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

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Lecture 32
Linear response of electron correlations

Greetings, we now have the last class of this unit in which we will have some further discussion on second order diagrams and higher-order diagrams and we will discuss the random phase approximation its extension the relativistic random phase approximation which you can also do in some other ways.

Which basically are inspired by the process of linearization which is the linearization of the time dependent Dirac fork or the Dirac Hartree Fock method? So, these are some of the things that I will sum up to provide an introduction to research literature.

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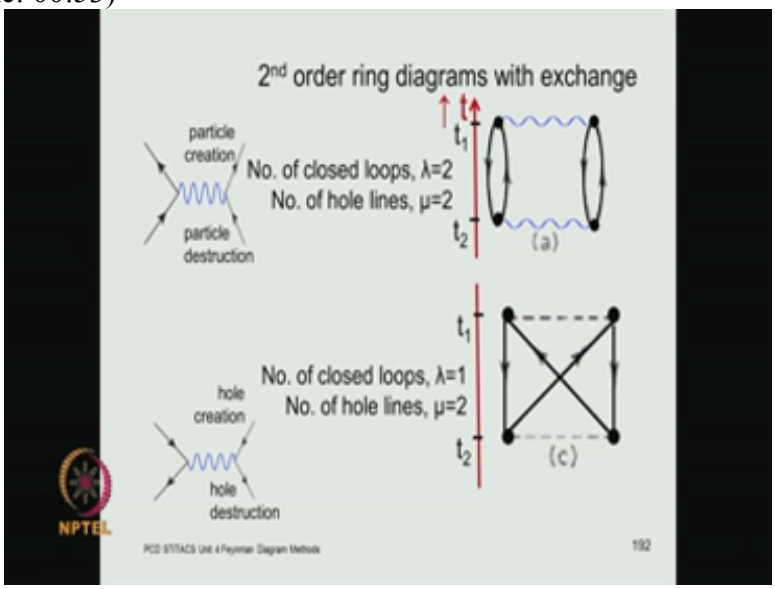

So, we were dealing with these second order diagrams in our previous class so we had the Coulomb diagram the direct and the exchange. And we had started talking about the number of loops and the number of hole lines and in the exchange you have got one closed loop as you can see and the number of hole lines is 2 which is written as mu following the notation of Raimes.

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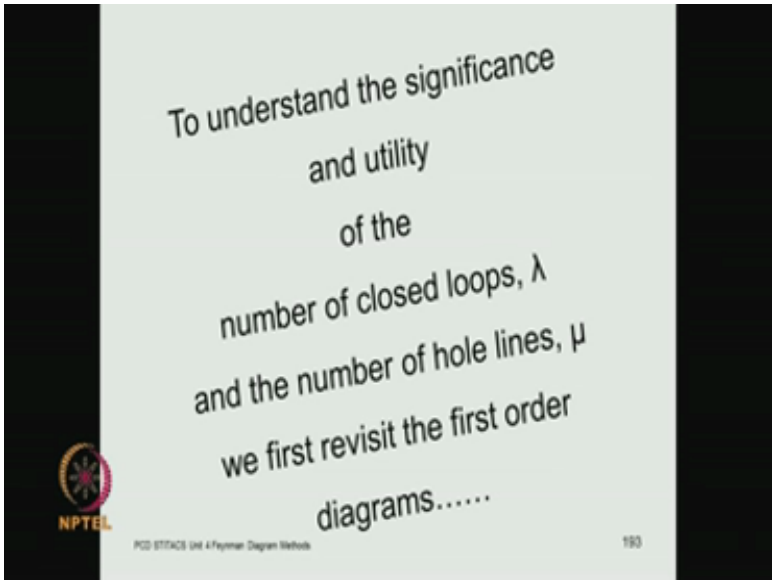

Now to understand how the number of closed loops and the number of hole lines is used in interpreting the Feynman diagrams.

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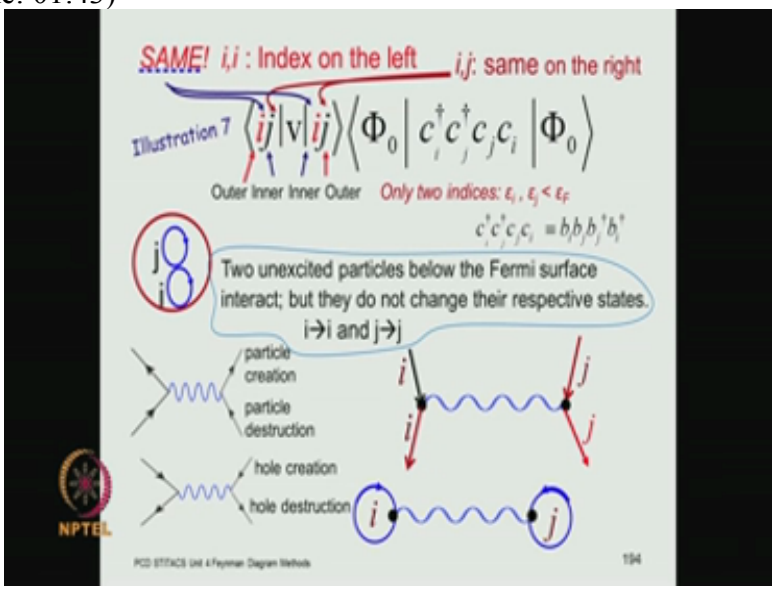

Let me go back a little bit to the first order diagrams. So, let me refer to the first order diagram which we considered earlier and here in the direct term you have the double bubble which we have discussed earlier.

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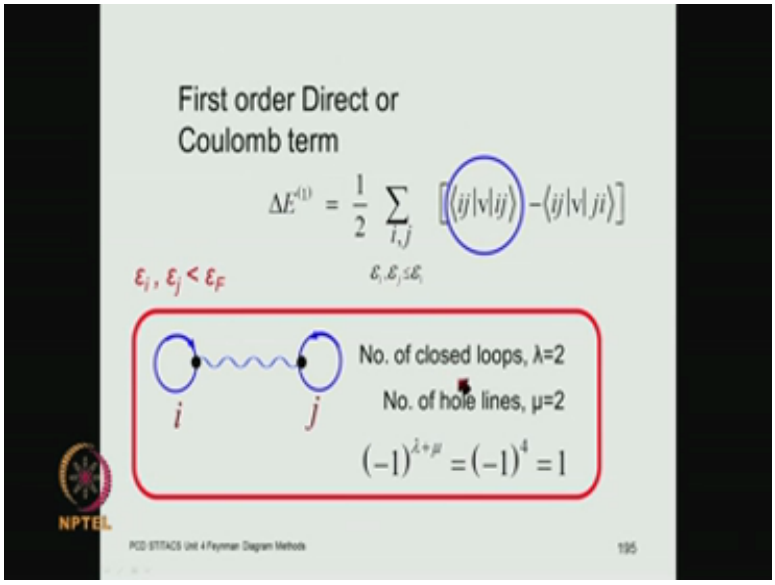

And in this double bubble if you count the number of closed loops you have 2 and the number of hole lines is also 2 okay. So, this is the situation and what does is if you take the contribution of lambda and mu together you get a phase factor which is -1 to the power lambda + mu which in this case is = +1 and what this diagram does is to contribute a +1 sign to this matrix element okay. So, this contributes a +1 sign to the first order correction.

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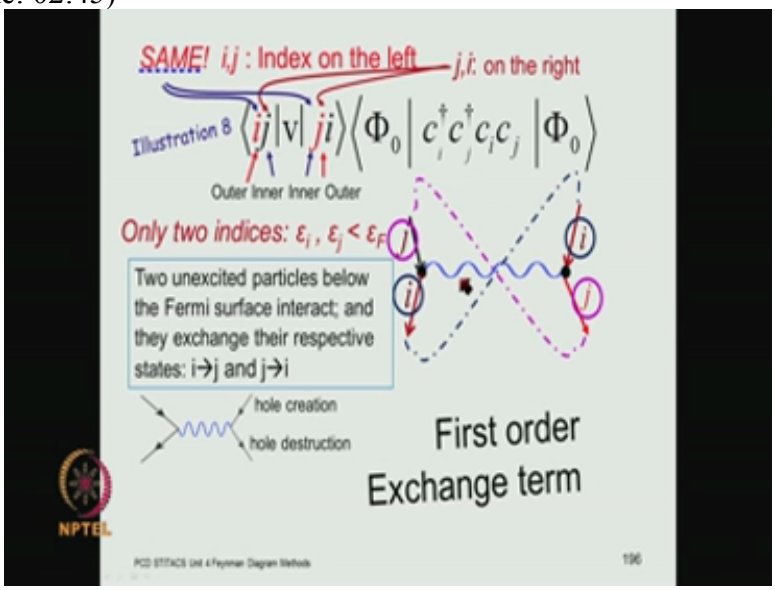

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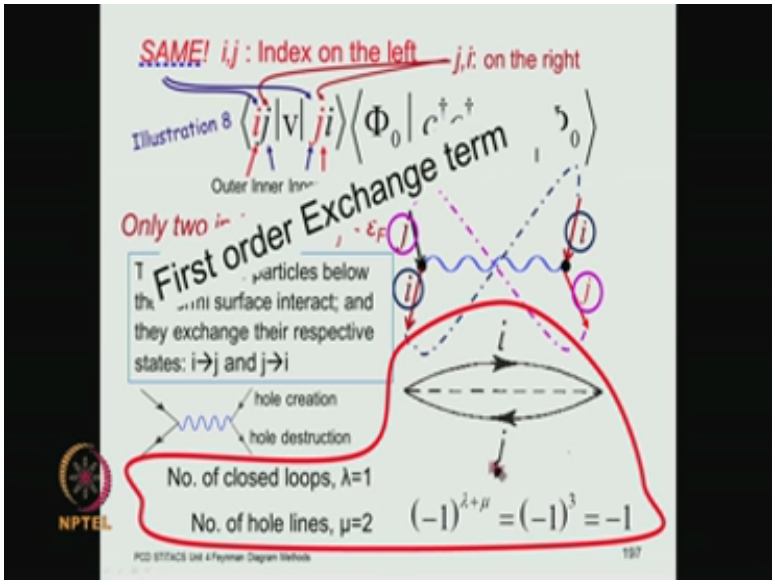

Now if you look at the exchange term you have a ji here and as a result of this you have, in this case the oyster right. This is the exchange correction from the first order exchange correction to the free electron energy. Now what does this does is to contribute -1 sign which you get by getting the phase as -1 to the power lambda + mu lambda being 1 because there is only one closed loop and mu being = 2.

So, this contributes a phase -1, so you can pick the number of loops and the number of lines by simply following by looking at the picture. So, just look at the topography of the picture and you will get the number of loops and lines number of loops and hole lines which is what you count for the consideration of what is used in a very famous theorem known as the Wick's theorem.

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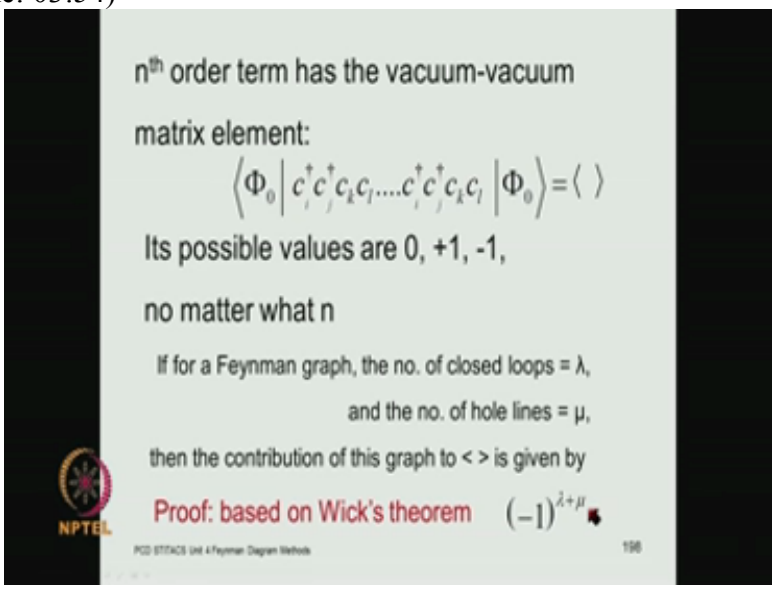

So, I will tell you how it is used, so you have in general nth order correction which will have you know contributions will be either 0 or they could be +1 or they could be -1 they cannot

be anything else because no matter what n is those are the only diagrams which will contribute to the corrections because unless you destroy a certain number of particles from occupied states.

And then create those particles in the very same states you are not going to get a nonzero contribution okay. So, that puts certain restrictions and depending on whether it corresponds to a direct or in exchange term the contribution is either +1 or -1 otherwise it is 0. So, no matter what n you are talking about whether it is n = 1.

For which we have seen this explicitly but even for the second order and higher order terms you always have a contribution to the graph which goes as -1 to the power lambda + mu. Now this is a result which is based on the Wick's theorem and the details of the proof I will not work out it is a little laborious but the techniques which go into the proof are essentially those which we have already used.

So, if you spend enough time you will be able to get a proof of this theorem it is worked out in considerable detail in the book by Raimes but I will not actually prove this theorem it is little laborious to do takes a while. But the result can be very simply stated that with reference to this particular application of the diagrammatic techniques.

That the contribution of a diagram to the correction to the nth order correction goes as -1 to the power of lambda + mu. So, that is where the number of loops closed loops and the number of hole lines becomes a significant factor to work with.

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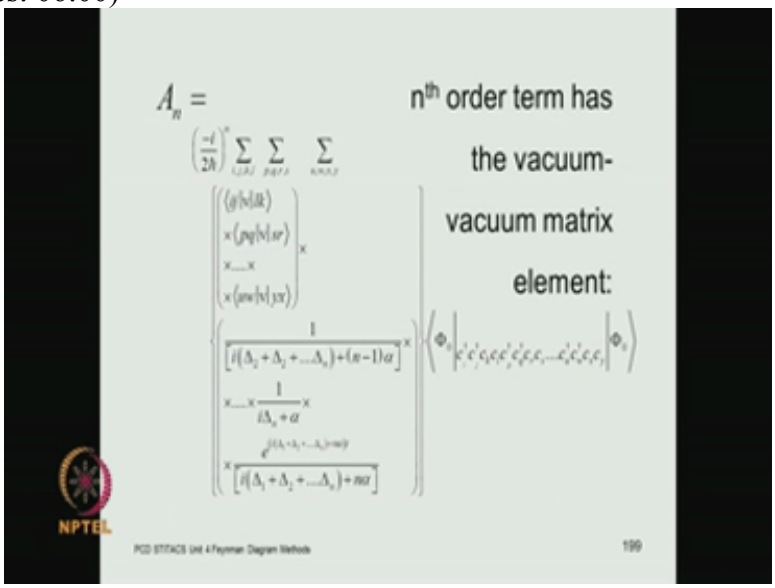

These are the nth order terms, so these terms are quite complicated as such but then because of these theorems the diagrammatic application of the results turns out to be quite handy and

rather neat which is what means the Feynman diagram methods so powerful and so nice. So, let us have a quick look at the third order terms okay just to get a little hang of it. So, the third order terms will have these corrections least contributions from the time integrals.

You will have these two center integrals and there will be a product of three of these terms and then you will have three sets of these four operators ci dagger cj dagger ck cl then you have got the next four likewise and then you have a third set. So, you have got a set of twelve operators sitting in the middle and you take their.

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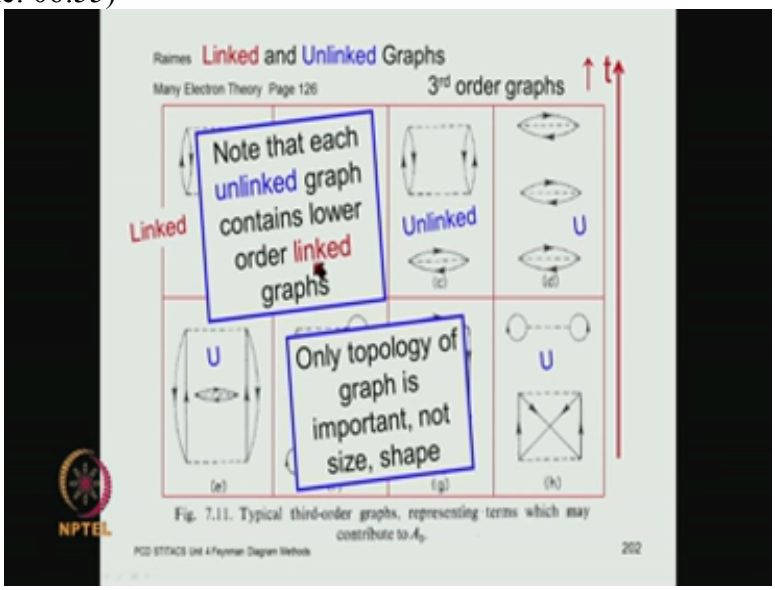

So, these are third order graphs okay, now they are built following exactly the same techniques that we have discussed in the earlier cases and you get a variety of third order graphs and what I would like to draw to your attention and I am not going to discuss the third order and higher order diagrams in great detail because the foundations we have already become acquainted with.

And we can then apply these techniques to interpret higher order diagrams. There is only one thing I would like you to notice over here which is the fact that you can recognize that some of these diagrams are linked and some are unlinked. So, if you look at the link diagrams, so here this one is a link diagram, this is linked and you can see why these are called as link this is a link diagram this is also a link diagram whereas this one is unlinked.

And the linked and unlinked terms are self-explanatory by looking at the pictures you recognize which are linked diagrams and which are unlink diagrams. So you do not really have to define them very extensively but you can recognize them from the pictures. So, these are the unlink diagrams and then there are some linked diagrams.

So, now in many body theory there are some other theorems which are proved, which can be proved using essentially the same techniques as we have done in this unit and in the in our discussion on second quantization using is essentially these methods. And you what you can see that if you look at the unlinked graphs these are made up of lower order linked graphs. So, this one is independently linked, this one is independently linked.

And every unlink diagram, so these are three unlink diagrams but each is a first order linked diagram okay. So, all the unlink diagrams contain lower order laying graphs in general. Now the only the topology is important the size of the graph or the shape of the graph is not important this comes from our fundamental consideration that whether these arrows point to the left or right really does not matter.

And that is used only for convenience to see what is happening at which vertex and only to distinguish between features when the two arrows tend to fall on top of each other that is when you make them lean to the left or right otherwise it really does not matter. So, only this topology is important.

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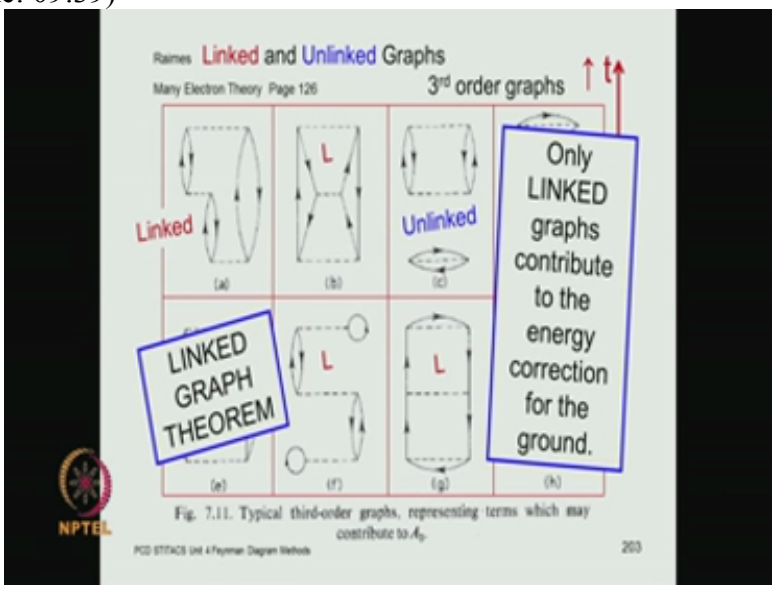

And there is a theorem which is known as the link graph theorem what this theorem tells us is that only the linked graphs contribute to the energy correction for the ground state. The unlinked graphs will contribute nothing. So, those contributions will go to 0 and some of these theorems are a matter of detail.

Which I will only mention and it is for you to follow up and there are extensive proofs and discussions in the book by Raimes, Fetter and Walecka and so on. Which are the primary references that we have used for our discussion here?

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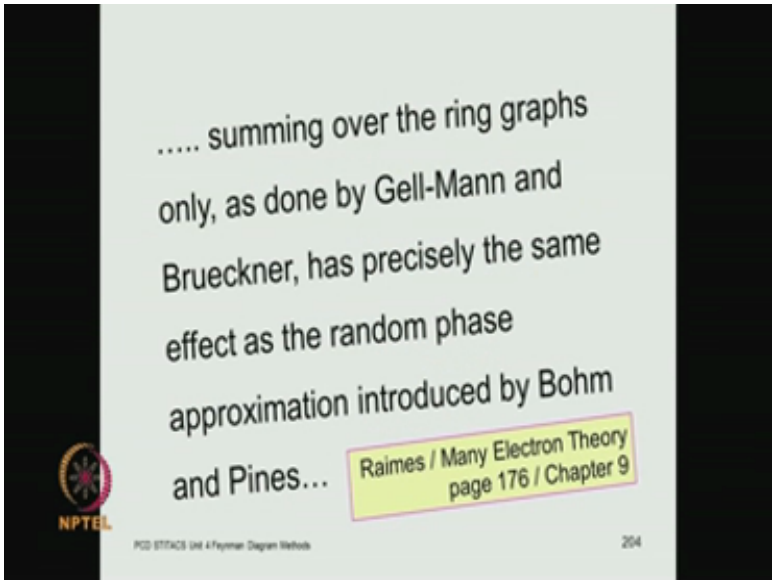

Now let me come to an important result because I am essentially summing up this discussion and I just want to in this last class of this unit give you some further leads okay. So, leads into other applications and developments which I will not be discussing in any great detail but these are like loose ends which come out of this which is for you to follow up in later discussions.

And an important result is that if you sum over all the ring graphs okay you already know that now there are graphs of different kinds. Now you know what are the ring graphs okay you have seen second order ring graphs, you will have third order ring graphs, you will have fourth order in graphs and so on right.

So, if you sum over all the ring graphs and this was done by Gell-Mann and Brurckner then the result of the approximation, now there is an approximation which is going into this what is the approximate that you are restricting your consideration only to the ring graphs and excluding everything else.

But what you are not excluding is the corresponding exchange terms because as I emphasized in the previous class when you take the direct terms it goes almost without saying that you would actually include the corresponding exchange terms although they are not exactly rings okay. But those are the exchange terms corresponding to the rings and there is a one-to-one correspondence for every direct term there would be a corresponding exchange term.

So when you sum over all the ring graphs and implicitly or explicitly whether you say it or not you also include the corresponding exchange terms. Then you get a certain approximation, the approximation being is that whatever is not the ring and whatever is not the corresponding exchange is excluded.

So, whatever you are excluding is it is not nobody is claiming that those terms will not contribute to the correlations they bill but in this approximation which we are discussing which is the choice of certain class of correlations which we refer to as the correlations corresponding to the ring diagrams and the corresponding exchange.

Now this has got exactly the same result as the approximation which was introduced in the previous unit. In unit 3 we discuss the Bohm Pines method extensively we carried out a series of canonical transformations you remember that, that in the unit 3 we had a number of classes some six or seven or eight classes, so we had a fairly detailed discussion on the Bohm Pines method.

And we did in the Bohm Pines method was to carry out a number of transformations but then when we went to higher order terms we agreed that we will remove certain terms from our consideration why because it is too complicated it is too messy. It is not that we do not like them or something but it is too messy. And that is how approximations are developed which is to solve part of the problem which is mathematically tractable.

And you can always go beyond it or make a different approximation and that is a choice that a theorist makes depending on which correlations he or she thinks are important for the consideration. And the kind of problem at hand often determines what approximations are made. So, this particular choice of retaining only the ring diagrams is completely equivalent to the random phase approximation which was done by Bohm and Pines.

Why it was called as a random phase is what we discussed at great length in the previous unit. Because the terms that we neglected involved certain phase factors and we discuss the cancellation of some of those terms and these are for a detailed discussion of this topic I will like to refer you to the unit 3 in which we have discussed this point at great length.

So, there are certain terms which cancel each other because of the phases and it is only for this historical reason that this approximation is called as the random phase approximation. Gell-Mann and Brurckner what they did was to sum over all the diagrams and they got precisely the same effect as was obtained by falling out following the method of Bohm and Pines.

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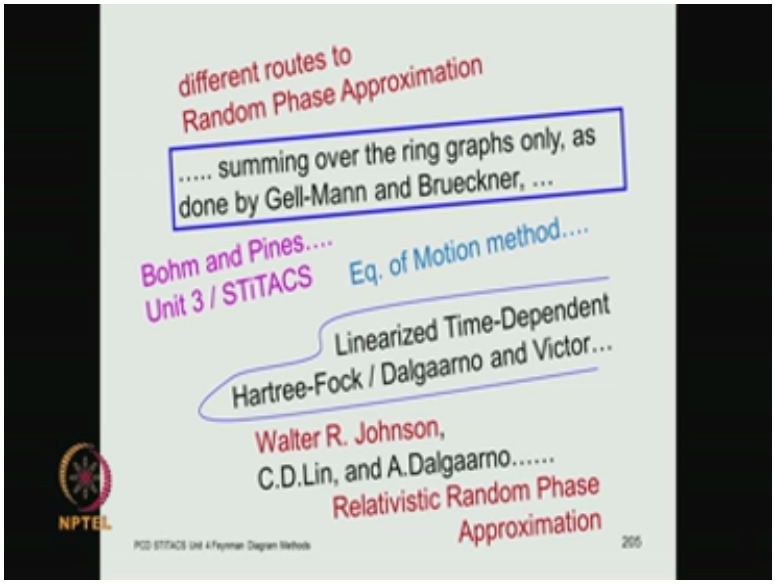

And there are this different routes to the random phase approximation you have the Gell-Mann Brurckner ring diagrams. So, that is one route to the RPA to the Random Phase Approximation or RPA as it is called. So, you have the Gell-Mann Brurckner summing over ring diagrams. Then you have the Bohm Pines method which we discussed in the previous unit. And there are some other methods and there is a equation of motion method.

There are propagator methods and then there is a method which is a particular interest to some of us because this is the form in which we make use of the random phase approximation in some of the studies that we many of you who are sitting over here in these classrooms are using and this is the linearized time dependent Hartree Fock method which was originally introduced by Dalgaarno and Victor.

And then it is relativistic you note formulation of the same technique which was done by Walter Johnson and his collaborators Lin and Dalgaarno which is called as a relativistic random phase approximation. So, all of these different routes are essentially equivalent okay. All of them amount to retention of certain correlations and exclusion of certain correlations. The correlations which are retained are those which correspond to the ring diagrams.

And the exchange which goes along with that, these are the same terms corresponding to the retention of those terms by excluding the terms in the Bohm Pines approach of removing the terms which are random phases which is why it is called as random phase approximation. And the terminology random phase approximation is applied to all of these including the method of the linearized time dependent Hartree Fock because they all amount essentially to the same set of correlation.

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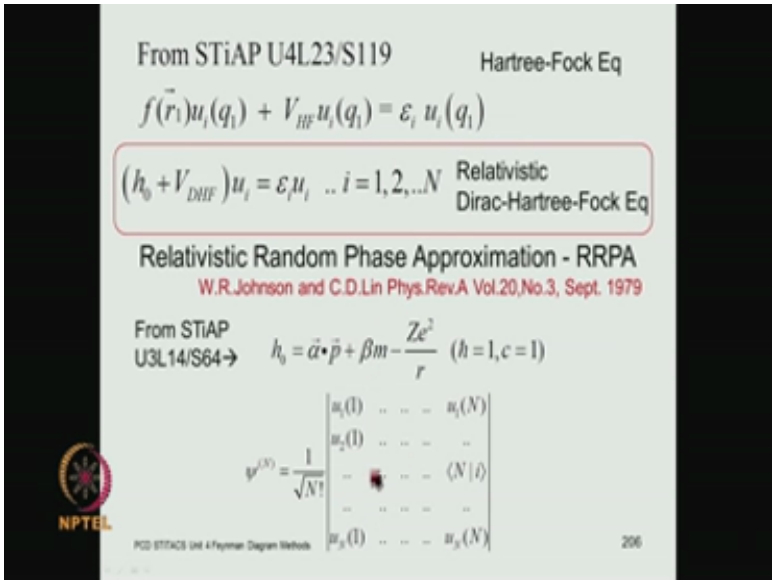

So, let me refer to the time dependent Hartree Fock and the linearization of the time dependent Hartree Fock which is the form of RPA which many of us make use of in our research studies. So, let me remind you the Hartree Fock equation and we have discussed this at great length in our earlier course on atomic physics. And we have the Hartree Fock single particle equation right.

So, I refer you to this particular unit 4 of the course special topics in atomic physics lecture 23 and you have the Hartree Fock equation in this. So, you have set of one electron operators and then you have got the Hartree Fock operator over here. And this looks like an Eigen value equation it is not an Eigen value equation as we know it. But some of these points we have discussed earlier, so I will not discuss them.

Now what would be the relativistic analog of this is what is called as a relativistic Hartree Fock but because it is starts with the Dirac equation rather than the Schrodinger equation it is called as the Dirac Fock equation or more correctly and more fully the Dirac Hartree Fock because Hartree is after all the person who really introduced the self-consistent field methodology.

So, I think it is not fair to drop his name in the middle. So, this is the Dirac Hartree Fock method and this is completely identical to the relation at the top which is the Hartree Fock okay. So, what we did in our courses is to do the Hartree Fock in detail, we did the Dirac equation in detail in the same course.

And now we put the two together and if we were to follow the self-consistent field methodology of the Hartree Fock beginning with the Dirac equation rather than the Schrodinger equation. We would get essentially an identical result with the difference that

these spin orbitals were two component functions in the Hartree Fock theory. But in the relativistic Dirac Hartree Fock theory these will be four components bi-spiners okay.

We have done this in great detail in the context of the Dirac equation. You will have a one electron operator which is h0 and then you will have a Dirac Hartree Fock potential corresponding to the Hartree Fock potential of the non relativistic model. So, you have an exactly identical equation with the difference that now your operators are represented by 4 by 4 you know matrix operators.

And the wave functions are now bi-spiners, so they have 4 components and the Hartree Fock wave functions are the spin orbital's which are the 2 component functions. So, with the difference we now carry over the discussion of the Hartree Fock into the domain of the relativistic Dirac Hartree Fock.

So this was the starting point for what is called as a relativistic random phase approximation which is inspired by the method of linearization of the time dependent Hartree Fock but the relativistic version being the time dependent Dirac Hartree Fock. So what does it do it begins with the relativistic Dirac equation.

So, you are one electron operator is not this non relativistic operator of the Hartree Fock but it is the relativistic operator of unit 3 in our previous course on atomic physics. And this operator has got these alpha and beta operators, so we have discussed them in our previous course on relativistic quantum theory okay. So, we have done the Dirac equation we did the Foldio Dyson's transformations.

And all of this discussion is available in the previous course this is the special or select topics and atomic physics we did this mostly in unit 3 and then lecture 14 and you know the lectures around it you will find all the details. So, this is the single electron operator and then you have got the Dirac Hartree Fock interaction term. And you will have just like the solution to the Hartree Fock is given by the Slater determinant.

You will have a Slater determinant giving you the solution of the N electron Dirac Hartree Fock problem with the difference that the elements of the Slater determinant are now 4 component bi-spiners and not to component spin orbitals. So, it has the same form it looks the same it is not the same.

The Slater determinant that we now on this have on the screen has got for its elements the relativistic single particle functions which are bi-spiners, so this is the solution for the relativistic Slater determinant.

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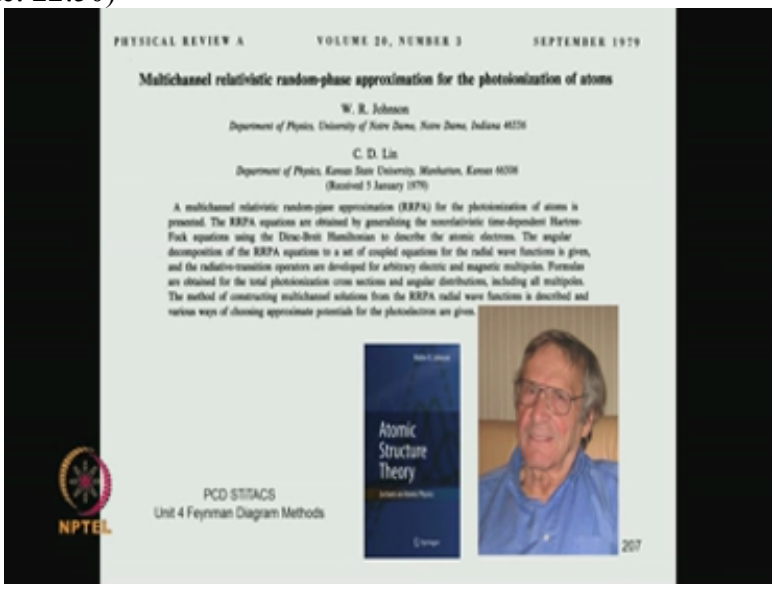

Now this is the solution to the Dirac Hartree Fock and this its extension and what the relativistic Dirac Hartree Fock does is to include the statistical exchange as we know it okay. It includes the statistical correlations it includes the relativistic effects because it started out with a Dirac equation rather than the Schrodinger equation what it does not include are the Coulomb correlations.

The Hartree Fock did not include the Coulomb correlations and the Dirac Hartree Fock does not include the Coulomb correlations. So, direct Hartree Fock solution is a single Slater determinant it includes the statistical correlations, the Fermi correlations, the exchange correlations they are all synonymous terms right, so all of those correlations are included in the Dirac Hartree Fock.

It is certainly one level better than the Hartree Fock because it is starting point is the Dirac equation and not the Schrodinger equation and therefore spin comes naturally in the Dirac Hartree Fock. Whereas in the Hartree Fock spin was sort of introduced on an ad hoc basis you work with the Schrodinger equation which does not really provide for the electron spin but you plug it in on an ad hoc basis and then go with the 2 component spin orbital's.

So, you have got the Hartree Fock two component theory then you have got the Dirac Hartree Fock for component formalism which gives you for its solution the Slater determinant. But what the Dirac Hartree Fock does not have is the Coulomb relation and to introduce these Coulomb correlations.

You can follow Bohm and Pines and do the RPA or you can follow Bruckner method and do the ring diagrams or you can follow Dalgaarno and Victor and do the linearized time dependent Hartree Fock which is what Walter Johnson did and this is the classic paper which I like to show this picture on the screen and Walter's lectures are also now available as a springer book.

So, that is where you will find a very rigorous treatment of most of the atomic physics that I have attempted to cover or I have attempted to cover just a small fraction of what you will find in this book not a small fraction maybe a very small fraction or a small fraction of a small fraction if you like okay. So, this is where you will find further leads.

And this is the famous paper which is cited in almost every work on the relativistic random phase approximation.

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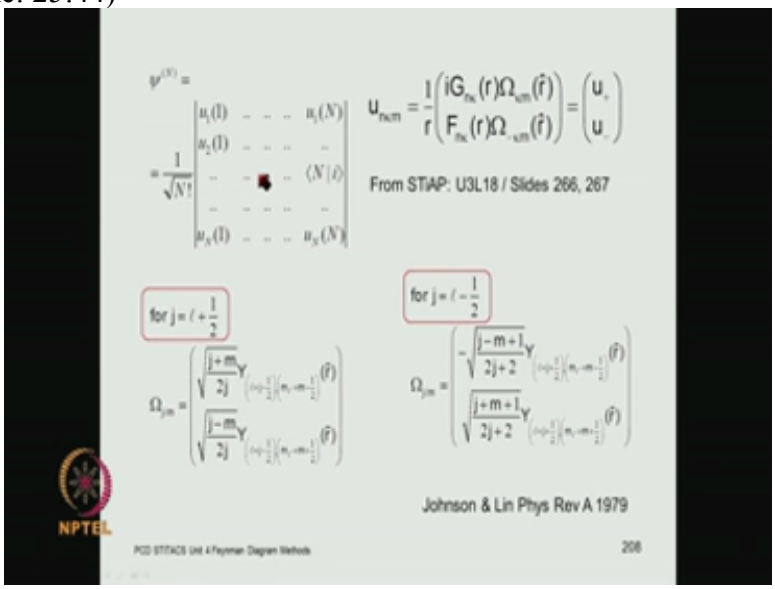

So, what it has are the Slater determinants in which each element is a 4 component bi-spiner okay. So, you have got these radial functions F and G coming from the Dirac equation right are this again I will not spend any time discussing it but refer you to what we did in unit 3 of our previous course a special or select topics in atomic physics. So, you will find a detailed discussion on these 4 component functions in the previous course okay.

Now here you have got the vector spherical harmonics and these vectors spherical harmonics you have two of them one for l + half and the other when the total angular momentum for the single electron is l - half. So, you have got two components over here, so that is what makes this two into two of four component wave function or a bi-spiner okay. So, you have these two and these two so you have got four component functions over here.

And this is the kappa quantum number which we have introduced in the previous course. So, these are the quantum numbers which go into the description of these one electron wave functions which are solutions of the Dirac equation and these are the elements of the Slater determinant. So, now you can do a Hartree Fock like treatment completely with the four component relativistic wave functions. You will get an exactly identical form.

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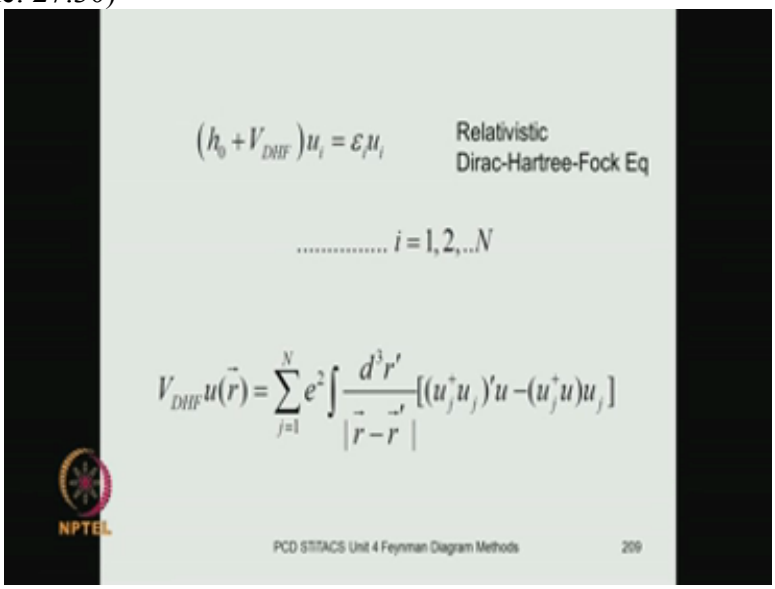

And essentially you will get the relativistic Dirac Hartree Fock equation which you already see is exactly the same as the non relativistic Hartree Fock equation with the difference that now you are single particle operator is the Dirac operator at h0. And your Coulomb exchange term is represented in terms of this Dirac Hartree Fock potential.

So, you have the Coulomb term and the exchange term but these are now the relativistic wave functions okay. So, you have got exactly the same form and if you go back to the previous discussion on the Hartree Fock you will find exactly the same term. Same symbols with the difference that in the context of the Hartree Fock they will refer to the 2 component Hartree Fock Schrodinger wave functions.

Whereas in the present context the same symbols now represent for component Dirac Hartree Fock bi-spiners okay. The 4 component wave functions, so you have the same results.

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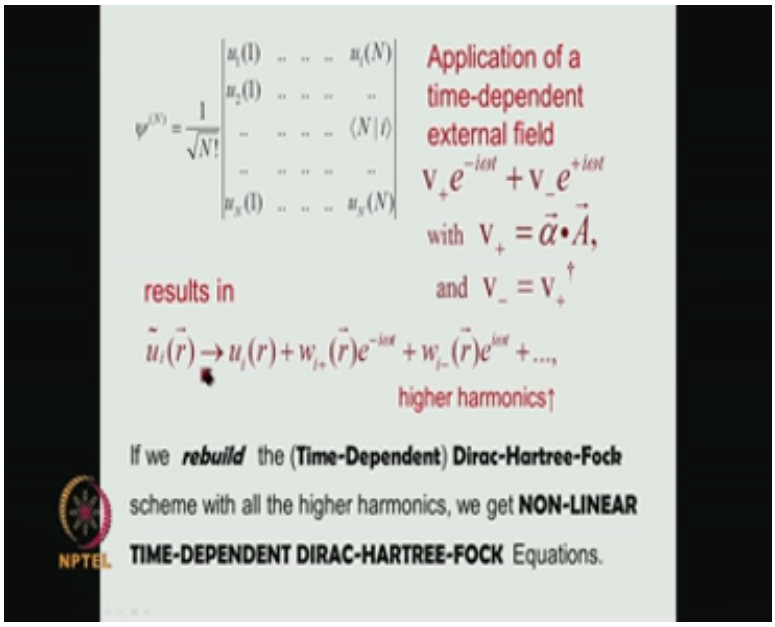

But what they have excluded are the correlations now how would the system respond to correlations. So got an electron system you have taken into account all this statistical correlations. You have also taken into account all the relativistic effects and we have come a long way by describing this an electron system by a relativistic Dirac Hartree Fock formalism with a single Slater determinant.

Whose components are the 4 components bi-spiners that is done what is left out are the correlations. But the reason to do this is also to study the response of the system to a stimulus such as an electromatic radiation which will cause transitions from a certain initial state to a certain final state and this is the photo absorption process in which many of us are deeply interested.

We discussed in collision physics that if you have a target and you want to probe its properties you can do so either by shining electromatic radiation on that or is by firing some particles a beam of projectiles which can be electrons, positrons, alpha particles. So, you can either do a collision experiment or you can do photo absorption, photoionization.

We have also discussed in our previous course how the two methodologies are related to each other through the time reversal symmetry which is why the entire quantum mechanical machinery of collision physics gets applied in photoionization physics. And here we are now talking about a particular probe which is electromatic radiation and we represent this electromatic radiation as a time dependent external field.
Which is represented by this operator here which is the alpha dot A and it is adjoint. So, you have got a combination of terms with e to the - i omega t and e to the +i omega t. So, let us

say that this term represents the interaction, so this is very similar to the p dot A term in time dependent perturbation theory of the Schrodinger formalism.

The time dependent Schrodinger formalism time-dependent perturbation theory in which you consider the application for example to the famous what is it called Fermi's golden rule okay. So, in that context you have got the p dot A coupling between the atom and the applied electromagnetic field.

But that is a non relativistic formulation in the relativistic formulation as we have discussed at great length in the previous course in the unit 3 I believe of the course on atomic physics instead of the p dot A you have got the alpha dot A term. So, that is the coupling to an external field but we could use it commonly also to represent the response of the N electron Dirac Hartree Fock system to whatever was not included in the Dirac Hartree Fock.

What was not included the Coulomb correlations okay Coulomb correlations were left out of the Dirac Hartree Fock and what this stimulus would do inclusive of the correlation effect is that these Slater determinant functions the single particle functions are no longer what they were. They would change what were they, they were the solutions of the Dirac Hartree Fock and they were the solutions of the N electron system.

When the statistical correlation was included in the relativistic avatar in the relativistic formulation of that theory what did they include in addition to the statistical exchange they included the relativistic effects because they started out with the Dirac equation. But both left out something and that was the Coulomb correlation.

Which is what we did what we addressed using the Bohm Pines method or the Brurckner method the ring diagrams and so on right. So, this was excluded and as a result of this these single particle functions will no longer be what they were in the Hartree Fock or the Dirac Hartree Fock method they will change.

How will they change each element of the Slater determinant will change to what it was to something new? And this new is something it is a consequence of what was left out of the Dirac Hartree Fock. What was left out of the Dirac Hartree Fock was the correlation and the coupling to the electromatic field okay.

So, if that is that effect is taken into account then you have new orbitals and these are not just our orbital's these are the bi-spiners. So, these are the 4 components, so every single u that we

are talking about we are looking at in this later determinants. And what we see over here is not the same as the Hartree Fock spin orbital.

But it is the four component bi-spiner function which is which comes from the Dirac theory. Now these by spiners will be mixed by certain perturbed orbitals, so this is the space dependent part and this is the time dependent part. These will be perturbed by these perturbed orbital's the wi + and the wi- and with these new 4 component functions you can rebuild a variational method.

How did we get the Dirac Hartree Fock equation? How did we get the Hartree Fock equation? We essentially did a variational methodology right. We used a variational technique variation technique subject to certain constraints. What were the constraints in the Hartree Fock that the one electron wave functions remain orthogonal to each other and they remain normalized?

So, now we are going to have to do the same, we did it in the Dirac Hartree Fock by requiring the one electron 4 component functions to be orthogonal and normalized and we would have introduced some Lagrange variational multipliers and carried out that entire variational technique using that.

But now we have to do it one more time because now we are not using the same elements of the Slater determinant but new single particle states which will take into account the correlation effect. And these will then require you to carry out a variational methodology once again on this which will give you with these time dependent terms because this is the interaction term that you are now going to include okay.

These are the consequences that you are now going to include, so you will essentially have a time dependent Hartree Fock theory okay. So, this will require a time dependent Hartree Fock theory or it is a relativistic version is what you will call as the time dependent Dirac Hartree Fock formalism. And you can rebuild the time dependent Hartree Fock or the time dependent the Dirac Hartree Fock.

The time dependent Hartree Fock is what was done by Dalgaarno and Victor the time dependent Dirac Hartree Fock was done by Johnson and Lin and also Dalgaarno of course so he was also one of the key contributors to that. So this is the time dependent Dirac Hartree Fock. But now when you have all of these higher harmonics you will have nonlinear terms because of this okay.

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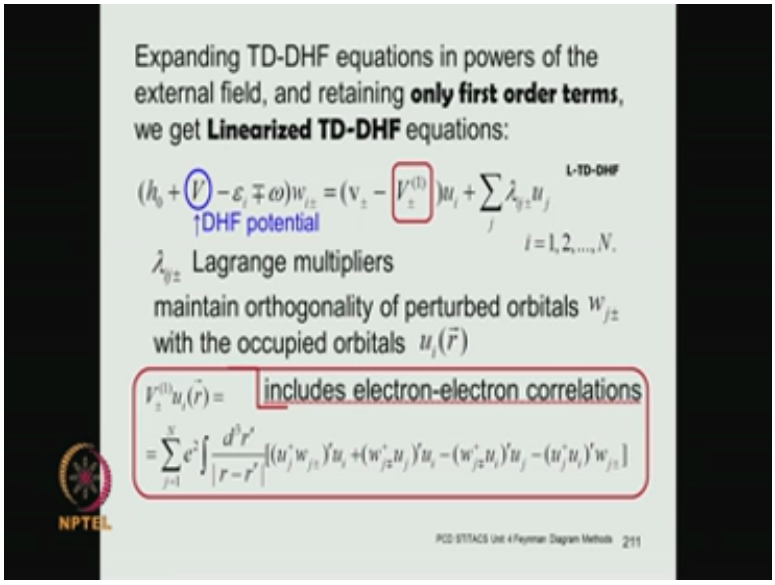

And out of these non-linear terms then if you make an approximation, so you can rebuild the time dependent Dirac Hartree Fock equations and retain only the linear terms. Now linearization if you remember was this key element in the Bohm Pines method because when we excluded those terms with random phases it amounted to throwing out certain nonlinear terms the terms that we did retain had linear term.

So, it is the linearization process which is common and which is fundamental which is why all of these methodologies these different routes to RPA are completely equivalent to each other. So, you have the linearized time dependent Dirac Hartree Fock equations that you get by retaining only the first order terms in this process.

And but when you do the self-consistent field methodology you have to introduce certain constraints. Because now the perturbed orbital's that you are including the w orbital's okay. These are the additional perturbed orbital's which are coming into our formalism which was not there in the Dirac Hartree Fock.

You will have to maintain that these perturbed orbitals must be orthogonal to the occupied orbitals. So, you have an additional constraint and because of that you have some more multipliers, variational multipliers which are again Lagrange method of variational multipliers.

So, the technique is exactly the same what you do is make use of these Lagrange's variational multipliers and carry out a self-consistent field variational methodology on the time dependent Dirac Hartree Fock, linearize it throw away the higher harmonics and then you get the linearized time-dependent Dirac Hartree Fock.

So, this V is the Dirac Hartree Fock potential which we have seen on also in the relativistic Hartree Fock or the Dirac Hartree Fock and this V plus or minus is what includes the correlation effects which was missing in the Hartree Fock and it was missing in the Dirac Hartree Fock.

So, these are the terms which include the electron-electron correlation effects and all of these relations are directly from the paper by Johnson and Lin using essentially the same notation as used in Johnson and Lin papers.

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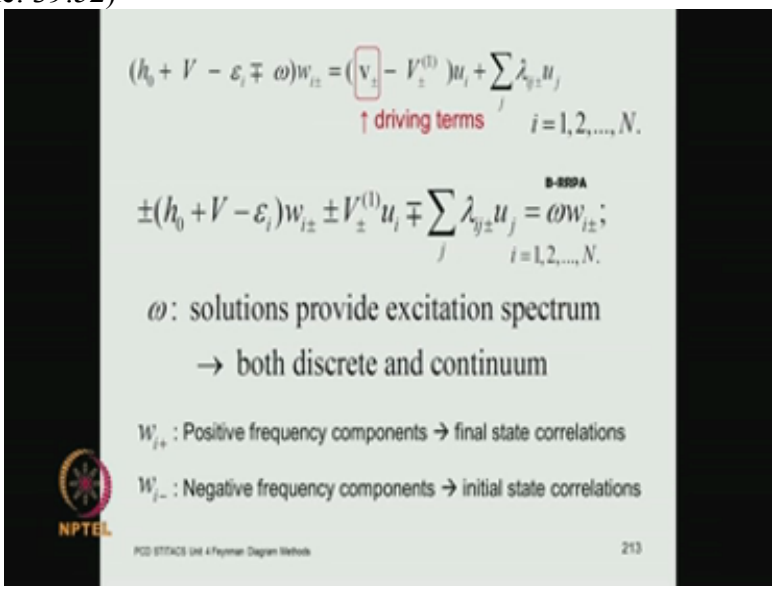

So, this is the term which includes the correlation effects and of course it has got these perturbed orbitals that W. So, it has the driving terms, so this is what is contributing to the correlation and you have got you get you can solve them at various levels what you do is first drop the driving terms and get what are called as the basic RPA equations.

Then of course you can write the solutions inclusive of the driving terms in terms of the solutions you get for this. So, this is a matter of detail and what this methodology enables you to do is to take into account the effect of the correlation which manifests as these perturbed orbitals.

And they take into account correlations in both the final state and correlations in the initial state because you know when you go backward in time you pick up the correlations you know if you identify a photon vortex. I am going to show you those diagrams and when you go backward in time you pick up the correlations in the initial state.

And you also pick up the correlations in the final state which we do in the RPA and in the relativistic RPA literature we refer to it as inter channel coupling when we are talking about the correlations in the final state.

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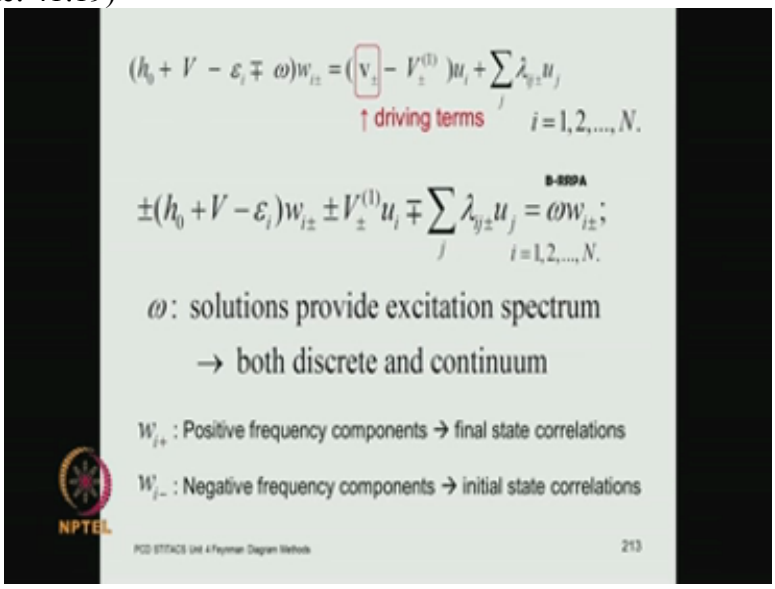

So, these are the corrections that were introduced by Walter Johnson Dalgaarno and Lin. And the solutions will give you the excitation spectrum, you get the bound state spectrum, you get the continuum and all the solutions can be obtained using this method in response to the driving term. So, both the final state and the initial state correlations are included in this.

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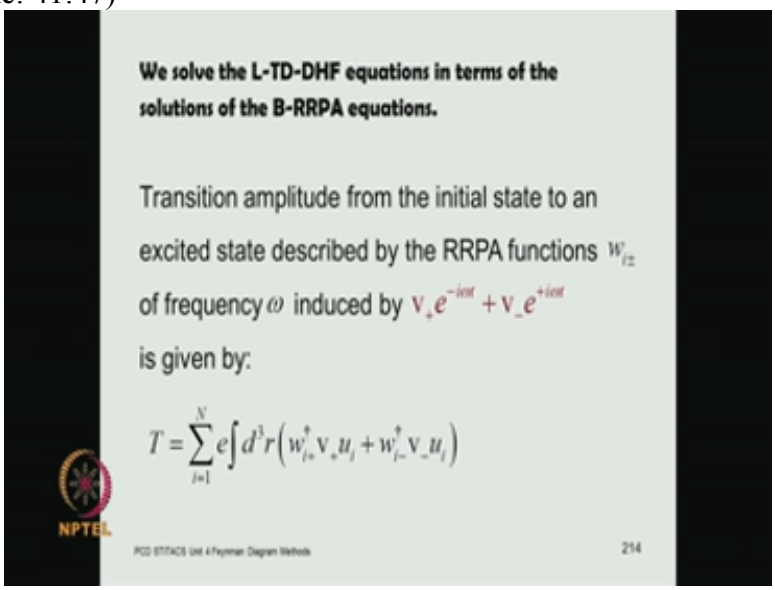

So, you can solve the inhomogeneous equation first get the basic RPA equations and then do the full RPA inclusive of the driving terms. So, you solve the linearized time dependent Dirac Hartree Fock equations in terms of the solutions to the basic RPA equations and then ultimately as is developed in great detail in this paper by Johnson and Lin. And there is no substitute to studying that paper.

So, I will only refer you to that literature you it the transition matrix elements there are other consequences which are of importance we discussed. I think in our previous course on the course and atomic physics then you can determine the matrix elements in the length form and also in the momentum form okay. And when you are dealing with a non-local potential we found that they often give you different results.

If you make use of a local potential like if you do a further approximation like the Slater approximation to exchange you get a local potential and you will get essentially the same result that is not because the method is better but only because the approximation makes the potential local. So, now we do have a non-local potential okay.

We do have the Hartree Fock potential or rather the Dirac Hartree Fock potential. We do have the exchange terms, so we do have the non-local terms nevertheless this is a beautiful feature of this approximation which is the random phase approximation that if you determine the transition matrix element.

And the transition amplitudes it does not matter whether you do it in the link form or the velocity form. And this was shown by Dong and Lin in one of the earlier papers I can give you the references many of you probably already have it. It turns out that this when you carry out the summation over all.

The possible correlations which are included within the subset of the choice of the random phase approximation which are the ring diagrams and the corresponding exchange then the length form of the matrix element and the velocity or the momentum form of the matrix element give you essentially the same result.

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So, this is a matter of detail and what you do is to determine not just the transition matrix element and the photoionization cross section but you get a number of other properties because as a physicist you will always like to do a complete experiment. You will like to get maximum information about a system and what kind of information you can it depends on what measurements are compatible.

Because certain measurements are not compatible with each other in quantum theory this goes down to the uncertainty principle itself okay. So, you have got a fundamental measurement process which results in a superposed system to collapse into an Eigen state corresponding to the measurement to the property that you are measuring. And all the properties which are compatible with each other can be measured together.

But those which are not compatible cannot be measured together and the operators corresponding to them would not commute. So, you like to do a complete measurement and what constitutes a complete measurement is determined essentially by the quantum uncertainty principle and its consequences to measurement and how it is reflected in quantum theory by the choice of operators which commute with each other.

So, these complete set of commuting operators that we talked about the CSCO or the complete set of compatible observables. And then what goes into the complete set of measurements in the photoionization process is not just the cross-sections but you can also determine the spin polarization states of the photoelectrons.

You can determine the angular distributions okay. So, you get the angular distributions and all these relations for the angular distributions and the spin polarization parameters these are

worked out in details in the papers by Johnson and Lin in this phase Drive 1979 or 1980 this paper by Johnson, Cheng, Huang and Le Dhorneu okay.

Huang is the one who wrote the codes for the spin polarization techniques along with Walter Johnson. So, you can measure all of these properties and here of course I am referring only to the dipole approximation okay. In the quadruple approximation you have these angular distribution parameters that you call as what is it delta zeta and so on right.

So, those are the things which go into this and all of these parameters can be determined using the very powerful techniques of Walter Johnson.

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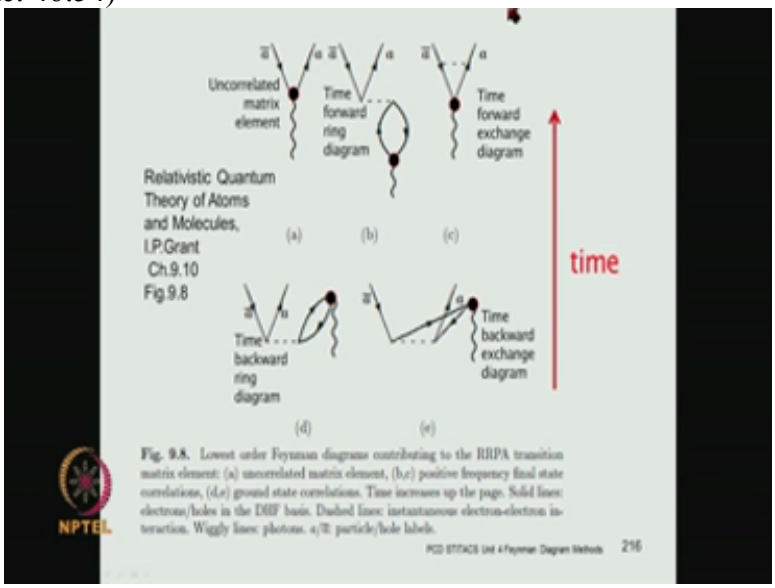

Essentially these are the diagrams which go into the analysis, so you have got this photon vertex over here. You have got time going from bottom to the top okay. What the RPA does is to take into account the ring diagrams which are both time backward as well as time forward.

And these diagrams are from Grant's book relativistic quantum theory of atoms. You will also find them in various papers by Johnson and some others. So, you have in this diagram the photon is represented by this wiggle okay and the interaction by this dash line. So, this photon interaction takes place at this vertex and you have got a ring diagram.

So, with reference to this point of interaction between the photon and the atomic system this is the time backward ring diagram. And here you have got a time forward ring diagram okay. So, what the RPA does is to take only the ring diagrams but also the exchange corresponding to it and these are the interactions these are the correlations which are included in the RPA.

But you of course you can go beyond the RPA you can go beyond RPA in the sense not necessarily better than RPA whether it is better or worse depends on whether it gives you a

better account of the experiment or not okay. But then you can do a time dank of by taking only the time forward diagrams. You can do a multi configuration time dank of which some of you have done.

In which case you take the initial correlations into account by doing an explicit configuration interaction you can do so by using a multi configuration Dirac Hartree Fock code which is developed by Grant and his group or which is typically known as the Grasp code okay. So, using Grasp you can do a multi configurational Dirac Hartree Fock to represent the initial state.

And to take into account the correlations in the final state you can do an inter channel coupling as you did in the random phase approximation okay. So, you can have the time forward diagrams corresponding to that to the inter channel coupling and that will be some sort of a mix of an RPA and a non RPA technique.

Now in some sense it is better than RPA because it will let you take into account some of the non RPA correlations but in some case it will not be as good as RPA because some of the terms that you would have included in the RPA have to be compromised with. Because what the RPA does effectively and that is a matter of detail which we have not discussed that you can take into account the ring diagrams to all orders of perturbation theory.

You cannot do that when you do a limited basis like you take a few configurations to go into your grasp self-consistent field. So, you do a multi configuration Dirac Hartree Fock or a multi configurational Hartree Fock and then you get some of the correlations but not to all orders of perturbation theory. So, you get some non RPA correlations but not to all orders of perturbation theory.

Whereas in RPA you get some of the correlations but to all orders of perturbation theory, so there is a matter of give and take and there is a price to pay you cannot do everything and get an ideal solution which is good in every respect. The reason you cannot do it, is what was stated at the very beginning even of the Hartree Fock formalism.

That if you are looking for exact solutions having no body at all is already too many you there are no exact solutions even for the vacuum state. So, when you have an electron system you do not have exact solutions you have to make approximations and the challenge which theories has is that you make as good an approximation as you can to explain the experiments you are interested in that is where the challenges.

So, you need a consistent theory and what you do in the RPA or the relativistic random phase approximation is to take into account all the time forward diagrams. So, here you have got the interaction taking place at this vertex you have got a ring diagram this is the direct term, this is the exchange term here this is the time backward ringing diagram.

So, this takes into account all the correlations in the initial state and then there is a corresponding exchange term because exchange is something by default as I mentioned automatically it ought to be included and it is included in most studies okay. Whenever it is not done of course you will get some errors.

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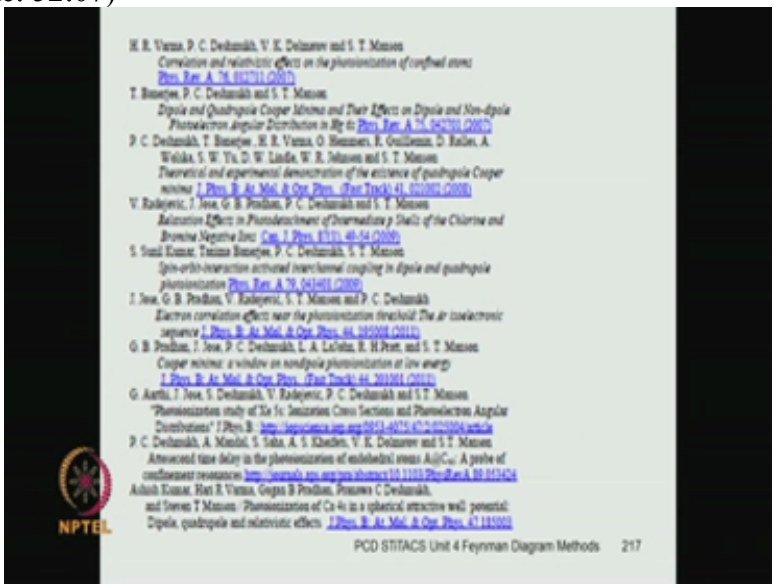

So, I would like to acknowledge the contributions of all of you who are taking this course and you have the first paper here by Hari but there are many others who have contributed Tanima, Sunil, Jobin, Gaghan, Aarthi, Ashish, Sindhu, so many have contributed and even prior to Hari of course there are various at the students who have contributed to this.

This is only the set of some of the references to papers in which the relativistic random phase approximation has been used in our group purely IIT Madras and of course in collaboration with many others and the principal collaborators of course are Walter Johnson whose codes we have been using all the original codes were written by him.

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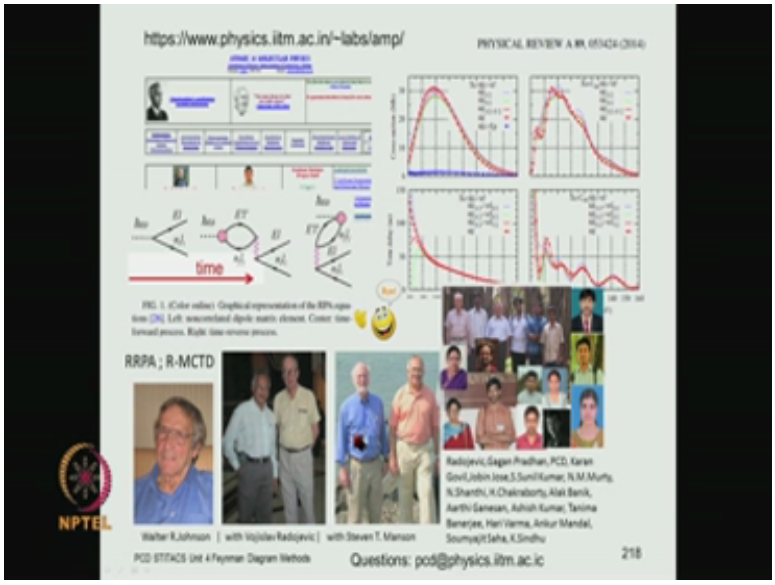

Voya who many of you have worked with, Steve is of course a long term collaborator and he has been with us throughout this development for more than three decades, beginning with some of the earliest papers that I was involved with although the earliest ones were of course with Walter and then many others students graduate students post docs other collaborators there are many whose pictures are not here.

In particular some experimentalist like Dennis Lintel and so on who have contributed a lot to many of our studies. So, you will find all the references and so on at our web page which is this and this is one of our latest contributions because the methodology has been used to many different kind of situations not just the photoionization of free atoms.

But photo ionization of confined atoms and Hari was the first one to start working on confined atoms then we studied photoionization not just in the dipole approximation but also in the quadrupole and there are various contributors to that and Tanima and Gaghan and many of you.

So, your are the pictures of many over your some of you are sitting in this hall some of you in these remote locations and some elsewhere or maybe having just a cup of tea or a nap. So, with that I think I will conclude this unit and there are several leads to follow up and I would be very happy to take some questions.

So these studies have been applied to confined quantum systems then to studies in which the dipole studies have been carried out, the quadrupole studies have been carried out, the interference between the dipole and quadrupole which gives rise to peculiar angular distributions have been studied.

There are various other applications including the determination of the phase shifts and the time delays where these are some problems of current interest because earlier on it was believed that when a photoelectron is knocked out of the atom it is kicked out instantly but there is a little bit of delay which is of the order of some auto seconds.

So Ankur, Samajit, Ashish there, Hari some of you are working on these problems Jobin also. So, what is done in these studies is that these time delays are determined and in this particular figure that we have over here we have the time delay in free atom and in the confined atom. So, you feel you see certain oscillations which come as a very beautiful signature of confinement.

But this is the matter of detail and you can refer to the original literature for these applications. Any other question, if not let us conclude this unit.