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

Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 23
Bohm-Pines approach to Random Phase Approximation

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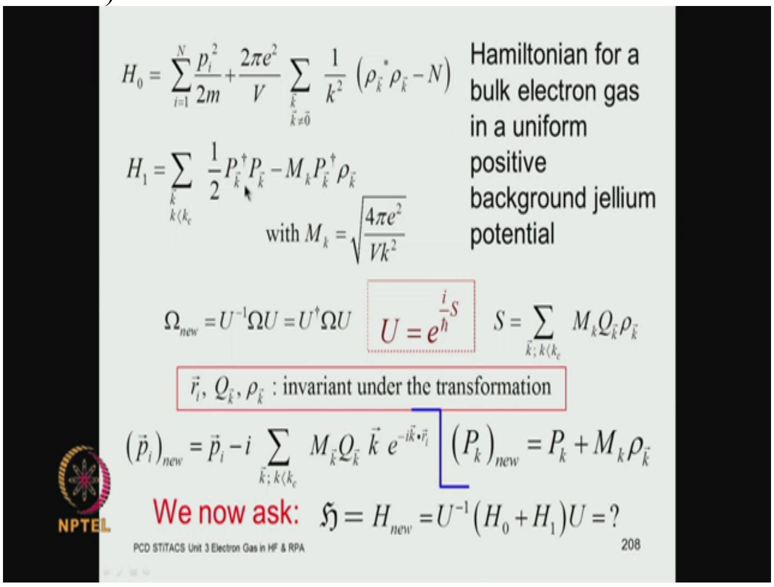

Greetings, we have today, the RPA in the classical model that we had already discussed, so we are going to get the quantum treatment completed which we already initiated in the previous class. So, let me remind you that we are dealing with a Hamiltonian for a bulk electron gas in a uniform positive background Jellium potential and this is the Hamiltonian for this system.

So, I will recapitulate some of the essential results that we got in our previous class, so spend a few minutes on that and then we will continue from this point. We introduced an auxiliary Hamiltonian in which Mk is defined as such. This is an auxiliary Hamiltonian it is made up of these operators P and Q which is sitting over here okay.

So, this is the operator that we use because this generates a unitary transformation on the Hamiltonian to a new Hamiltonian. And we choose this auxiliary Hamiltonian because of some special properties that it has. So, let us quickly recapitulate what these special properties are.

So, under this unitary transformation the new coordinates and the position operator and the components of the Fourier components of the charge density they are invariant under this unitary transformation. The momenta however change okay, the new momenta which are introduced. So, these new momenta are canonically conjugate to the new coordinates Q. So, capital ki capital Q and capital P are the new momenta and coordinates.

They are canonically conjugate, so they do not commute and their commutator is according to the QP of quantum theory. They are not hermitian but they are used in a term H1, which is the auxiliary Hamiltonian which is hermitian. And the question we are going to discuss today is if you now transform the Hamiltonian H0 + H1 then what does the new Hamiltonian describe? What kind of a system does it describe? Okay.

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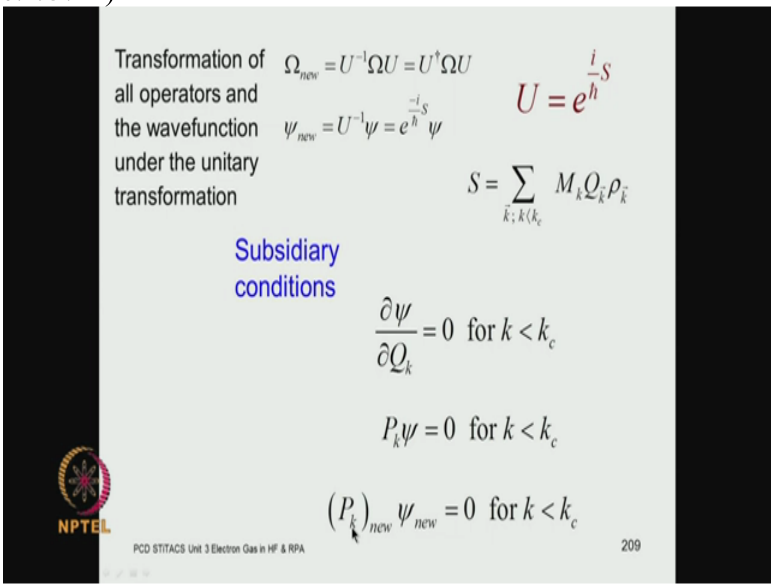

How do we interpret that system which is represented by the new Hamiltonian? So, this is the transformation of an arbitrary operator and the new wave function will be U inverse psi. So, these are our unitary transformation operators. We do have the subsidiary conditions that the wave function cannot depend on any additional degrees of freedom. We already recognize that k must be less than kc.

And whenever k is less than kc the new the wave function cannot depend on any additional degree of freedom because all the dependence on coordinates is already explicitly spelled out on the dependence on the lower case q which are the original coordinates we used in setting up the Hamiltonian for the electron gas.

Which means that the derivative of the wave function with respect to the new coordinates, the auxiliary coordinates vanishes which means that the momentum operator operating on this wave function would vanish because the momentum is nothing but - ih cross del over del Q. And it also means that this relation which is the result of the operation by the new momentum on the new wave function this would also go to 0.

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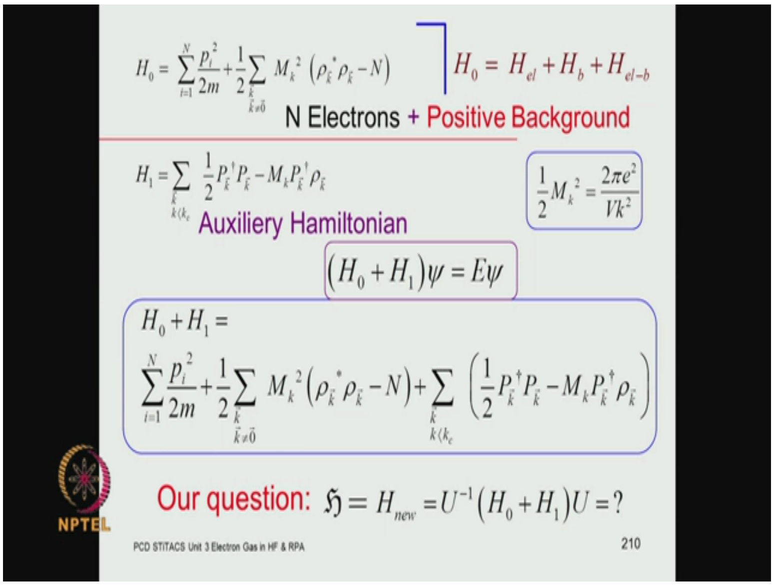

So, essentially the idea of this auxiliary Hamiltonian is a very clever one because what it helps you to do is to write a Schrodinger equation in which the Hamiltonian is not the original H0. H0 was the Hamiltonian for the N electrons together with the positive background. So, all the background effects are certainly included over here there is the background-background interaction.

There is an electron background interaction all of these three terms go together to define this H0 which is written here, so this is the same H0. But what we have done is remove the k = 0 component that is the one which kills the background and the electron background terms. So, this auxiliary Hamiltonian helps us describe the same system. It gives you the same Schrodinger equation as such.

And we now add these two terms, so you have got two terms in H0 another two over here. So, we write this summation which is the new effective Hamiltonian which is made up of the real Hamiltonian for the electron gas together with the auxiliary Hamiltonian and we ask how will this sum H0 + H1 transform under the unitary transformation that we have defined. This is our question and what kind of physical properties does the system have.

And how do we interpret it. So, the system is already there we are not getting a new system out of it but we are interpreting the system in a new form.
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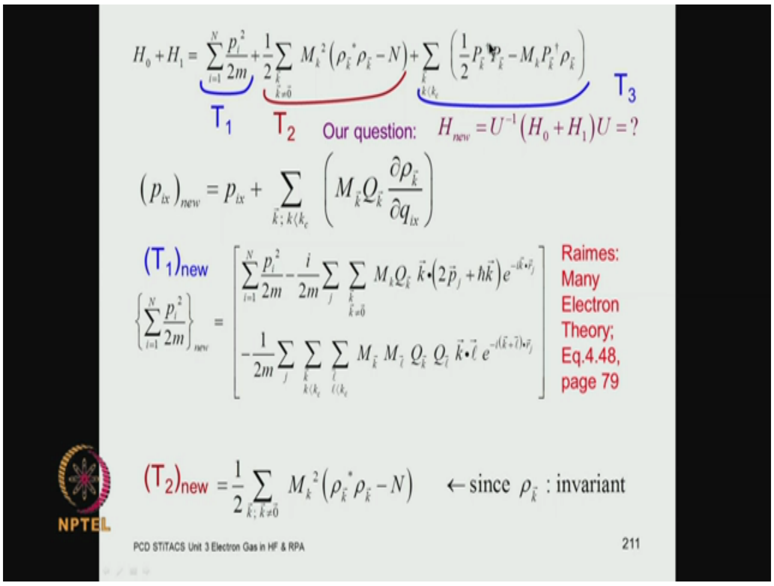

So, let us look at it term by term and there is a little bit of cumbersome mathematics. It is not very cumbersome as such but a little bit cumbersome. It is certainly not any difficulty mathematics, it is elementary mathematics but it is slightly cumbersome because there are large number of terms which are involved. You have to keep track of which term goes where okay and then assemble all the terms.

So, I am going to do it piecewise. So, first I will deal with the kinetic energy term which is T1 then I will deal with the second term which I will call as T2 and then the third term which I will call as T3 and then we will look at the transformations of each of these terms and then put it all together. So, there is a good bit of bookkeeping to be done and these equations will flash on your slide they come up just at the stroke of a key.

But you cannot write them fast enough in your notebooks but the good thing is that you do not have to because the PDF files for all of these slides will be uploaded at the course webpage very soon. So, you will have access to all of that. So, you do not have to write anything but just keep track of how the terms are kept, are developed and then we will assemble all the terms.

So, there are plenty of terms which will come because whenever you carry out a transformation you get a new set of terms and we have done this when we did the other transformation big transformation exercise and quantum theory. When we did the Foldio Dyson transformations of the Hamiltonian, we had plenty of terms popping out of the transformations. So, this is somewhat similar in some respect.

So, this is how the lower case momentum operators were transform okay. This we have seen already, we have seen that the coordinates do not transform but the momentum operators they do change under the unitary transformation. And the lower case momentum transforms according to this relation. And therefore you have to take, find how the term T1 will transform.

Now this is already a large number of terms and it takes a little while to do this. So, I have not spelled out all the results but if you just put in the right hand side of this relation and carry out the transformation of the T1 this is what you will get. Some of the intermediate steps are given in on page 79 of the book by Raimes.

So, you can catch up with that if necessary okay. Look at the other term T2. Now T2 term is easier to handle but we are going to you know discuss the T2 term in some details. It is easy to handle so far as this transformation is concerned because it actually remains invariant because it is made up of the Fourier components of the charge density.

And these terms do not transform Mk does not transform. So, T2 new will be the same it will remain invariant okay. The first term transforms according to this relation over here. Now we have to work with T3 and this has got two parts one is coming from the P dagger P and second term is coming from Mp dagger rho.

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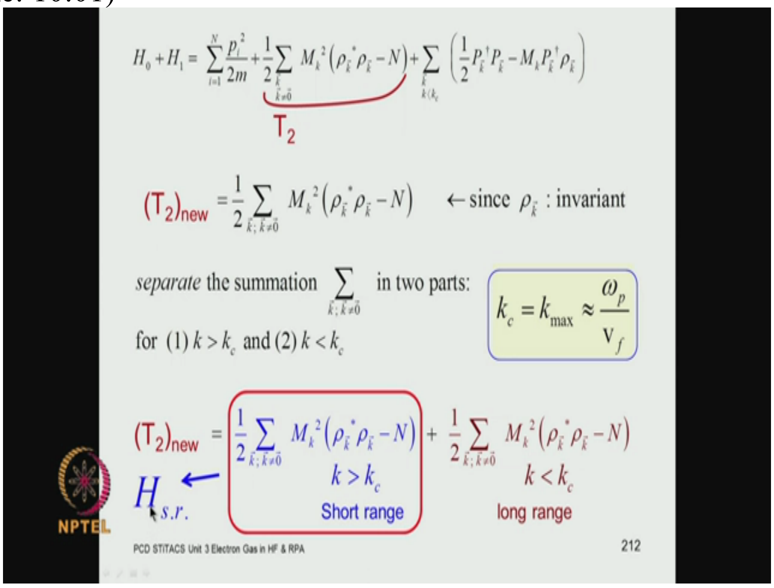

So, these are the three terms T2 we know is invariant, what we will do is to separate the term T2 into two parts there is a summation over k for k not equal to 0 okay. But we know that there is a certain upper limit on k. So what we will do is to break this sum into two parts one for k greater than the upper bound of k and the other corresponds to the values of k which are less than kc.

Now kc is this upper bound on the wave number we have discussed this in our earlier discussion. So, this corresponds to k larger than kc distance is the inverse of it, so this is the short-range term okay, k is 2pi by lambda. So, the distance appears in the denominator, so this is the short-range term and this is the long-range term.

In other words whatever interaction is represented by the term T2 in the full Hamiltonian is broken into a short-range interaction and a long-range interaction. This is the short-range interaction which I will write as H subscript sr for short-range.

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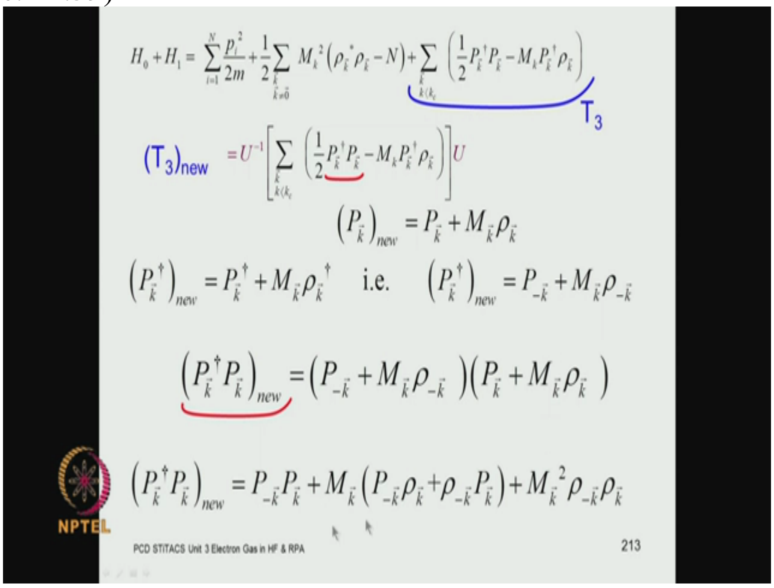

What about the term T3, now T3 is made up of these two parts, so the transformed operator resulting from the unitary transformation of the term T3 will be U inverse T3 U, so you need the new momenta okay. And we know that these new momenta the uppercase momenta these are the auxiliary momenta that we introduced. These momenta are not invariant under the unitary transformation you get new operators.

And the new operator is the old operator plus Mk Rho k of this result we obtained in our previous class, so we will use this. So, this is the new momentum this is its adjoint. So, P dagger is P dagger this is the adjoint of the first term. And then the joint of the second term, so which is Rho dagger but Rho dagger you know can be written as Rho - k that also is is a result that we have discussed in our previous class.

So, you have to transform this term, so this transformation will be made up of P dagger P this is P dagger okay which is P - k + Mk Rho - k keep track of the signs over here they are very important okay. We have all; the reason you are having this difference over here is because P dagger is P of - k right. This is not a self-adjoint operator okay. The auxiliary coordinate and momentum operator’s capital Q and capital P are not self adjoint.

But the hermitian they generate the Hamiltonian they generate the H1 the auxiliary Hamiltonian that they generate is in fact a hermitian. So, this is the new P dagger P and you expand these terms, so you have got P - k Pk then you have got Mk which is common from this term and this term and in this term and this term and the last two will give you a term which is quadratic in N.

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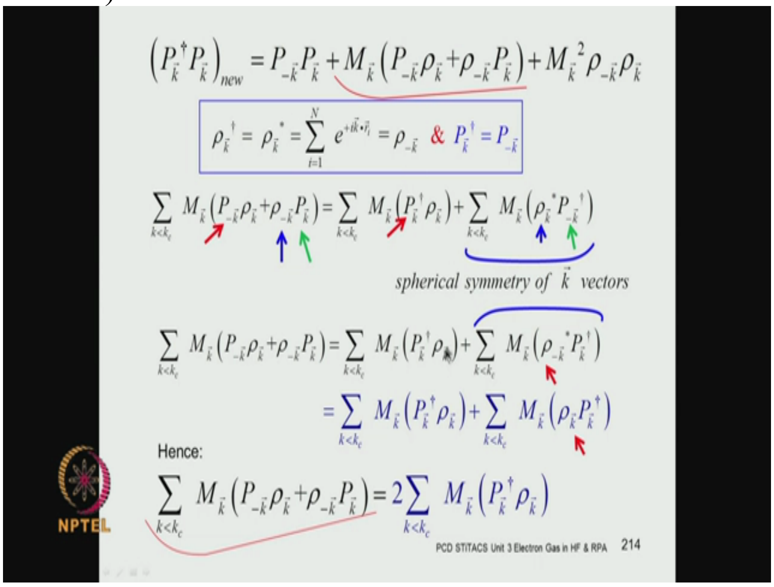

So, these are the four, these are the terms which come out of this. So, these terms have been written here at the top of the slide. Let us look at this middle term okay and this is what I had warned earlier then there are a large number of terms and on one slide only so much as can be written. So, at the end we are going to compile all of these terms and then figure out what they all add up to.

So, you just have to follow the reasoning and how these terms are handled are not worried about taking down notes and writing them out explicitly because all of this information is available. So, here you are, so you have to find what this middle term is and you will have to sum over k for k less than kc okay. So, this is that summation that you have to carry out. So, I now have written these two terms separately.

The Rho of - k is Rho k star okay, Pk is the same P - k dagger. So, I am only substituting it is very simple mathematics but a little bit cumbersome. So, notice that instead of P - k you get Pk adjoint. Then over here you have Rho - k which is Rho k star. Then here you have Pk instead of Pk you have got the adjoint of P - k okay. That is according to how we have chosen these auxiliary operators.

Now here you have got a summation over all the wave vectors. But this there is a symmetry in the k space which we discussed yesterday also. So, we can easily carry out this summation over - k just as well. It does not matter whether you carry out the summation over + k or -k because you are going to pick up under the summation all vectors in the momentum space. So, you can write this Rho k star as Rho - k star and P - k dagger as P + k dagger.

And that is because of the symmetry; Mk of course is symmetric because Mk is defined through the square of the magnitude so it does not matter okay. So, now what is Rho of - k star Rho of - k star is Rho k itself okay, Rho of -k is Rho k star. So, Rho of - k complex conjugate is the complex conjugate of this term which is Rho k alright.

So, now look at these two terms this term is the same as this term, so the right hand side becomes twice one of the two terms. So, this is a result that we will use now.

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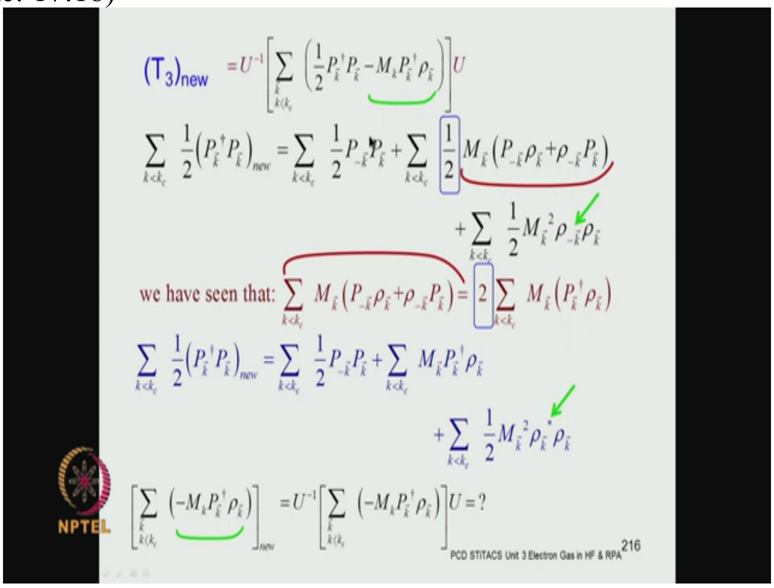

This is the whole transformation that we have to look at. This is the transformation of the first term right, it has got a term which is quadratic in N and it is this term that we were examining and this term we find is twice this term okay. So, we will keep track of all the terms and then put it all together all right. Now this we have done we have seen this part remember that there is a half over here and there is a 2 over here.

So, when you rewrite this you will have to keep track of this half term and this 2 over here. So, using this half and this 2 over here, you can write this left-hand side same left hand side as the same first term and instead of this second term you write this term but you take care of this half and 2. So, this is a sum for k less than kc of Mk P dagger Rho k right, so this is the last term.

In the last term, we have also made use of what we know about how Rho - k and Rho k star are related they are equal to each other because of our result that we obtained yesterday. Now we have to ask how does this term transform okay. We got this one we got the first term, we now have to find how the second term transform second term in T3 second of the third term if you like okay.

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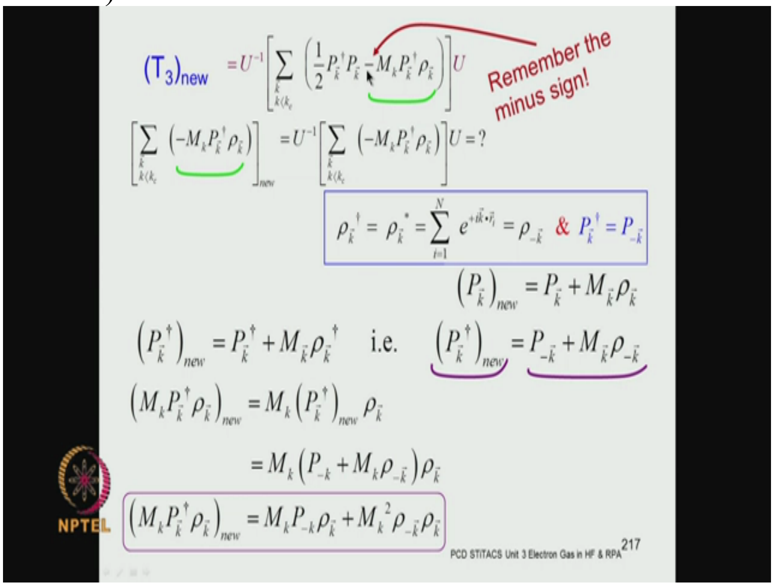

So, here we are we have to find out the new which is the U dagger operating on this and what will this give us. This is our question now, we have to remember that these are the primary relations that we are using. We know that the new momentum operator is not invariant you get Pk + Mk Rho. You have the relation for the adjoint because it is the adjoint which is important over here in the second term okay.

So, this adjoint we know how it transforms, we know that Pk dagger is not equal to Pk because this operator is not self adjoint it is instead equal to P - k right. So, what does it give us, we know that this term when you transform it will give you Mk Rho dagger new Rho k right. So, it is the transformation of this term, this and this remains invariant, P dagger is given by this right hand side and we put these two terms over here.

And now again you get a term which is linear in M and another term which is quadratic in M, so now we have got the transformation of this term but remember there is a minus sign over here. So, when we put all the terms together we will have to plug in the minus sign.

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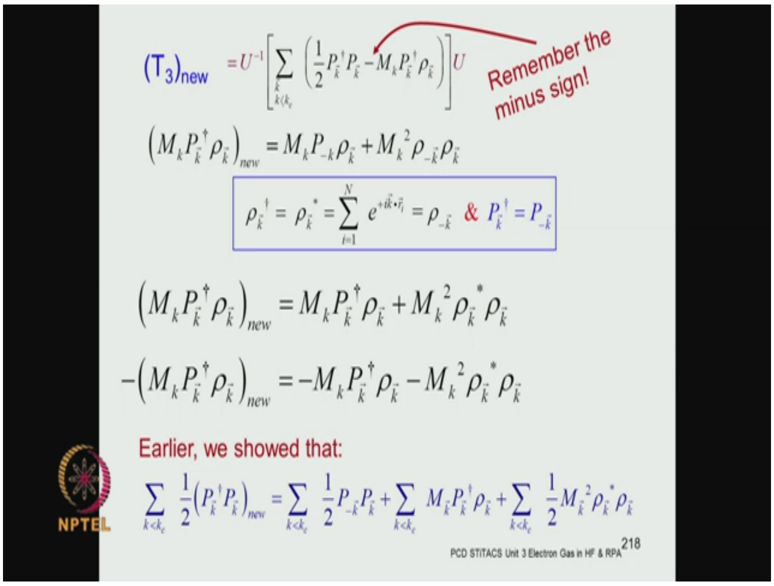

So, this is the transformation of the second term here. These are the primary transformation relations that we are using, P - k is the same as Pk dagger right, because this operator is not self adjoint you have got the quadratic term here, Rho - k is the same as Rho k star. So, you have got the Fourier component Rho k complex conjugated. And this is Rho k. Now we need the minus sign, so let us put it here, so this is the minus sign.

So, you get a minus sign behind this and a minus sign behind this. Earlier we have already found this term, so now you can get the complete transformation of the term T3. So, essentially we wrote the expression for the transform term T1, T2 was invariant and the transformation of T3 is given on this slide over here okay.

So, now we have got all the terms right. You have to remember that k, the magnitude of k this summation is restricted to k less than kc.

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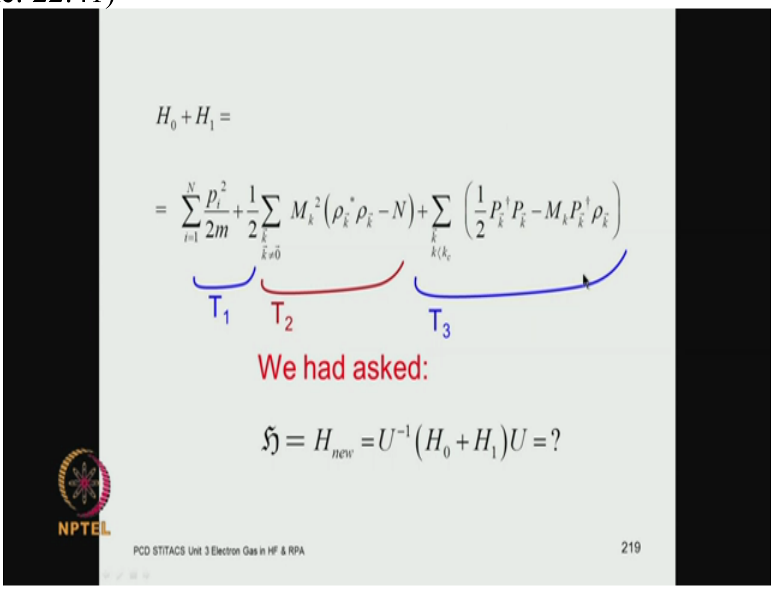

So, these are the three terms and this is the question that we had raised and now we can answer it because we know how the first term transforms which is the kinetic energy term. We know that the second term remains invariant and we know how the third term transforms. So, we can transform the complete Hamiltonian.

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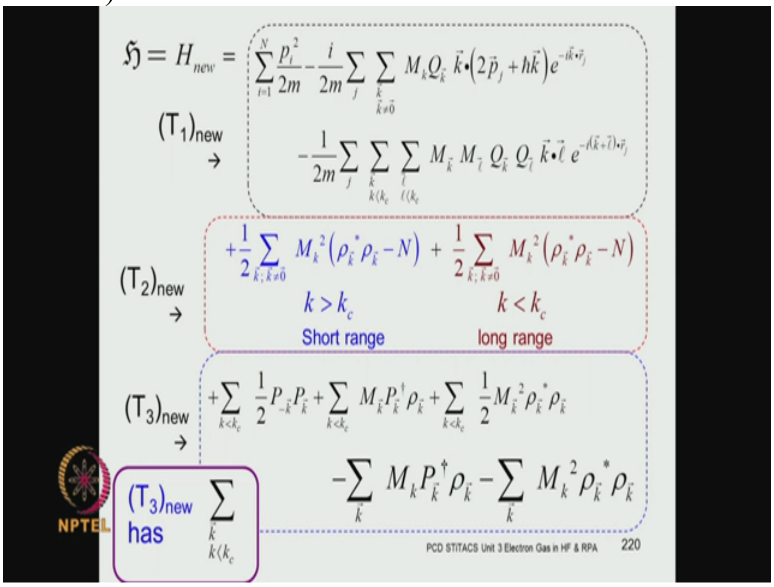

So, let us write the new Hamiltonian, so this part comes from the term T1 which is transformed okay. Then you have the second term which is invariant however we wrote the second term in two pieces. The second term is a part of the Hamiltonian and as a part of the Hamiltonian it is going to represent a certain interaction of the system. The system is whatever the system is as described by the new Hamiltonian.

That is the system that we have to interpret, so it is made up of the kinetic energy parts and the potential energy parts which are the interactions. And the interactions are represented by everything which does not correspond to the kinetic energy part. So, those interactions, these are not new interactions you are adding on. They already belong to the system; they are internal to the system.

It is only that they were not dealt with in the Hartree Fock theory nor in the perturbation theory. Where are they coming from they are coming from the correlations because the Hartree Fock formalism does address the statistical correlations namely the spin correlations which are also equivalently called as the Fermi Dirac correlations.

The Hartree Fock theory also does a static average of the Coulomb interaction including the exchange which is coming from statistics which is why the Hartree Fock wave function is an anti-symmetric determinant. But what the Hartree Fock leaves out are the Coulomb correlations. So, they are already there in the system.

So, they are already there in this Hamiltonian but they will now become manifest because of the transformations and they are sitting in some of these interaction terms in the new Hamiltonian okay. We have not ignored them and this is the transformation of the third term which we just discussed few minutes ago in our previous slide okay.

So, we have put all of these terms together and this physical system is now represented by a combination of T1new + T2 new + T3 new and we expect to find the plasma oscillations in these terms. So, it is there but it has to manifest itself right.

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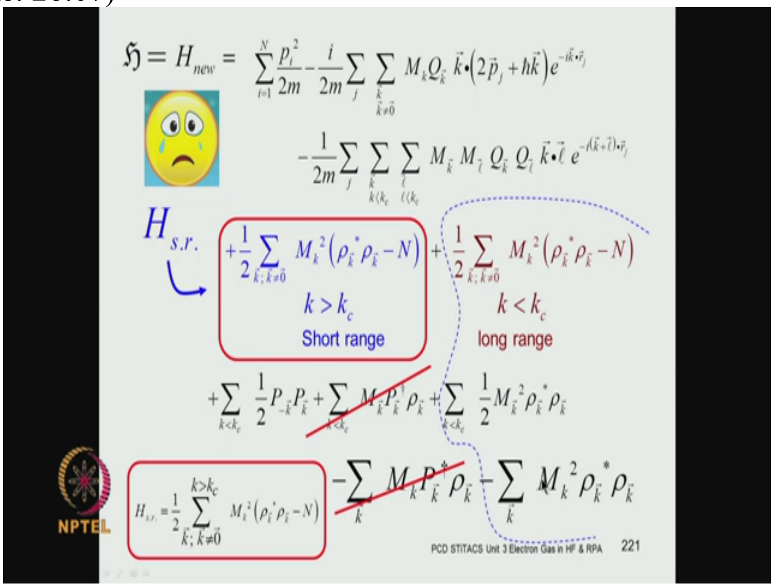

So these are the terms and this is a lot of work we certainly expect that this system will represent to the collective behaviour. The correlated dynamics of the electron gas everything is included in it. The electron-electron interaction, the electron background interaction, the background-background interaction, so this is the Hamiltonian for the full system its exact there is nothing is no approximation made so far.

It is exact but it is a lot of terms and what is the physical content of each term is not very apparent at least in the form in which these terms present themselves to us on this slide. Now good thing is that this term cancels this, so there is some relief okay. If you notice this is the same term as this, this comes with a plus sign this comes with a minus sign, so you can cancel them okay.

So, there is some relief. Now what else can we do to simplify them because there are too many terms and you have to recognize some patterns in them. (Question time: 27:28-not audible) No you even in that you still have the summation which is less than kc. It is only the second term in which you have separated the summations over k less than kc and summation greater than kc.

So,(Question time: 28:00-not audible) so in these two terms you have got the same range of k okay. This part is already recognized as a short-range part.

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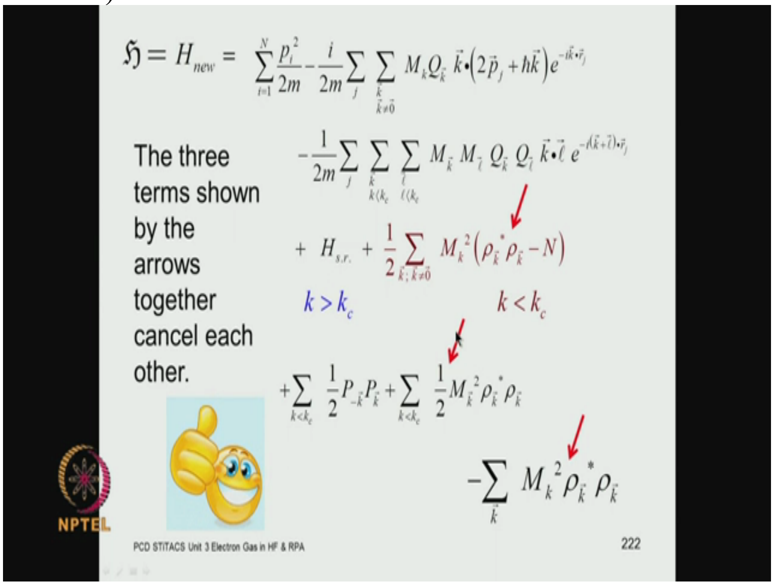

Here you have; if you look at this term on this term and this term okay, if you look at these three terms you will find that they are they together cancel each other because this is this comes with a plus half sign this also comes with a plus half sign and this comes with a minus sign. So, these three terms together they cancel each other okay.

So, the only term with k greater than kc is here. So, these three terms together cancel each other and that gives us a little bit of respite because we managed to get rid of two terms which were equal and opposite. Now we have three terms which combine to cancel each other.

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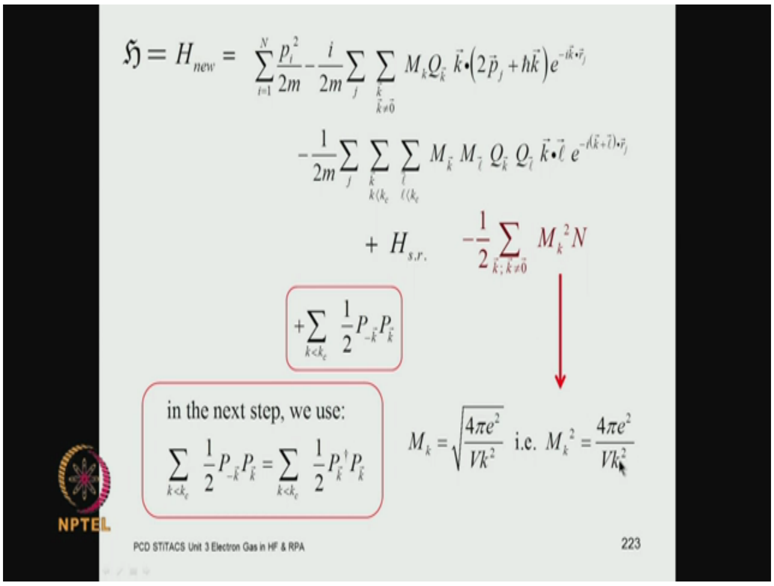

So, now there are less terms to work with okay. The relationship is beginning to look a little compact but it is still cumbersome but certainly there is some respite. Now Mk square N you know that Mk depends on this k square in the denominator. So, Mk really does not matter with us it does not change with respect to sign. You are working with Mk square, so you can redirected this term in terms of this 4pi e square by Vk square factor.

You have this term but P - k is the same as Pk dagger and Pk is written over here. So, we will rewrite this whole expression which is now looking a little bit of little bit compact but we will rewrite it by substituting this box by this box which we know is correct and by replacing this M square by 4pi e square by Vk square.

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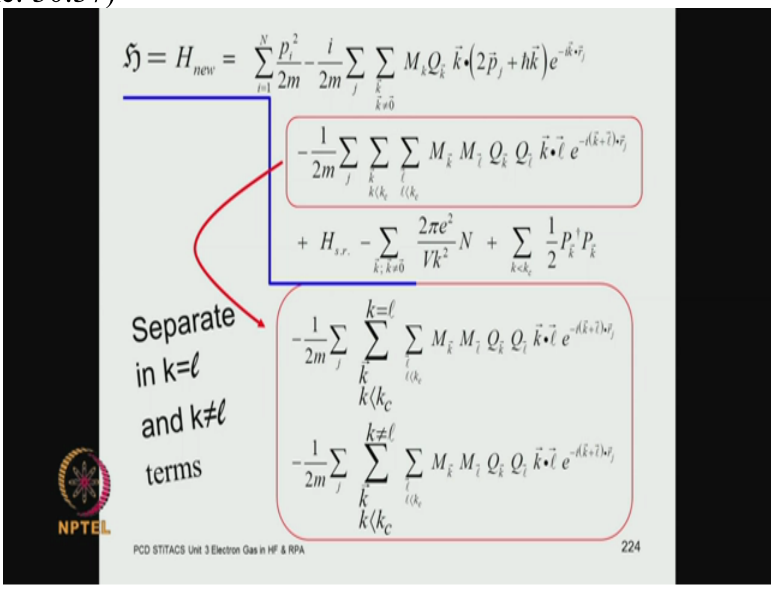

So, when you carry out these substitutions. Now the relation looks like this, so this is the form that we will actually analyze further. Nothing is lost all the terms have been kept track off they are collected together explicitly. Now look at this term over here, this looks a little messy and before we simplify it we will make it messier okay.

So, what we will do is to separate this double sum this is the summation over k in summation over l. We will separate it one for l = k and the other when l is not equal to k. So, we will deal with this term separately.

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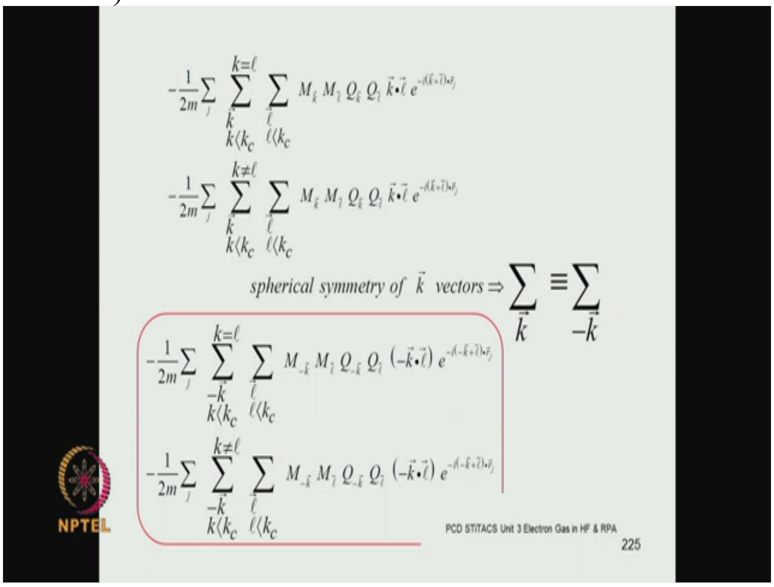

So, these are the two pieces one corresponding to l = k and the other corresponding to l not equal to k. Now what happens with these terms you also have the spherical symmetry, so summation over the vector k and the summation over the -k give you the same result, so we take advantage of that.

And write this term as summation over –k. So, if this was some over +k, so instead of +k, we have a -k this was some over +k, we have a sum over –k here. Here you had Mk, you have a -k which we know is the same as Mk because Mk does not change but then you have Qk going to Q-k that is Qk dagger as we know right. So, we will use that in the subsequent step. So, this is Ql it is the k which goes to –k. So, this k goes to –k, Ql remains the same as Ql.

But k goes to -k okay, and it is the same thing in the second term. So here also this k has gone to –k, this k has gone to –k, l remains Ql remains the same as Ql. But look at the exponents also you have k + l over here, which goes to -k +l here then likewise the k +l over here goes to -k + l over here okay. So, we have to do it systematically for every term.

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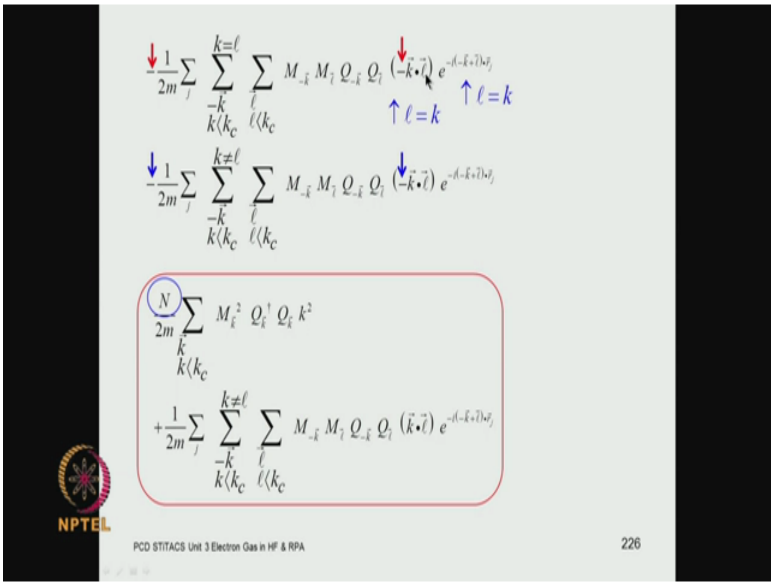

So, I have just written these terms together here at the top of this slide. Now notice that there is a minus sign here in a minus sign here. So, these two minus signs will give a plus sign for the first term. Likewise there are there is a minus sign here in a minus sign here. So, again you get a plus sign right. What else you have l = k over here. So, you will get k dot k, so you get a k square.

What else we have you have got l = k here as well right. So, l - k will give you zero, so you get e to the power 0 here. So, you get a factor of k square because of this and you get e to the power 0 which is equal to 1 which means that you are going to add one to itself as many times right. So, you have for l = k, you will get e to the 0 and when you add 1 to itself as many times and how many times would you add 1 to itself?

As many as the single particle fill states are as occupation number of states are. So, that will give you the total number of electrons this is the k square coming from this l dot k when l = k. So, you have got the k square, so this is what you get from the first term and this is the second term where this sign has already been annulled by this minus sign. So, you get a plus here and a plus here you got a k dot l.

But in the second term k is not equal to l, So, these are the two terms Mk of course does not change when the vector k goes to - k and now we use the spherical symmetry again and go back to the +k notation. So, we had done this intermediate step just for some intermediate convenience that we got. We will go back and exploit the symmetry over the k vectors. So, once again we change the sign over here.

So, instead of Q -k we have a Q +k this is the term corresponding to l = k, so this becomes Qk, so you get a quadratic term in Qk here this is Q dagger Q but this is not self adjoint. And then you have got a k square coming from this l dot k for l = k from here you get 1 and this 1 has been added to itself N times giving you this factor N over here. So, this is the summation of the two terms.

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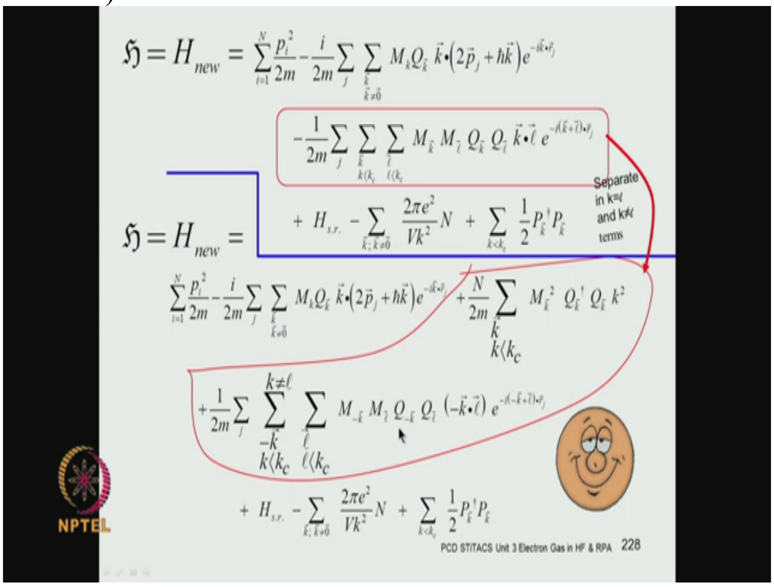

Now put all of those terms over here now, so all the terms are kept track off now, the transformation of T1 the transformation of T2 and the transformation of T3 and all of these terms are together over here. Now this term looks a little complicated right. This is the messy term it is quadratic in the coordinate in the auxiliary coordinate Q. This is the one which we separated in k = l and k not equal to l terms right.

And on separation it gave us a combination of this term and this term. And this new Hamiltonian is now rewritten everything else is written as the same. But this part is now written separately in two pieces one term coming from k = l and the other coming from k not equal to l. So, all the terms are over here.

Now this looks a little better but not quite and I think we have done a lot of bookkeeping we have to put all of these terms together. And figure out what how to deal with this, so I think this is a good point to take a break and then continue from this point in the next class. So, in the meantime that gives us a little bit of breathing time to make sure that we have kept track of all the terms and we have not lost any term.

This Hamiltonian is completely exact there is no approximation made anywhere. Only the auxiliary terms have been added they are added because H0 + H1 Psi1 = e Psi there is no problem there. H1 has to be hermitian otherwise you cannot use this result. So, we do have a hermitian H1 which is the one we are working with you are not measuring these auxiliary momenta. So, they are not hermitian and that does not worry us.

But they are used as an intermediate mathematical step and we now have the transformed Hamiltonian. But the transform Hamiltonian has a form and we still have to work with these terms a little bit figure out how to rearrange these terms which we will be doing in the next class. So, until then I will take a break if there is any question I can take it now. In the next class I will be concluding unit 3 on the RPA okay.

Because we are almost there, so this is the completely quantum treatment we began with the Hamiltonian. We carried out transformations of the Hamiltonian. We will now do the random phase approximation and we will see how it leads us to the collective oscillations to the correlated dynamics of the electron gas.

So, we go beyond the Hartree Fock and that enables us to do, to take account of the electron correlations which we had ignored earlier on. So, thank you very much and we will take it from here in the next class.