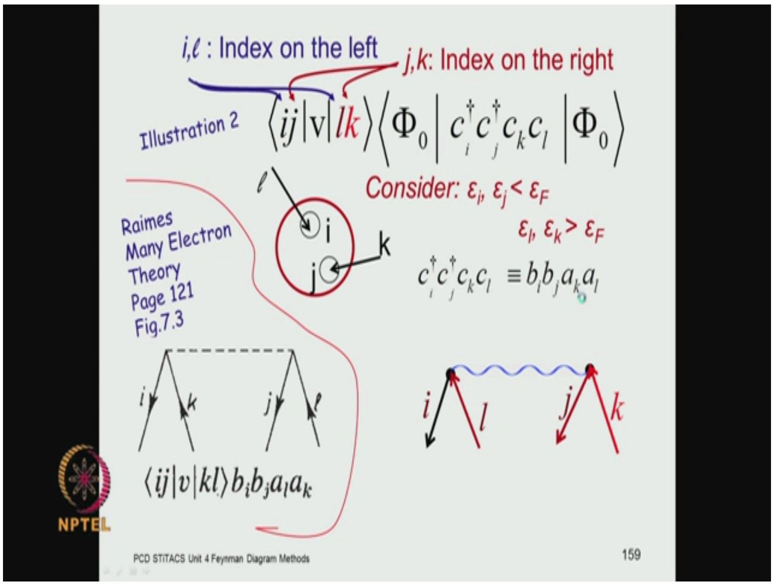


Now this is the first illustration that we considered now let us take another consideration another example. So, in the second example what I am going to do is deal with two electron states i and j but i and j below the Fermi level now in the previous case i and j but above the form in this case we have i and j below the Fermi level. And l and k are above the Fermi level how will you represent this diagram.

Again you follow the same prescription that your operator ci dagger cj dagger ck cl effectively involves the destruction of these holes bi and bj because i and j are below the Fermi level. So, you are creating two electrons below the Fermi level and you create two electrons below the Fermi level by destroying two holes over there that is the only way you can create two electrons below the Fermi level.

But now you are not talking about electrons you are only talking about the slanted *p* particles which are electrons above the Fermi level but below the Fermi level you have got the hole states. So, you have got the ci dagger cj dagger becomes bi, bj, ak, al and now you draw the wiggle you draw the vertices, then you draw the pictures for what is on the left and you have i and l are on the left, i j in the pair ij, i’s to the left j's to the right.

In the pair lk, l is to the left k’s to the right okay. So, you keep track of that and then you have got i which is an arrow pointed downward you have got a whole destruction in the i state. So here it is ci dagger is bi what is bi it is destroying, it is first of all a hole operator, so it has to be represented by an arrow pointed downward and it is a hole destruction so it has to get out of the vertex.

So, here this is the arrow pointed downward getting out of the vertex. So, this is your i and j be corresponding to bi and bj and corresponding to ak and al you have particle destruction in the kth state and the lth state and how do you represent particle destruction here it is this is the particle destruction. So, particles are represented by arrows pointing upward destruction by arrows getting into the vertex.

So you have l and k over here okay, so quite simple actually once you get used to it then you can do it quite simply. So, this is your second example here you can represent it drawing some sort of a physical diagram to represent this process. Now if you see the corresponding example in the book by Raimes then in Figure 7.3 you have got a similar diagram.

So, these the diagrams on over here from Reims book is the same as what you have over here okay. It is exactly the same you have got an arrow pointed up and an arrow into the vertex and arrow going downward out of the vertex. So, it is the same diagram but here the labels are ik and here the labels are jl.

Whereas we have il and jk and it is only because Raimes has al ak over here and we have ak al there okay. So, we have used different indices so there is no need to get confused all you have to see is what is what and there will be no inconsistency.

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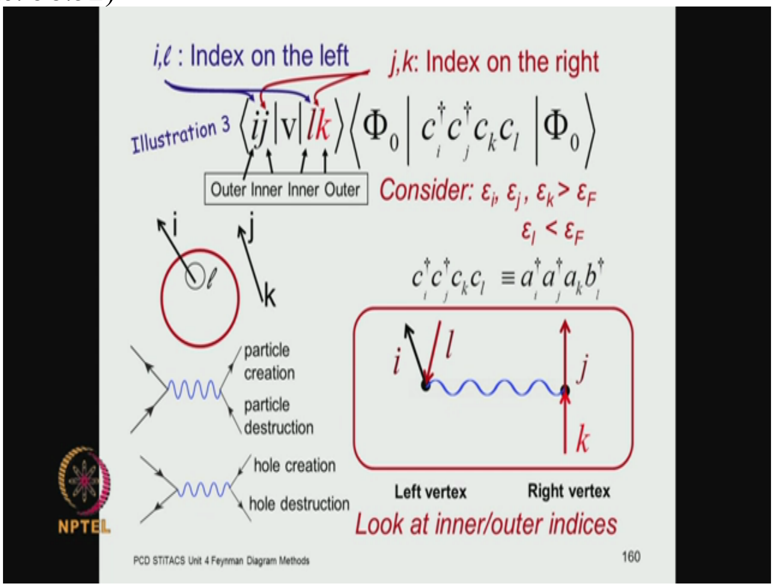


So, let me take another example here which is the third example I am considering today. Now I have got three indices ij and k above the Fermi level in this case in the previous two cases I had two above and two below but different sets. Now in the third example I have got three indices ij and k above the Fermi level on the fourth cl below the Fermi level.

So what would it mean the ci dagger cj dagger ck cl would correspond to ai dagger aj dagger what is ck, ck is destroying a particle above the Fermi level so that is a destruction represented by ak. But these two are creations, so you have got ai dagger aj dagger ak and cl will be represented by the creation of a hole in the state l right.

So, again you draw the left vertex the right vertex have the wiggle in place and draw the arrows corresponding to ai dagger aj dagger ak and bl dagger and you will have i coming to the left j going to the right and k going to the right and l going to the left. And now you notice that whether these arrows are leaning to the left or right really does not matter over here okay. Over here it was useful not to draw them on top of each other okay.

Because if you were not to make these arrows lean they would end up coming on top of each other which is why they are drawn with a little bit of slant but otherwise it really does not matter and then when you provide a slant then you keep track of what is an outer arrow and what is an inner arrow. So, that slants becomes useful to represent this when otherwise they would come on top of each other.

But j and k they have no chance of coming on top of each other because one is getting into the vertex and the other is going out of the vertex, so you do not really need the slant. So, that is not the most important thing and you have to keep track when you have them, when you have the possibility that they would come on top of each other. So, you could represent that picture by showing you know these physical kind of pictures.

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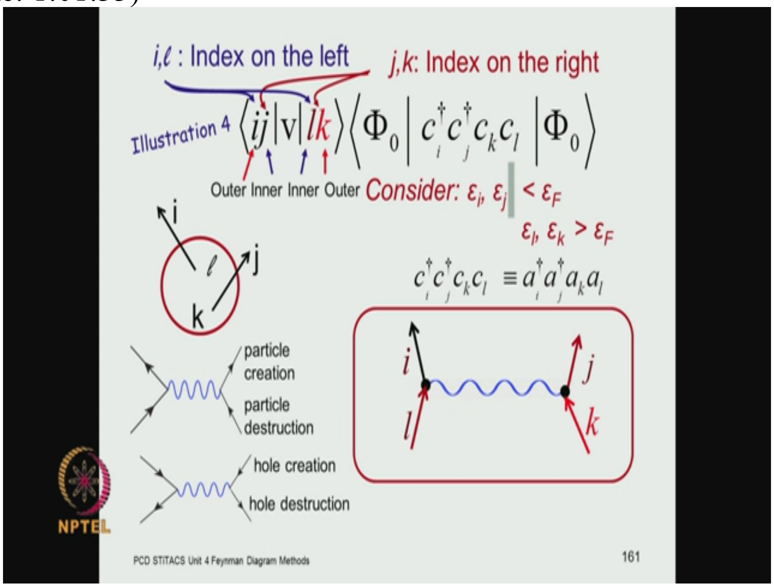


Let me take the last example for today which is the fourth example I am taking and in this case I am taking these two epsilon i and epsilon j below the Fermi level and epsilon l and epsilon k above the Fermi level and this can also be drawn using the same kind of convention. So, now you have got a picture of this kind okay. So, I will not get into too many details here now you know how to generate these diagrams.

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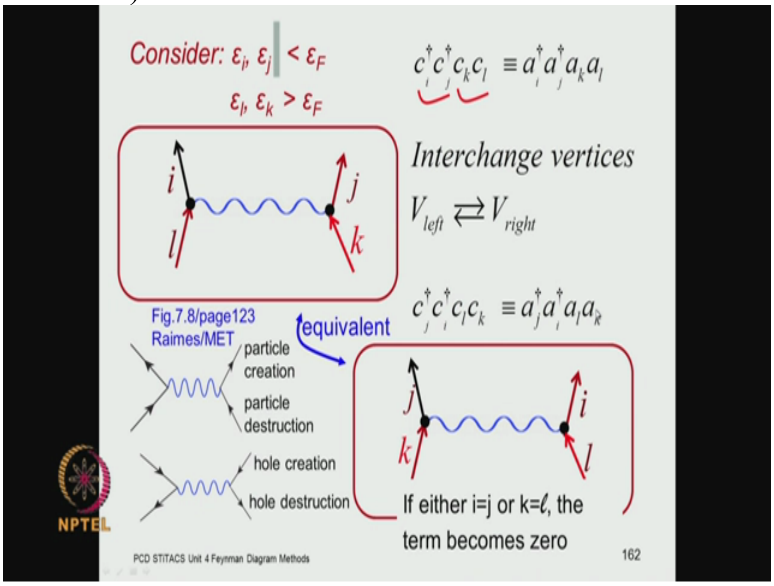


So, these are the first order diagrams that you can get. Now the reason I gave this example is because if you change the vertices okay. Interchange of vertices amounts to swapping these labels right. And what happens if you put cl behind ck these operators anti commute, so you will get a minus sign right. But you will get a minus sign also from ci dagger cj dagger when you interchange their positions right.

So if you interchange the word choices you will get a similar diagram. So, you have got li over here and this li has now gone from the left to the right because you have interchange the left vertex for the right vertex. So, these diagrams are equivalent, so that is the reason I gave this example the fourth example okay. That when you interchange the vertices you have equivalent diagrams.

You have got the same kind of structure on the other hand you should know that if i = j you would end up attempting creation of an electron in the ith state and creating an electron in the ith state yet again in what is already occupied and you cannot create a Fermi particle in an occupied Fermi particle.

Because the occupation number of fermions is either 1 or 0 likewise you cannot destroy a particle a hole state twice. So, if l and k are the same then the term would vanish.

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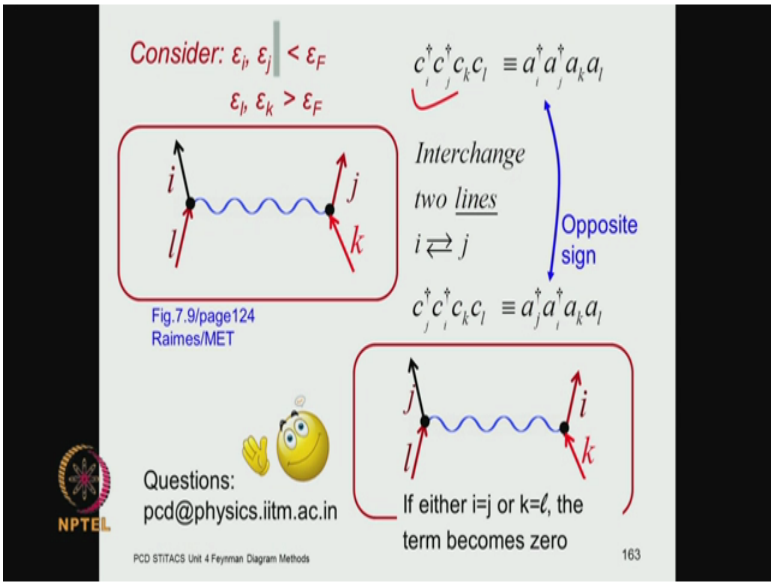


So, these are some of the considerations what would happen if you interchange two lines we discussed what would happen if you interchange two vertices, so you have the same result. But if you interchange two lines then you will be swapping only i with j and then from the anti commutation you will pick up a minus sign.

So, you can write the corresponding set of operators but then you would have terms with opposite sign. So, these are some of the things that you can remember and in the next class we will get into some more examples of this kind and we will also then subsequently get into second order diagrams and higher order diagrams okay.

So, when we get into the second order and higher-order diagrams you will also meet the ring diagrams and other diagrams as are used in the diagrammatic representation of these electron correlation terms. Questions (Question time:1:05:05) yes It is related to the first part of the lecture yes the you said earlier that we should write a combination of Slater determinants to represent a state right.

So, my question is that by defend Slater determinants which corresponds to some excited state yeah, so they will have difference of this according to the Hamiltonian i am right. Well that is it Thejes or Afsul who is this; it is Thejes okay, Thejes, see when you talk about excited states you are referring to an excited state with respect to the Dirac Hartree Fock Slater determinant okay.

So, go back to the example of the magnesium that we first talked about. So, you had the electron configuration with the neon core and two electrons in the 3s state and then you had the second configuration in which you had the neon core the 1s2 2s2 2p6 and then the remaining two electrons were in the 3p state right. Now 3p is what you will call as an excited state only with reference to the Dirac Hartree Fock ground state.

Otherwise 3p is not an excited state what the correlation does is it is telling you that your ground state in fact is a linear superposition of those and those together will have the energy which is an Eigen value of the full Hamiltonian inclusive of the correlation. So, you are not making a difference between the energies of the 3s2 configuration and the 3p2 because they are mixed by the configuration interaction.

So, you have to stop thinking about the energy states in terms of the single Slater determinant because that represents what was an unoccupied what it was a ground state only with reference to the original Slater determinant. But now your system configuration is the linear superposition of Psi1 and Psi2 and you can have even more terms.

So, they all have a single energy, they all have a single energy which is the Eigen value of the full Hamiltonian inclusive of the correlation. It is not that the s2 configuration has a lower energy and the p2 configuration has a higher energy they are both components they are Eigen functions your system Eigen function your full Schrodinger equation is H Psi = E Psi okay E is the energy of the full system inclusive of the correlation, Thejas.

And you have to Slater determinants which are getting into the linear superposition. So your system wave function is c1 Psi 1 + c2 Psi 2 and that linear superposition is an Eigen function of the full Hamiltonian belonging to one Eigen value which is your E inclusive of the correlation. And c1 and c2 give you the amplitudes the probability amplitudes that if you do a measurement.

What is the possibility that the system will be found in the states Psi 1 and that is not equal to unity because c2 is not 0. So, the sum of the squares of all these coefficients c1 square + c2 square will be, will add up to unity. (Question time: 1:09:40-not audible)So, the different Slater determinants degenerates states; degenerate because of the correlation okay.

In the presence of the correlation they are different components of a wave function it is like doing simple quantum mechanics in which a particular wave function is not in a pure state. When you have a system which is not in a pure state then it is in a mixed state right. It is in a superposition state and the superposition consists of a linear superposition of various basic elements.

Which are, which give you the complete set of bases to represent an arbitrary wave function and the coefficients give you the probability amplitude that a measurement will cause the system to collapse into one of those states okay? So, you have to stop thinking about them as belonging to different energies one being ground state the other being excited because they are just different components of the total Psi.

Total Psi is c1 Psi 1 + c2 Psi 2, now what is the Eigen value of this, this is a new energy which is E Psi okay. The H Psi = E Psi the new energy is E which is inclusive of the correlation now. Now this is the Eigen value of the full Hamiltonian okay. So, you will think about the 3p state to be an excited state only in the single particle approximation not when you are doing a configuration interaction.

In which you have taken both of these and your system wave function is recognized as c1 Psi1 + c2 Psi 2 does that answer your question Thejas okay. Any other question (Question Time:1:11:56- not audible) yes Hari tell me yes When we talk about creation and destruction yes these are mediated by the correlation there is no external photon no, no what your talking about the ground state correlations yeah.

The ground state correlation always present because the Hartree Fock or the Dirac Fock, the Dirac Hartree Fock is only an approximation. So, the correlations are always present and as a result of these correlations you do not need an external field to generate these correlations they are intrinsic to the system.

They are intrinsically present in nature you cannot switch off these correlations if N electrons exist they will exist along with all their intrinsic properties and these intrinsic properties will be like their intrinsic angular momentum with their electron-electron interaction and electron-electron antisymmetry because of the spin right.

And also because of the correlations which there is no way you can ever switch off they are always present only while doing an approximation you can turn off certain interactions. So, they are always present you do not need an external field and as a result of these correlations you always have a system wave function which essentially must be described as a linear superposition of an infinite set of Slater determinants.

Of course the complete basis requires these infinite Slater determinants but in practical situations a few of these later determinants will suffice and if you take just one of these Slater determinants which is the magnesium neon core + 3s2 if you take just one Slater determinant you get the Dirac Hartree form which is not a bad approximation to the magnesium atom. But then it is not a sufficient approximation either.

So if you just did the Dirac Hartree Fock representation of the magnesium atom you will not get correct results if you were to interpret collision data or photo ionization data and so on. So, to represent these correlations you require these many-body techniques but they are always there. They are not in response to any external field okay. So thank you very much.