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

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Lecture 20
Many-Body formalism, II Quantization

Greetings, we will continue our discussion on the random phase approximation and we are getting very close to the point that we can actually introduce the RPA and the primary references for our discussion will be the book by Fetter and Walecka quantum theory many particle systems.

And the book by Raimes many electron theory by Stanley Raimes and his review which he wrote in 1957 in the reports of progress in physics and there are a few other references which I will refer to as we go along.

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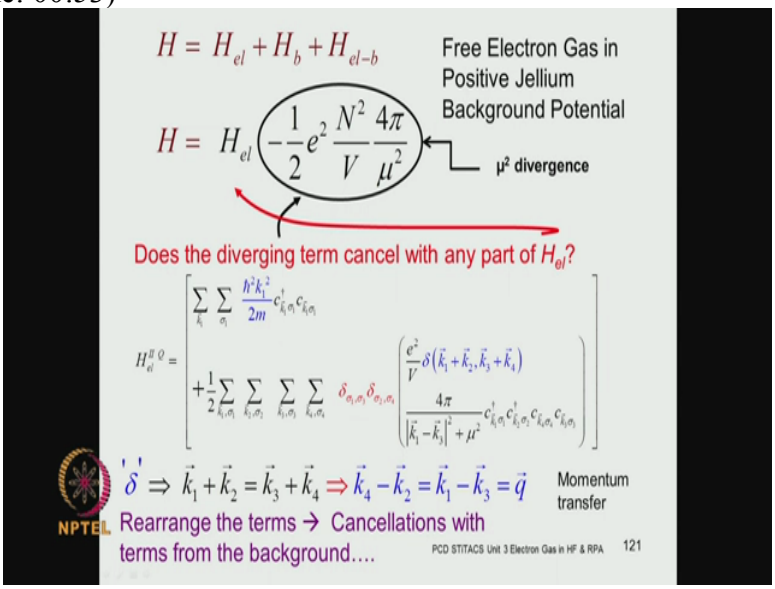

So, this is the picture we had before us. So, we have the electron-electron terms in this part of the Hamiltonian. And then you have the nuclear-nuclear interaction terms which is the interaction between all the positive charges of the Jellium plus the interaction between the electron and the positive charges which are smeared out in the Jellium potential.

So, these are the three pieces of the Hamiltonian and you have the 1 over mu square divergence coming from these two terms from the combination of these two terms is what you get over here. Now, before we proceed we should inquire if any part of the electronic Hamiltonian which is the first term.

Also has some contribution which goes as what you see in this circle in the circular loop you have got a term which goes as N squared over mu N squared over V 4pi over mu square. So, there is a term which is sitting inside this anywhere and that is something that we have to search for. Then there is a possibility that there would be a cancellation of this mu square divergence. So, that is something that we are going to examine.

And we promise ourselves that we will do that. So, let us look at this particular expression here, what we have now done is to we can write the electronic Hamiltonian in the second quantise form inclusive of the spin and we are going to inquire by rearranging the terms in the electronic part of the Hamiltonian if there is any cancellation. Now we have to remember that the in the electronic Hamiltonian there is a Kronecker delta over here.

So, that is going to put some constraint, so all the, there are four momentum indices k1, k2, k3 and k4. But all of them are not independent because k1 + k2 must be equal to k3 + k4. So, there is one constraint and that will reduce the number of momentum variables that we have to work with. So, we will write the momentum transfer which is k4 - K2 which is the same as k1 - k3 as q.

And then we will look at various terms for the momentum transfer. When the momentum transfer is 0 and when the momentum transfer is non-zero. So, we will examine these terms very carefully and ask if any of these terms leads to a cancellation of this 1 over mu square divergence coming from the background terms.

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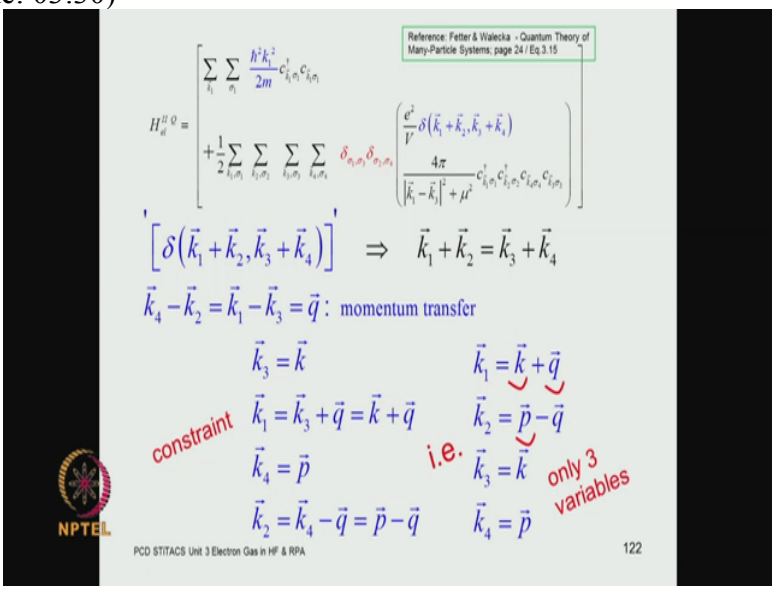

So, this is the Hamiltonian now and as we pointed out you have got the constraint which is k1 + k2 which is equal to k3 + k4 which means that you really do not have for momentum variables and if you write these four momentum variables in terms of a new parameter k, q

and p. So, k, q and p, so these are the three new variables that we introduced, so we write k4 = p, k1 = k3 + k. But k3 we set equal to k.

So, now instead of k1, k2, k3 and k4, k2 becomes k4 - q which is the same as p - q. So, instead of these four parameters we know that there are only three independent parameters because of the constraint. And these three parameters r, k, p and q okay. So, k1, k2, k3 and k4 are given by these relations and we really have to work with only three parameters instead of four because of the constraint which we have.

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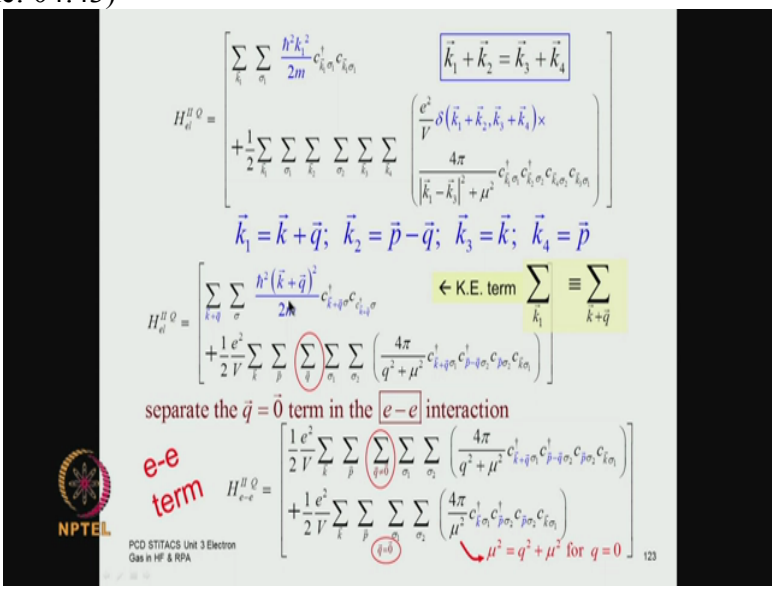

So, let us exploit this now, so we will write rewrite this Hamiltonian not in terms of k1, k2, k3 and k4 but in terms of the three momentum levels. Now what are these so you now have summations over these three k, p and q. We exploit the Kronecker delta, so that we are left with out of these four summations only one will be taken care of through the contraction coming from this Kronecker delta.

So, now you have summation over three indices k, p and q. And now you have 4pi k1 - k3 this over here you will have q square + mu square. So q is the momentum transfer okay, so this is the term that you get for your electronic Hamiltonian. Now, we will first examine this kinetic energy part of the Hamiltonian.

So, the kinetic energy part of the Hamiltonian is this here the summation index is k + q, it really does not matter because you only start summing from some index and turn over all the indices. So, whether you start with k or start with k + q it really does not matter effectively it is the same summation. So, now what we will do that we examine this electronic part the electron-electron part and over here you have summation over q.

And in this we separate the term corresponding to zero momentum transfer and then the remaining terms in which q is not equal to zero. So, we will separate this in two parts one is this q not equal to zero and this part is q = 0, when q = 0, here this term which is 4pi over q square + mu square becomes only 4pi over mu square this is because q = 0.

In the other term which is corresponding to q not equal to 0, you have q square + mu square okay. So, I have rewritten the electron-electron term which is the second term the kinetic energy part is separately taken care of and then in the second term in the electron-electron term you have the separation of the q = 0 term and q not equal to 0 term.

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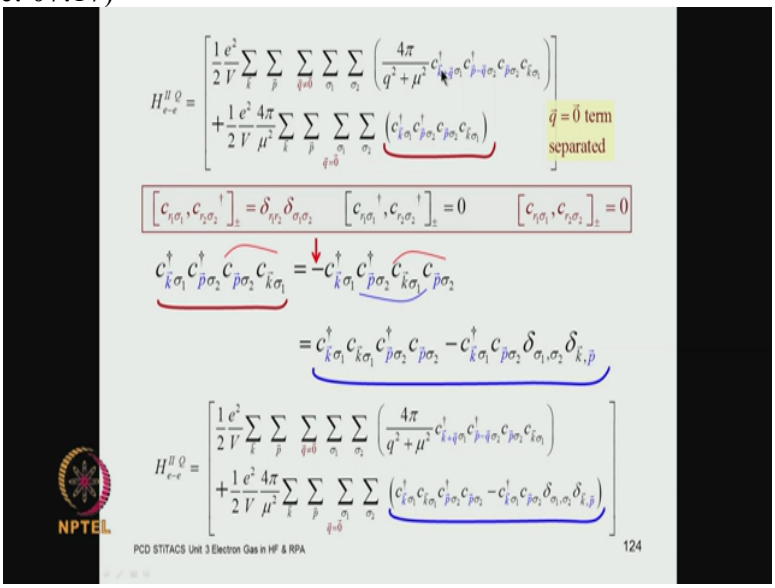

So, this is rather straight forward algebra but we will do it carefully. And we will make use of the commutation or rather the anti commutation relations further Fermion creation and destruction operators. So, these are the relation for the anti commutation relation the plus sign is for the fermions that the minus sign for the bosons. So, these are the general commutation relations inclusive of spin.

And what we have over here is this relation but this Cp and Ck we swap their relative positions and that is what gives us a minus sign here, so that is the first thing we do. Having done that we get a minus sign here and now we interchange these two. So here p and k are different sigma2 and sigma1 are also different. So, we will get a delta sigma1 sigma2 delta kp and then you have this additional term right.

So, this term these set of four operators two of them are creation operators and two of them are destruction operators together will give you these two terms now. So, these two terms take the place of this single term and the electron-electron Hamiltonian in the second

quantized notation the second q is written as a superscript in the second quantized notation becomes the first term is the same which is 4pi over q square + mu square.

And these creation and destruction operators and the second term, the first term is corresponds to q not equal to zero but it is the q = 0 term which is now written in these two pieces okay.

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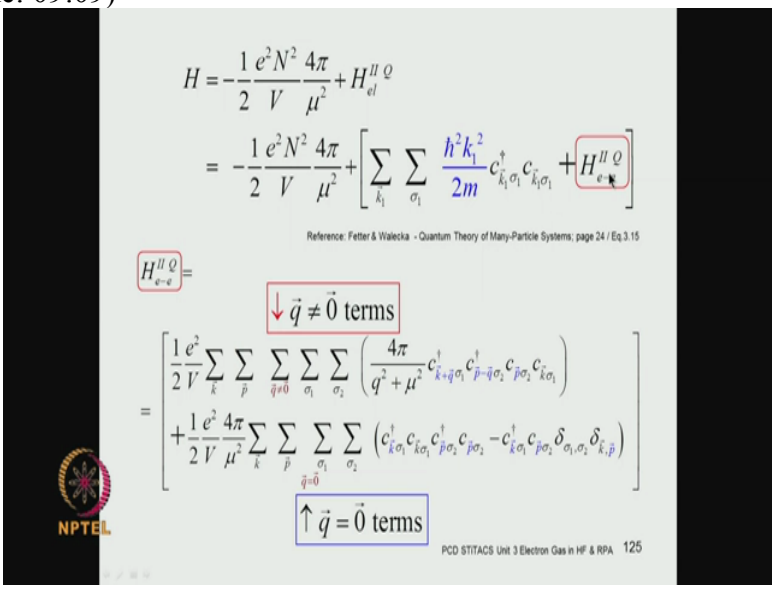

This is the complete picture you have got the full Hamiltonian which is made up of the electronic part of the second in the second quantized notation of the Hamiltonian and these are the terms which comes from the background, from the background, background and from the electron background of the Jellium potential.

Then you have got the kinetic energy part and then you have got the electron-electron part which is now written in terms of q not equal to 0. But the q = 0 term now is written in these two pieces by rearranging the creation and destruction operators by using their anti commutation relations. So, that is what we have got at the top of the slide.

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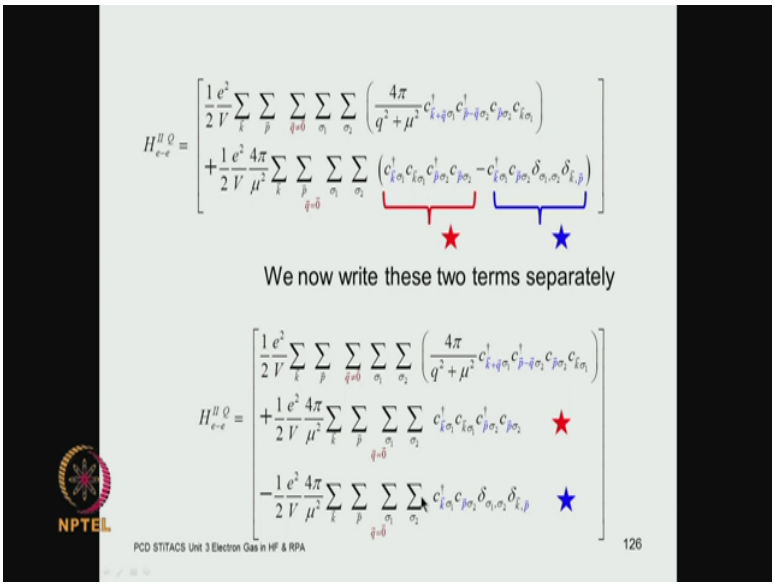

Now let us see, let us look at these terms carefully. So, there are two terms in the second part corresponding to q, q = zero one is what I indicate by the red Star and the other by the blue Star. And what I will do is rewrite this expression with these two terms written explicitly spelled out. Instead of putting them together in a bracket I will write them as two separate terms.

So, I have got the first term corresponding to q not equal to 0 which is this q not equal to 0 then this is the term coming from the term for which we have the red star and this is the term which comes with a minus sign for the blue star. So, these are the three terms which come in the electron-electron part of the Hamiltonian of the second quantized electron-electron Hamiltonian okay.

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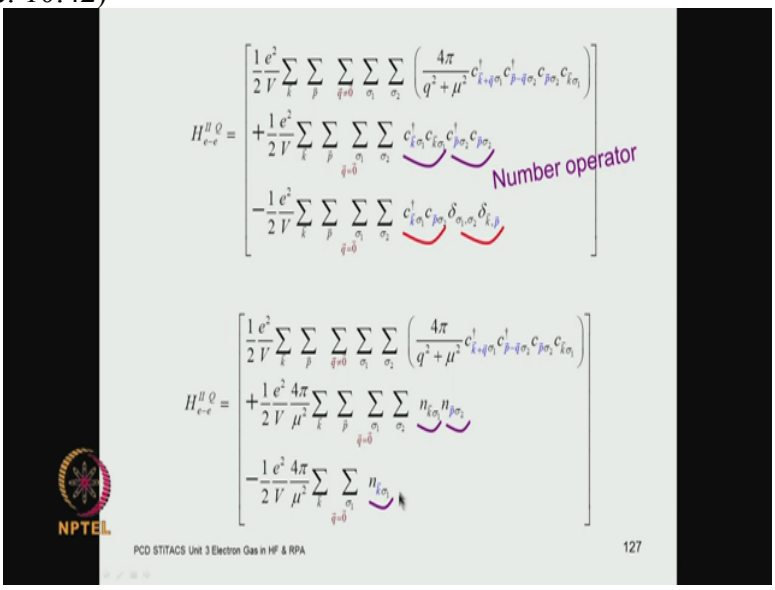

So, now let us look at this further you have got these two terms the first one is with a plus sign the other next with a minus sign. Look over here what is this, these two are nothing but

the number operators C dagger C right. So, this is nothing but the number operator, so is this. This is the number of for the state k sigma1 and this is the number operator for the state p sigma2 okay, C dagger C is the number operator.

What about this term this also has got the C dagger C but the subscript here is k sigma1 and the subscript here is p sigma 2 but no problem because sigma1 must be equal to sigma2 and k must be equal to p. So, because of this Kronecker delta this is also actually in number operator okay.

Because when you carry out these summations over k and p you will necessarily be left with terms for p = sigma and for sigma2 = sigma1 right. So, you will have a number operator coming from here as well. So, let us carry out those summations, so let us sum over sigma2 and we also sum over p. So, instead of having these four summations you now have only two summations because of the kronecker delta contractions.

And then you have a number operator here as well, so now you have got a number operator here, a number operator here and again a number operator here. So, these are the three terms and the last two this term and this term both correspond to q = 0 the q not equal to 0 terms are sitting over here.

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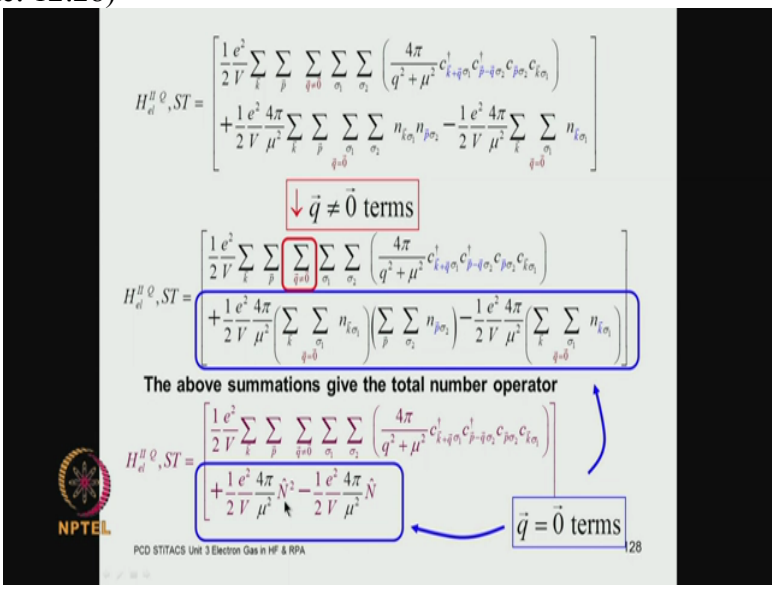

So, this is just a matter of you know rearrangement of terms and I will do it a little carefully and walk you through all the steps, all the important steps so that we make sure that everything is accounted for appropriately okay. Now this is the term corresponding to q not equal to 0 and the lower two terms in the second line over here these correspond to the q = 0 contribution, this is coming from q = 0 contribution.

This is also coming from the q = 0 contribution but for this you are summing over all values of k and all values of sigma1. So, that is really the total number operator right, you get the total number operator when you sum over all the states. So, essentially you get from here one total number operator capital N.

From here you get another total number operator which is capital N, so you get N square okay, from these two terms. And from this you will have only one total number operator coming from this term which is written over here. And both of these are coming from the q = 0 terms.

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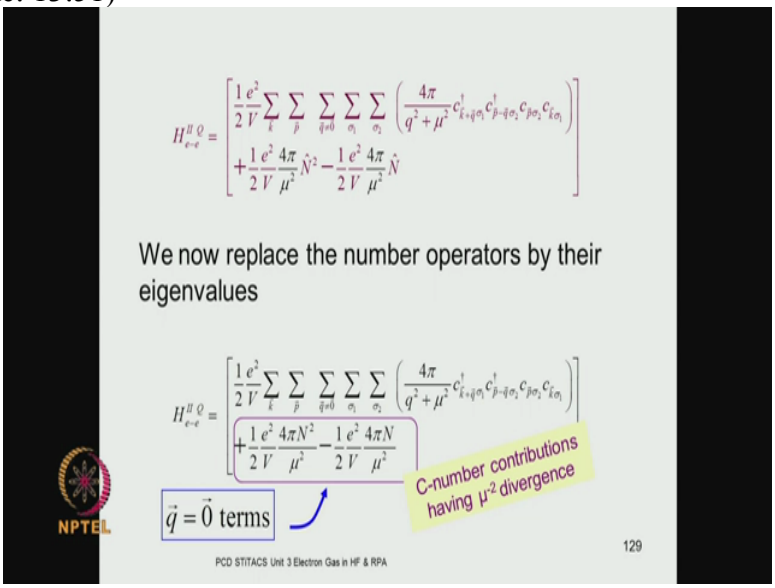

So, let us take this result to the top of the next slide and you have got N squared over here and N over here. And whenever you are dealing with occupation number space, vectors then the number operator will be diagonal in it and therefore whatever quantum algebra you do, you will be able to replace the number operators by their Eigen values. So, the Eigen value of the total number operator is nothing but the total number of electrons.

So this N operator square is replaced by N square effectively this is also an operator multiplied by the unit operator. But now we have anticipated the results that all the operations have been carried out. So, you have got the n square operator over here minus from the second term you have got the minus half e square by V 4pi N over mu square.

But these N do not have that carrot symbol on top which we had over here. Because this and this are operators whereas this and this are the Eigen values okay. So, we replace the number of operators by their respective Eigen values okay. So, this is just like a numerical contribution but both of these terms have got the 1 over mu square divergence and this is what we had anticipated.

That some part of the electron-electron term may have 1 over mu square divergence. And it could cancel the divergence which was coming from the background terms, from the background, background Hamiltonian and from the electron background Hamiltonian, so they were right. So, both of these are coming from the q = zero terms.

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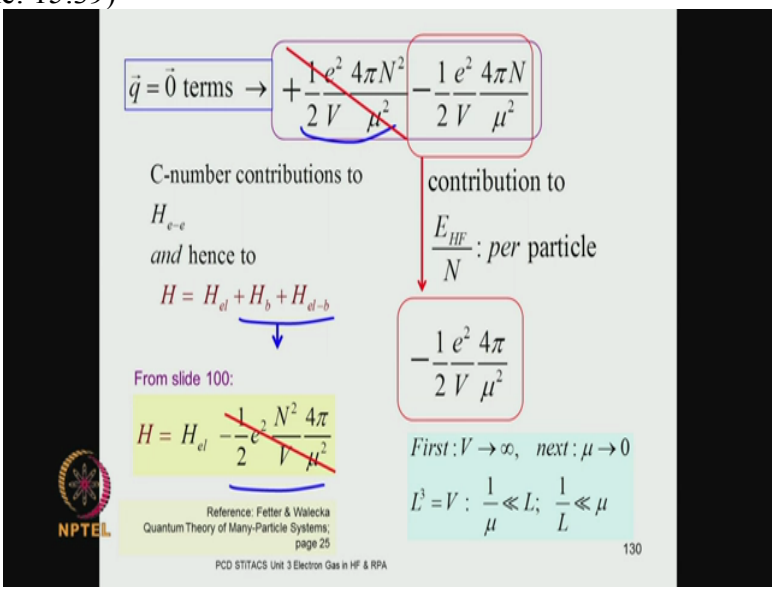

So, these are the two contributions these are the C number contributions these are just numerical contributions okay. These are just numerical contributions first one is with the plus sign here second one is with a minus sign. But mind you the first term has got N square and the second has got N okay.

So, you have to be careful with that and if you remember the mu square divergence coming from the combination of the background-background Hamiltonian and the electron background Hamiltonian was -half e square N squared over V 4pi over mu square this was a part, this is a mu square divergence that we were concerned with. And we find that because this comes with a minus sign this term comes with a plus sign.

This is this term is quadratic in N, so is this. So, these two terms will cancel each other okay. So, let us go ahead and cancel them and you are still left with this term. You are still left with this term but now what we will do is, you have if you look at the Hartree Fock energy per unit particle per particle. So, you divided this by N, so this n will go to the left side when you divide both sides by the total number of particles.

You get a contribution which is minus half e square by V 4pi over mu square this is the contribution that you get which has got mu square divergence as such. But then we know that

we can first take the limit V going to infinity and that already takes care of this term okay. And the limit mu going to 0 will be taken later okay.

So, it is a mathematical construct that we had introduced mu was the parameter which we introduced to make the potential screened Coulomb instead of the Coulomb potential. So, instead of the 1 over r, we had the e to the - mu r over r. So, that what that is the origin of mu and you can take mu going to 0 in that term but that can be done at a later stage.

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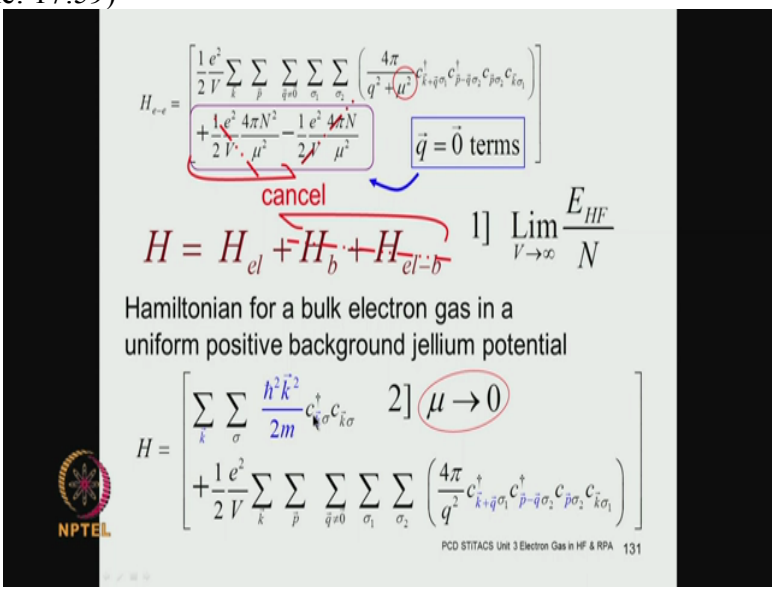

So, we have the q = 0 terms this part of the divergence cancels the background and the electron background Hamiltonian. This part is taken care of when you take the limit V going to infinity right. Having done this now this term is also lost and now we take mu going to zero okay. Note the sequence it is very important that you follow the sequence because otherwise the 1 over mu square will already give you a divergence.

So, this sequence of this is a mathematical procedure which is strictly correct but the order of taking the limits must be maintained. So, now you take the limit mu going to zero and when you take this limit mu going to 0, you have this mu square over here which will go to zero right. And if you now write the electron-electron Hamiltonian after taking these limits then you have the full Hamiltonian in which you have got the kinetic energy part.

And then you have got the electron-electron interaction term in which you have q not equal to zero because q = 0 terms have already been taken care of because they cancel the background right, the Jellium background, the background-background parts and also the electron background part. And then in this term for q not equal to zero because you are now taking the limit mu going to zero.

Instead of this q square + mu square you have only q square in the denominator but this q is not a null vector it will never be zero in this term right okay. So, this is the advantage of carrying out this mathematical construct and this procedure of taking the limit.

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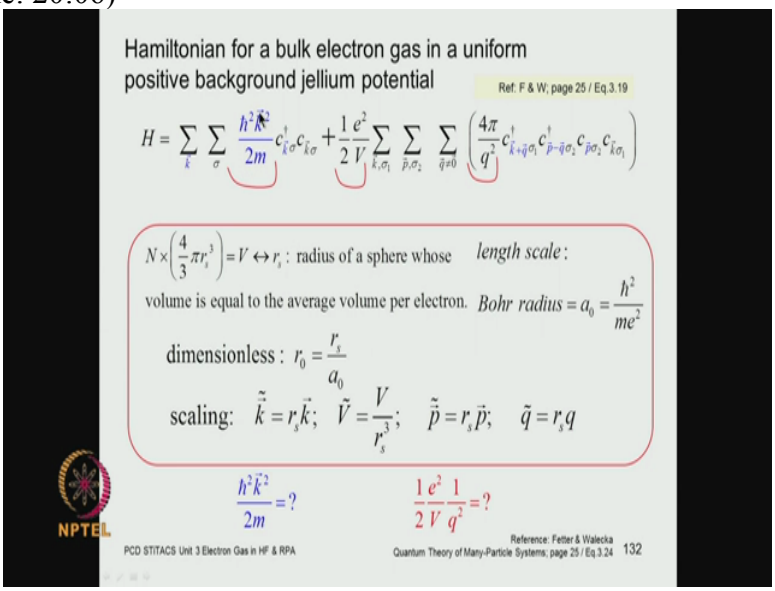

And we now have the Hamiltonian for a bulk electron gas in a uniform positive background Jellium potential everything is taken care of now the electron-electron terms the electron potential term, electron Jellium potential term and the mutual repulsion between the positive charges of the Jellium. Everything is taken care of, so this is the full Hamiltonian for the system for a bulk electron gas in a uniform positive background Jellium potential.

And these are the terms that you get mind you; you have got q not equal to 0 here. And now we do a little bit of you know simplification of these terms because the total volume which comes over here is nothing but the volume occupied by the number of electrons. And we had defined an average radius per electron which is rs, so that this is the average volume occupied by each electron.

These times the total number of electrons will give you the total volume. So, rs is the average radius of each electron and we do a little bit of scaling here, we rewrite this expression in a certain new set of scaled parameters. And the scaling is done to recognize that we could use perturbation theory as such.

Because if you look at this Hamiltonian over here there is; it is not obvious that you can solve this problem perturbatively by treating this part as the unperturbed Hamiltonian and this part as a perturbation. Because to be able to use perturbation theory you need to recognize that what you would add to the original unperturbed Hamiltonian is a small term okay.

So, the size of the second term of the electron-electron term is by no means is obviously small but it will turn out by rewriting these terms into using the scale variables we will find that you can actually use perturbation theory. Let me show you how, so we use new variables what we do is do some scaling through the Bohr radius. So, the length scale is now rs divided by a0, so this becomes a dimensionless length parameter right.

And likewise we scale the momentum volume this is just h cross divided by k will give you the momentum. And also the q everything is scaled by the factor rs which is the radius of a sphere, which has got an average volume occupied by a single electron. So, this is; these are the scaled variables that you introduced and in terms of these scaled variables, let us ask what is the value of h cross square k square by 2m, which is the kinetic energy.

Let us ask what is the value of this term which is half e square by V times 4pi over q square, so what is half e square by V multiplied by 1 over q square in terms how do we write it in terms of the change variables okay. So, this is just rewriting the same term but in change variables and that is what will help us recognize that we can treat this problem perturbatively okay.

Earlier, remember previous classes we discussed how the problem of electron gas in a Jellium potential is solved using the Hartree Fock self-consistent field method okay. So, using the self-consistent field method we found the solutions exactly right. Now we are showing how this problem is done perturbatively.

And before we do that we are actually demonstrating that perturbation theory can in fact be used at all okay. So, we are going to show that perturbation theory can be actually applied.

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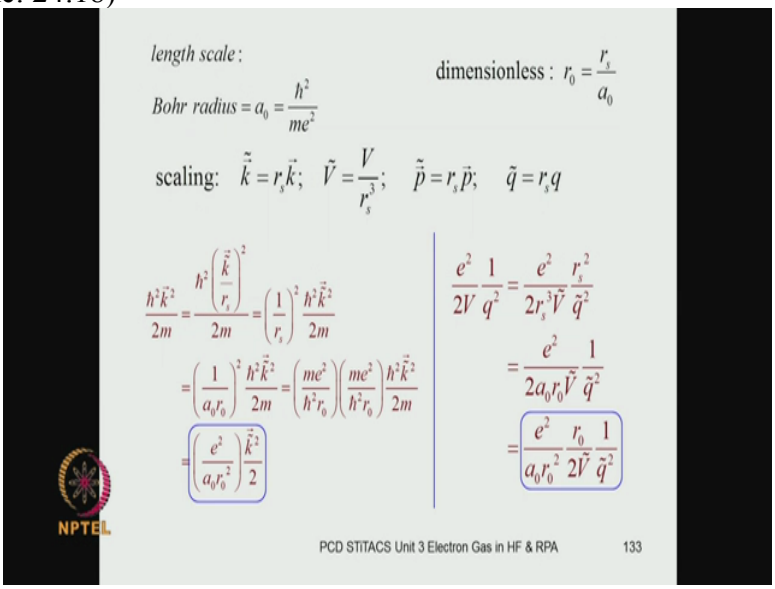

So, these are the new variables, the new variables are represented by this tilde on top this wiggle is the tilde symbol. So, you have got new variables and in terms of these new variables you can write this term h cross square k square by 2m and you simply carry out these transformations.

Plug in the corresponding substitutes and you get this result for h cross square k square by 2m okay. So, you get a transformation over here and similarly the other term that we wanted to examine was half e squared over V 1 over q square and this in terms of the new variables which is tilde and q tilde is given by this relation. And we will put these two in the Hamiltonian and rewrite the Hamiltonian in terms of the new variables.

Which are the tilde variables okay. So, all of this of course will be uploaded at the course website so you do not have to write down all these intermediate steps but just concentrate on how the analysis is done okay. Because the actual terms you can work out yourself or look at the detailed transformations when these slides are uploaded at the course website.

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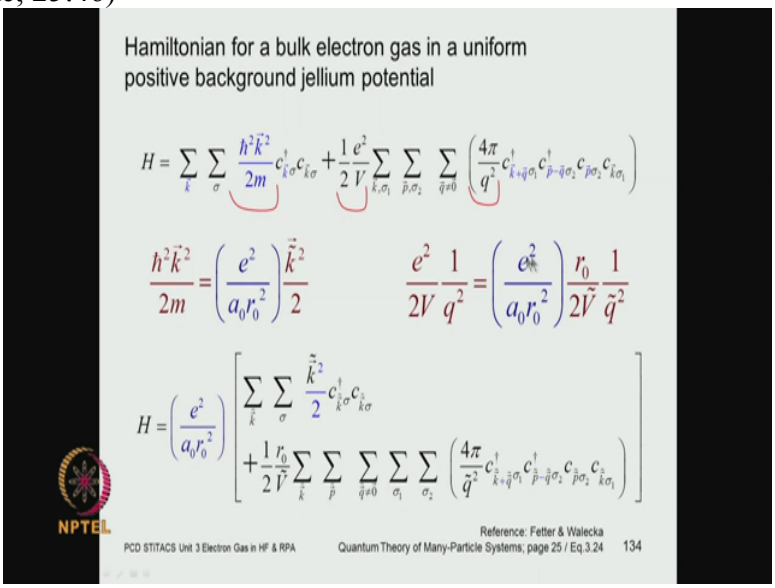

So, these are the two results that we will use to substitute in the expression for the Hamiltonian. So, this is very what we wanted to substitute or write this is the term we want to substitute in terms of the tilde variables and then e squared over V 4pi by q squared is what we want to substitute in terms of the tilde variables. So, let us do that, let us replace all of these by these tilde variables.

So, these are the substitutions that we know and in terms of these substitutions we factor out e squared over a0 r0 square which is common in both the terms okay. So, that is written outside the bracket and the rest of the terms are over here. Now this suggests something very interesting and some of you have possibly already spotted it that.

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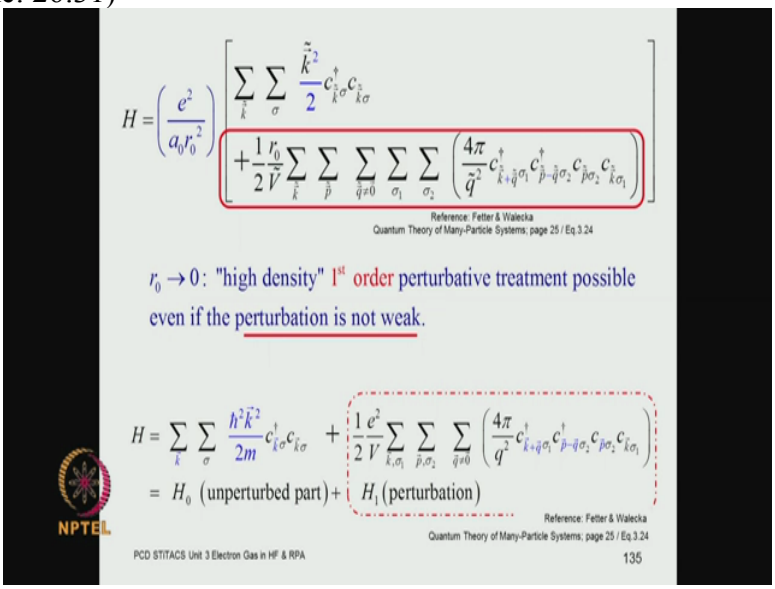

If you now look at this term okay, these are the two; these are the terms you find that the second term which is the electron-electron interaction term has got r0 factor okay which means that if r0 becomes small the second term which is in this red loop can be treated perturbatively okay. And r0 going to 0 is the high density limit because when you have a large number of electrons per unit volume right.

The average radius will become small right. Your scaled parameter r0 will shrink and in the high density limit you immediately see that the electron-electron term can be treated perturbatively. And now we can use perturbation theory on a remark that we had made earlier was that the result of the Hartree Fock self-consistent field method and the perturbation method turns out to be the same.

So, we are showing it now we have already got the results for the Hartree Fock self-consistent field method for the electron in the Jellium potential and what we are doing here is developing a perturbative approach and we will find that the end result will turn out to be the same as what we got from the self-consistent field.

But of course we had already remarked that second order and higher order terms diverged which is where you have to use many-body theory and the RPA was developed to address those issues. So, we are getting to that now, so first let us work this out perturbatively. So, you have got an unperturbed part which is just the kinetic energy part this is straight forward there is no big deal over here.

And this is the electron-electron part which is to be treated perturbatively. But everything is taken care off the background is taken care of, the background-background repulsion is taken

care of, the electron background attraction is taken care of okay. The q = 0, terms are taken care of, they are the ones which cancel the background divergence right.

So, that is taken care of and the only terms that remain to be taken care of are the terms coming from q not equal to 0, q is the moment of transfer of q not equal to 0 these are the terms to be taken care of and these terms go these are scaled by a factor r0, which means that this can be treated perturbatively.

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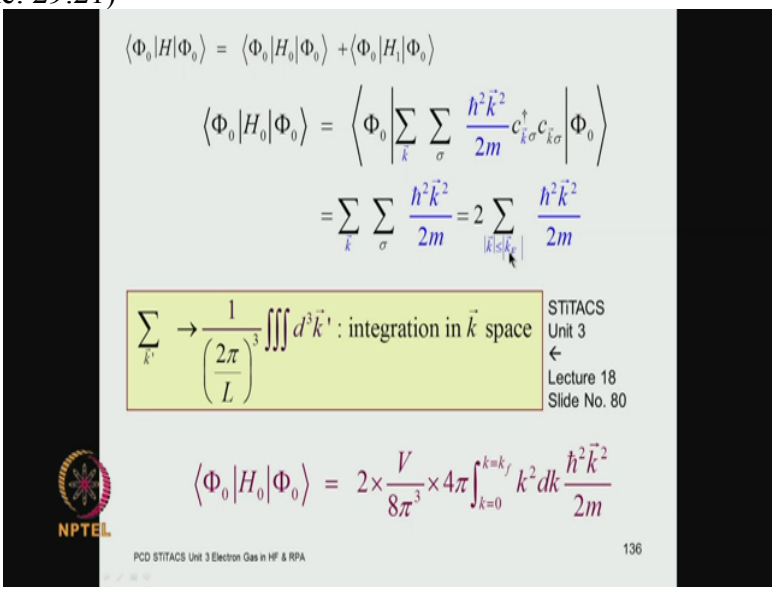

So, let us do that so now this is your expectation value of the Hamiltonian in the ground state in the unperturbed ground state. And this is the part coming from the unperturbed Hamiltonian and the first order perturbation theory correction will nothing but the matrix element of the perturbation Hamiltonian H1 in the unperturbed ground state which is Phi 0 okay. This is just the plane result of first order perturbation theory.

So, the first term is easy to evaluate because the kinetic energy part of the Hamiltonian is just the sum over k and sigma, so you get the kinetic energy of each particle right. But then you have to sum over sigma as well. So, you will get a factor of 2 because this term is independent of spin. So, both spin up and spin down they will give you the same contribution.

So, when you sum over sigma as well as sum over k you get a factor of 2. But then C dagger C is just a number operator which will give you a non zero value if and only if the momentum states that you are referring to are those which are occupied states. And only those states are occupied which are at or below the Fermi level.

So, that is the reason this summation must be restricted to k values which are less than or equal to the momentum at the Fermi level okay. So, this is a summation over all possible momentum states but that is now limited because of the c dagger c factor which is the number operator. And the number operator is going to give you a non zero Eigen value only for occupied states.

For unoccupied states like in value 0, so it will make 0 contributions to the total sum. Now the other thing we are going to do because we have a quasi continuous discrete spectrum we have done box normalization of the plane waves alright. So, you have got a quasi continuous discrete spectrum.

And the summation over k we have seen earlier in the 18th lecture of the unit of this course from the unit 3 we have shown already that the summation over k is completely equivalent to integration in the momentum space. But then you have got this factor 2pi over L whole cube that comes from the boundary conditions in which you have the plane waves which are not to be found all the way to infinity but they are confined to the length of the box.

So, that is the reason you have this 2pi over L whole cube coming here. And we will now go over from this summation this discrete summation to integration. This integration in the momentum space will have integration over the angles in the momentum space which are the angles in the reciprocal space.

But you will have the sine theta sine theta d theta d Phi type of term in the volume element which you integrate over all the angles of theta and Phi in the reciprocal space will give you a factor of 4pi which is here. And then you have to carry out integration over the momentum with actually integration over k.

Which goes from 0 to the value of k and the Fermi surface because here we know that the summation must be restricted to values of k less than or equal to the value of k at the Fermi surface right, so, the integration is from 0 to kf, k = 0 to k = kf then k squared dk comes from the volume element right.

It is 4pi k squared dk is the volume element, so this 4pi here and then you have got this h cross square k square by 2m over here right. So, V over 8pi cube is nothing but this term L cube is the same as V, so V over 8pi cube is just this term. So, this is the result for the expectation value of the unperturbed Hamiltonian.

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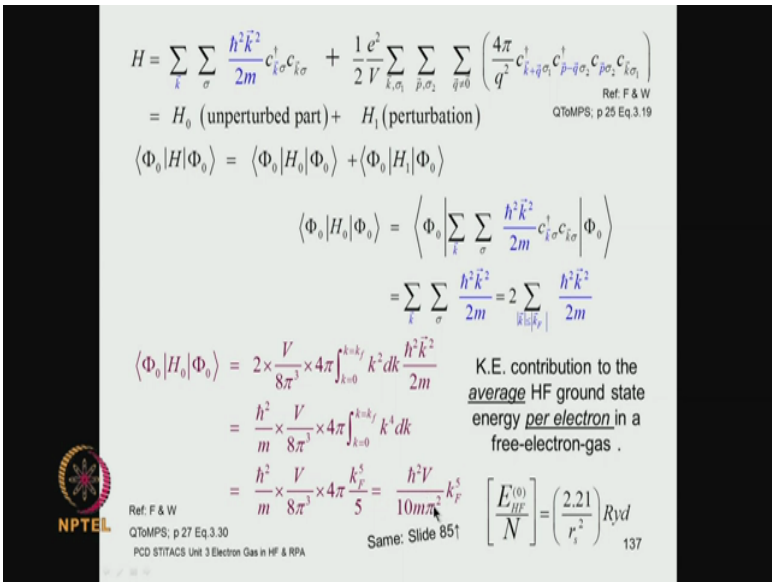

So, we now have got the result for the unperturbed part of the Hamiltonian we have this result which goes as k squared dk you have got h cross square k square by 2m. So, you have to integrate k to the power 4 which gives you a k to the power 5 when you put the limits k equal to 0 to kf.

You get k to the power 5 for the value of k at the Fermi level which is kf okay. So, this is the result of the unperturbed part of the Hamiltonian. And if you now put in all the values okay evaluate the result for energy per unit electron this we had evaluated, this is the same term as we got when we discuss the Hartree Fock technique.

And this is nothing but 2.21 by rs square in Rydberg units. So, this we have discussed earlier in our previous classes you can refer to the earlier slide to look at this results how this translates into 2.21 by rs square okay. So, this you will remember from our previous discussions. So, this is the same as the result that we got from the Hartree Fock.

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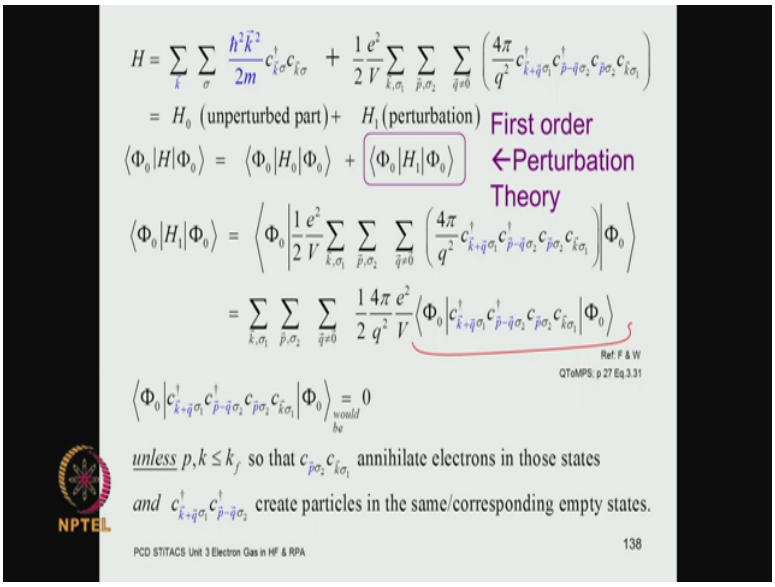

Now what about the perturbation okay let us evaluate this using first order perturbation theory. So, this is the term H1 we have written explicitly over here in this term this is the perturbation Hamiltonian. You have q not equal to 0, I have taken the 4pi e square over 2, 2q square V factored out. So, that I have got only the matrix element of the creation and destruction operators.

Now what we do know is that there are two destruction operators over here Cp and Ck and two creation operators C dagger p - q and C dagger k + q. Now certainly you will get a 0, when you operate by Ck on this unless the kth state is already occupied which can be the case only if it is at or below the Fermi level right not otherwise same thing over here. So, you must destroy two particles from below the Fermi level.

And then create the corresponding two particles otherwise you will get a 0 contribution from this matrix element this is simply because you cannot destroy a particle unless that state is filled and you cannot create a particle unless that state is empty these are Fermi Dirac particles, so that is all there is to it.

So, this would be 0 unless p and k are below the Fermi level. And these two creation operators create particles in the very same empty states after the holes have been created after the particles have been destroyed okay.

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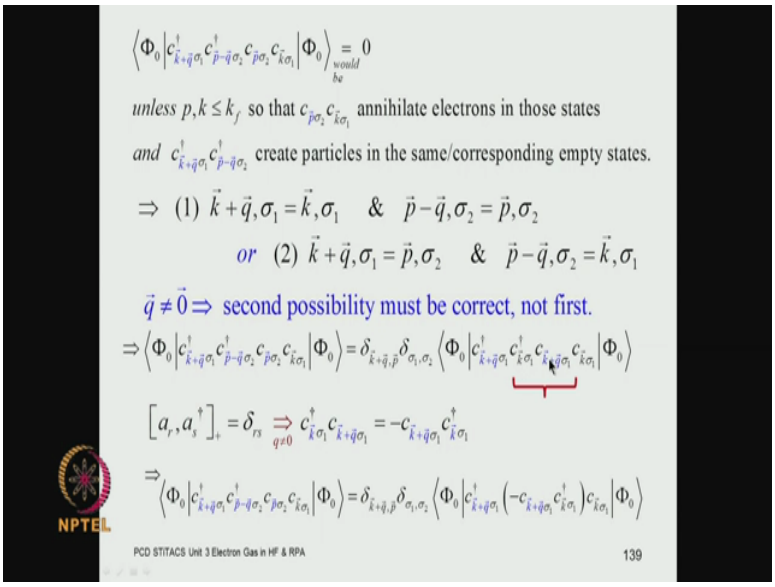

So, let us recognize that there are two possibilities now, one possibility is that this k + q sigma1 is the same as k sigma1 because then you destroy a particle in the k state and create in k plus qth state right. So, this is one possibility the other possibility is that k + q creates where this particle Cp has destroyed that these are the other possibility. So, there are two possibilities one is that k + q sigma1 = k sigma1.

The second is k + q sigma1 = p sigma2, now the first possibility is ruled out because q is q = 0 are the terms that we are looking for right. So, q not equal to 0 means that this second possibility must be correct and not the first right, so now the second possibility being correct you have k + q sigma1 p - this is the second operator is C dagger p - q sigma2 p - q sigma2 is the same as k sigma1 right.

So, this operator C dagger p - q is replaced by C k dagger sigma1, this is Cp sigma2, so Cp sigma2 is replaced by Ck +q because if p - q = k then p becomes equal to k + q, so that the k + q that comes here. And the corresponding spin variable is sigma1, so you have got sigma1 everywhere and then you have got the delta sigma1, sigma2 and k + q must be equal to p. So, k + q must be equal to p and sigma1 must be equal to sigma2.

So, that is the only condition when you will get nonzero contributions. So, that identifies the terms and now you can interchange the positions of this creation and destruction operator by using the anti commutation rules again. So, when you do that when you interchange these two positions right.

You interchange you swap these two positions, you get a minus sign and you get Ck + q sigma1 C dagger k sigma1. Which is this term moves to the right instead of the left but then you pick up a minus sign.

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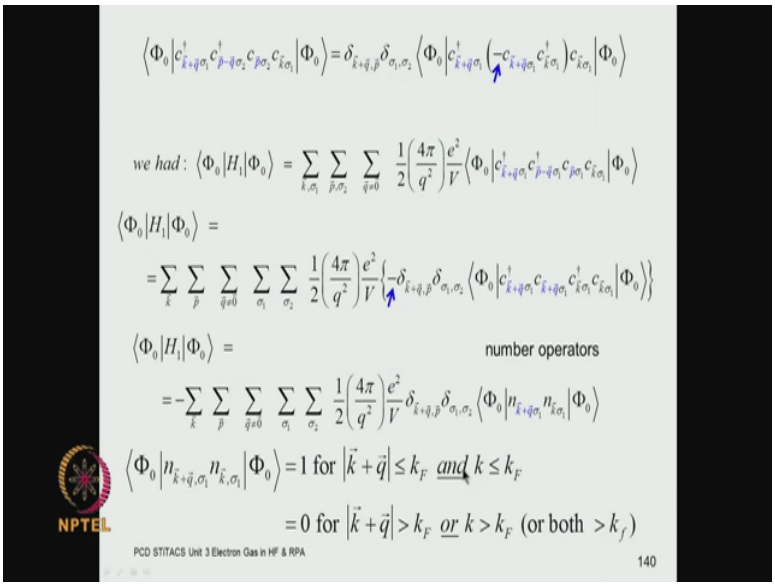

So, let us write it at the top of the next slide which is here okay. So, this is the term we are looking at. And this was just a part of the matrix element the full matrix element of the perturbation Hamiltonian has got all of these summations to be taken care of. Then you have got this factor of half 4pi over q square e squared over V.

And then you had the matrix element of the creation and destruction operators in the unperturbed ground state. So, this part of the matrix element which is the matrix element of the creation and destruction operators in the unperturbed ground state is evaluated over here. You have got a minus sign here, you have got the kronecker deltas over here and we can now use the right-hand side of the first equation which is at the top of the slide.

And use it to replace this term okay, what does it give us you get the matrix element of the perturbation Hamiltonian. Then you have got the sum over k, the sum over p, you have got q not equal to 0 which is here right. You sum over q only for q not equal to 0 and now you have got double summation over sigma1 and sigma2 which is written over here explicitly.

But then you also have the kronecker deltas, k + q must be equal to p and sigma1 must be equal to sigma2. So, this will help you contract some of the summations okay, that is coming because of the fact that we are dealing only with q not equal to 0 terms. yes (Question time: 41:24 not audible) yeah we have already considered that q not equal to 0, correct whether we have to write explicitly again that q not equal to zero.

Absolutely because you are summing over q, you are summing over q and you must carry out summation over all values of q except q not equal to 0 okay. Now the operators over here look at this is C dagger C and the indices are exactly the same this is k + q this is also k + q

and this is sigma1 this is also sigma1. So, this is the number operator look at the second one this is also C daggar C and look at the subscripts this is k sigma1 this is also k sigma1.

So, these are nothing but the number operators n corresponding to the state k + q and sigma1 and this is the number operator corresponding to the state k and the spin label sigma1 and now if you can go ahead and recognize that this operator, the number operator will give you a value 0 unless the corresponding momentum state is occupied.

And what are the two momentum states which are being referred to there are two number operators one for momentum k and the other for momentum k + q. So, the first number operator spells out that this matrix element will be equal to 1 for this k + q less than or equal to the Fermi momentum in units of h cross and the second condition should also be satisfied because if either of these gives you a 0 the matrix element will go to 0.

So, one condition is that k + q must be equal to less than or equal to kF and the second condition is that this k the magnitude of this k must be less than the Fermi momentum in units of h cross in which case this matrix element will be equal to 1 and if either of them is greater than the Fermi momentum then this matrix element will go to zero right.

So, this matrix element of the creation and destruction operators is going to contribute either 0 or 1. And the conditions when it will contribute a nonzero value are determined by when the sum of k + q and the magnitude of k itself is whether or not it is less than or equal to the momentum at the Fermi surface or greater than that so those are the determining factors.

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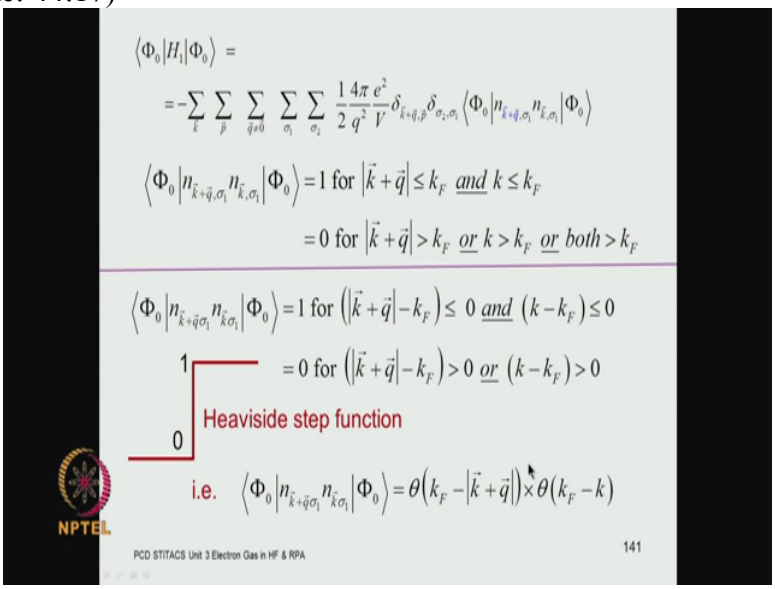

So, these conditions I have rewritten at the top of this slide there is nothing new in this relation at the top of this slide. And now you have a term whose; which can take only two

values either 1 or 0 and you are perhaps familiar with a function which has got two values, which can have only two values either 0 or 1. And this is nothing but the Heaviside step function okay. So, this is the condition which we have written.

So, k + f must be less than or equal to kF or if you subtract k from both sides of this inequality k + q - kF should be less than or equal to 0 and this condition becomes k - kF less than or equal to 0. So, it is the same condition written differently and this is the Heaviside step function which is popping up. Here Heaviside step function has got a value of 0 depending on a certain condition being satisfied.

If the independent parameter is less than or a certain value this value is 0 if it is greater than that value its equal this value is equal to 1. So, we can write this condition using the Heaviside step function that this matrix element of the creation and destruction operators which now manifests itself as a matrix element of the number operators.

This becomes a product of these two heavy side step functions. So theta is the Heaviside step function okay. So, we can rewrite this matrix element in terms of the Heaviside step function.
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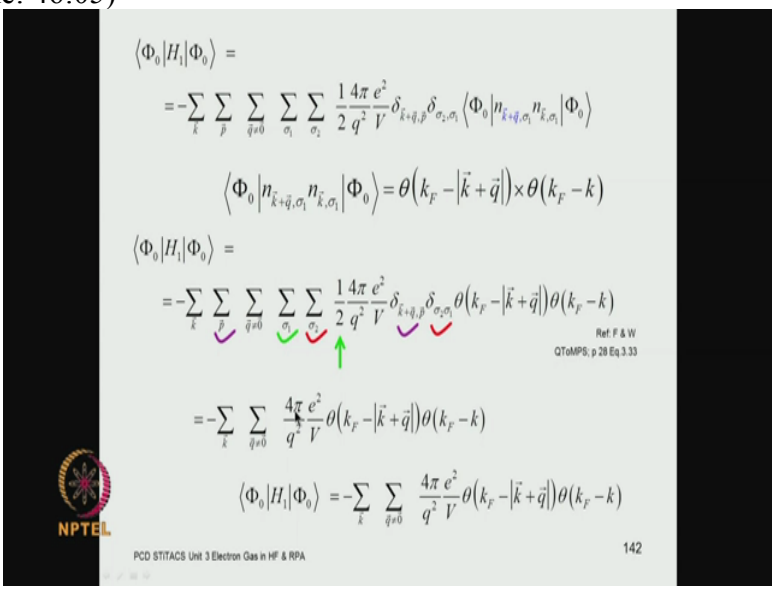

So, let us do it here this is the product of the Heaviside step function. Notice that it has to be product because if either of these two Heaviside step functions is 0 then the product goes to 0. So, this matrix element of the perturbation Hamiltonian in the unperturbed ground state is given by this minus sign is over here.

All of these summation indices this term is here you have got the kronecker deltas and instead of the matrix element of the number of operators you have now the product of the Heaviside

step functions. Now this delta sigma2, sigma1 when you sum over sigma2 will give you a term only when sigma2 is equal to sigma1 right.

But then you have a further summation over sigma1 but the terms are identical for spin up and spin down. So, when you do this further summation over sigma1 the half will be taken care of because you will get an equal contribution from spin up and spin down right, so that will be taken care of. And then when you sum over p only the term for p = k + q will survive right.

So, when you carry out all of these summations do the Kronecker delta contractions your result becomes minus sum over k sum over q not equal to 0, sum over p has been taken care of. The only term that is going to survive is when p = k + q and that is the only term that survives and now you have the product of the Heaviside step functions.

So, this is what you now have to sum up right okay. So, let us do that, so you have the result for the perturbation correction according to first order perturbation theory.

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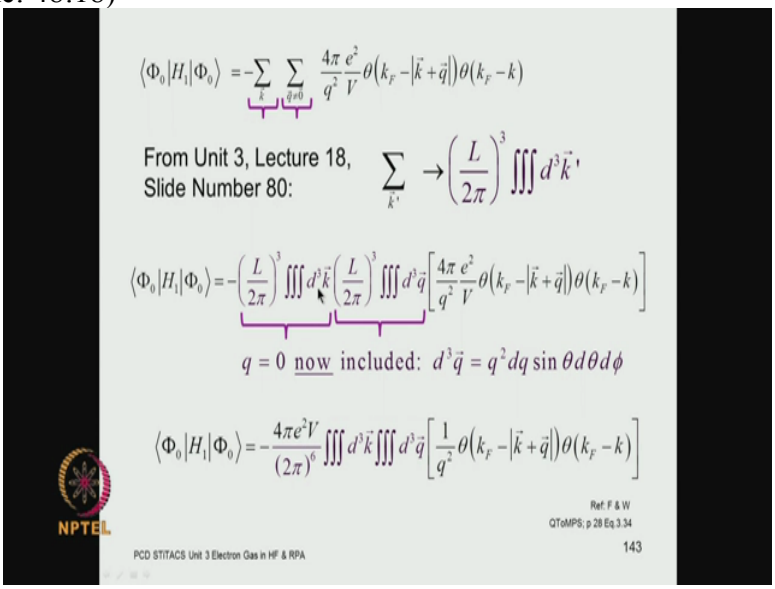

Now this is what we have to evaluate but we are not going to carry out a discrete summation. We are going to carry out an integration in the momentum space right. So, the summation over k goes over to this integration in the momentum space with this factor because of the volume occupied by every state right.

So, that is the term that was coming from, so this summation over k goes to the corresponding integration. This summation over q also goes over to the integration over the momentum space okay. But here we were taking care that q is not equal to 0 right. Now we

do not have to worry about it because the 1 over q square is what would cause the divergence right. Now when you do the integration you are not worried about it.

Because you have got the q squared dq in the volume element and that q square will cancel this 1 over q square. So, when you carry out this the corresponding integration you do not have to worry about it okay. So, q = 0 now can be included because you are doing this integration and you get the q square dq term in the volume element in the momentum space of course you will get a factor of 4pi.

So, that will come, when you carry out the integration over the solid angle. So, now we have this minus sign over here, you have got the 4pi e square, 4pi e square then you have got a 2pi to the cube and 2pi to the cube, so you have got 2pi to the 6 okay. Then you have got L cube which is V, this is also L cube which is also V, so you get V into V but there is a 1 over V over here, so you are left with one V in the numerator.

So, all those factors are taken care of right. You see that so you have got 4 pi e square V over 2pi to the 6. Then you have got integration over k, you want integration over q, you do not have to worry about q going to 0 which is included in the volume of integration. And then you have got the product of the two Heaviside step function.

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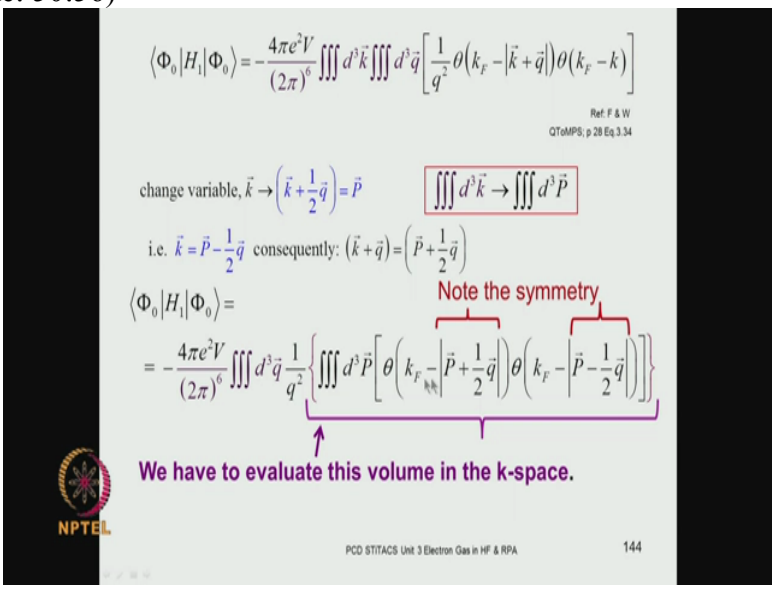

Essentially what you have to do now is if you do a change of variable okay. Now this is a very nice trick which is very nicely discussed in Fetter and Walecka's book that if you change the variable from k to k + half q which I now write as capital P. So, k + q becomes you are adding another half to the left side, so you add half to the right side, so this becomes P + half q right.

The integration you all you have done is to change the variable from k to P. So, you have got the same integration over the whole space for momentum the Heaviside step function will take care of the appropriate part of the momentum space to be dealt with. And the first order perturbation correction is now given by this term 4pi e square V over 2pi to the 6.

You have got integration over q d3q over q square which is written over here and instead of the integration over k you have integration over uppercase P of the product of these two momentums, these two Heaviside step functions. Now the advantage of changing the variable from k to k + half q is that in the Heaviside step function you are subtracting a term is certain magnitude of a momentum term.

From the magnitude of the momentum term at the Fermi level I am referring to k as momentum knowing of course that it is in units of h cross okay. So, kF from kF you are subtracting P + half q and in the second Heaviside step function again you are subtracting from the momentum at the Fermi level not P + half q but P - half q. So, instead of P + half q you have P - half q over here.

So, there is a certain symmetry and that enables us to evaluate this integral using very simple elementary geometry, I will show you how it is done. So, this is an evaluation over the momentum space okay, this is just a number which is either 1 or 0. So, there is a certain part of the momentum space. And we have to find the volume of that part of the momentum space.

So, if we identify that part of the momentum space correctly. Then we will know what the corresponding volume in the momentum space is? Which is the reciprocal space? Which is going to give you this integral?

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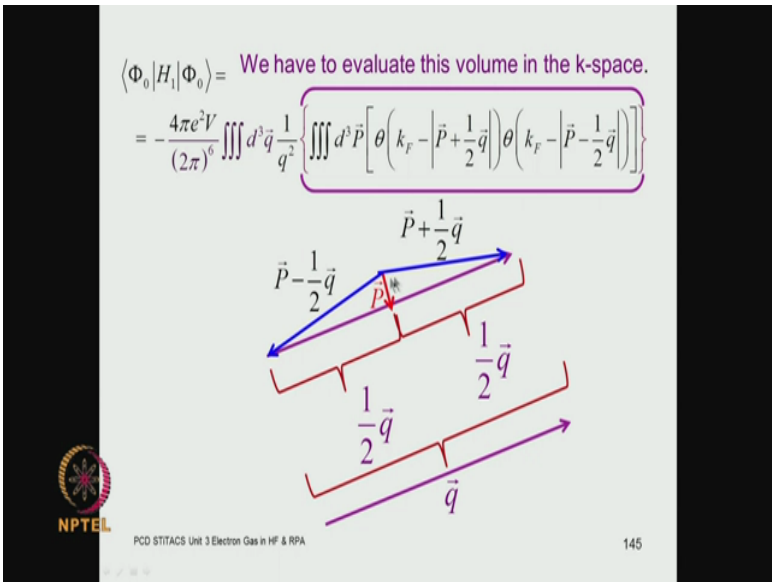

So this is the integral to be determined. This is the volume in the momentum space that we have to determine. Now let us consider the vectors P, this is a vector P and let this be the vector q okay. Let us begin with this geometry what I do now is I take half of q, I look at this q as half q + half q because in one case I am adding half q here in the other case I am subtracting half q because of the symmetry.

So, I write this q as twice half q, so this is the q vector which is twice half q, so this is the geometry now. And what it tells me is that this vector is P + half q and this vector is P - half q this is just from the triangle law of addition of vector. So, see how this transformation of vectors enables us generate the recognition of the volume element that we have to find okay. What is the total volume of which goes into this integral? That is all the question is.

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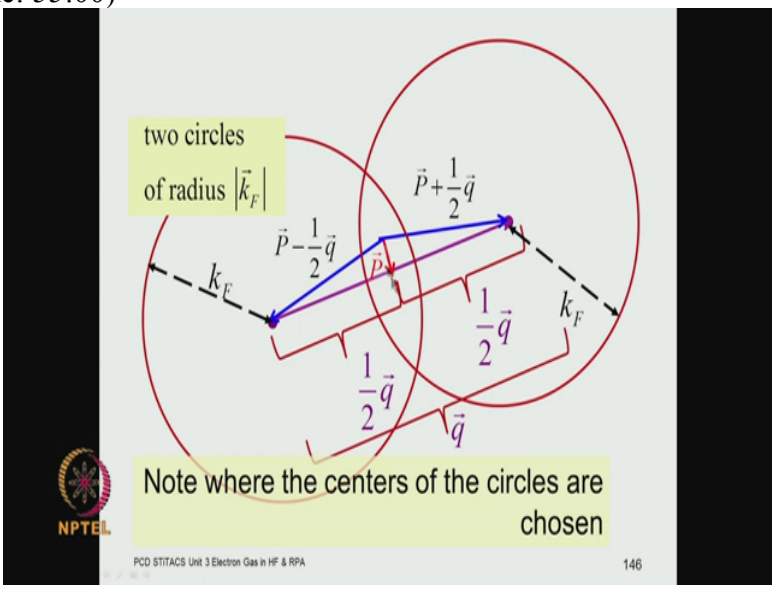

Now this is a very nice trick and by carrying out this transformation you find that this is the geometry that we have to work with. And to this geometry we what we do now is to take this

as a center and draw a circle of radius kF take this point as the center of another circle of radius kF so, at both of these points one which is at the tip of the vector P + half q.

We have seen how you get this vector this is and the tip of the other vector which is P -half q. At the tip of this vector you choose the center and you draw this circle over here.

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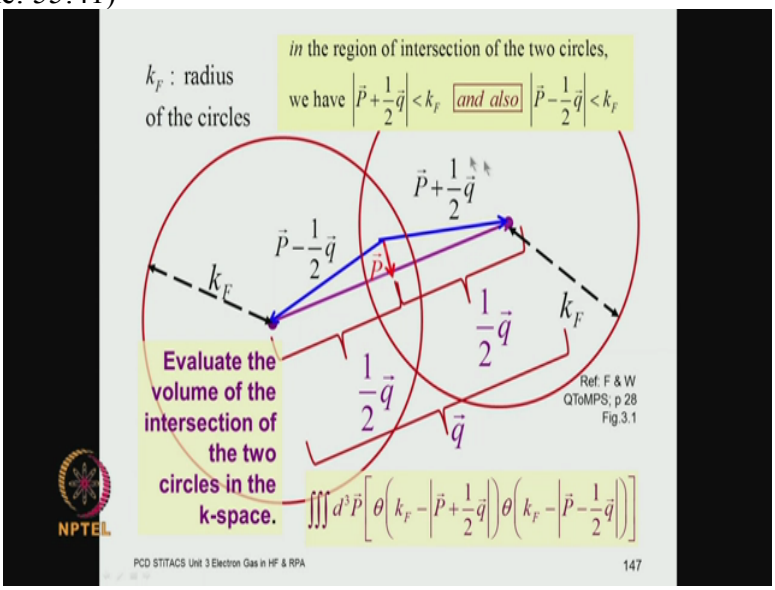

And essentially what it tells us that if you look at this region of intersection of these two circles you have this condition satisfied that P + half q is less than k F and P - half q is also less than kF. So, this carrying out this integration this is the integral that we have to determine.

This integration now becomes a problem in geometry all you have to do is to find the volume of intersection of these two circles okay. So, this is a very nice trick and having done this you now proceed to determine the volume of intersection of two spheres. With this kind of geometry.

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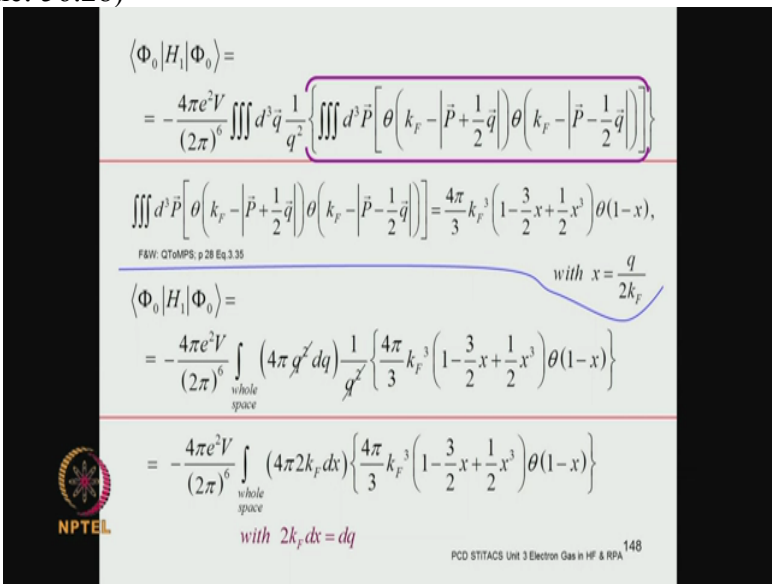

And that result comes straight from geometry. So, I will not work out through those steps you can work it out. And that result is 4pi by 3 kF cube and instead of writing in terms of q I am writing the result in terms of x which is defined as q over twice kF okay. So, this is the result of the volume and we can now put this back over here.

So, you had a q square dq over here, you have a factor 4pi q squared dq which is the volume element right. So, the 4pi is here which is coming from integration over the angles in the reciprocal space the q squared dq the q square cancels, this 1 over q square and this integration of this volume which is the volume of intersection of the two spheres is given by this result over here.

In terms of x but now you have to integrate over q over whole space but mind you x must be less than or equal to 1 because of the Heaviside step function here okay. So, this is the Heaviside step function and if you now proceed to evaluate this integral because this whole space integration now reduces to integration only from 0 to kF.

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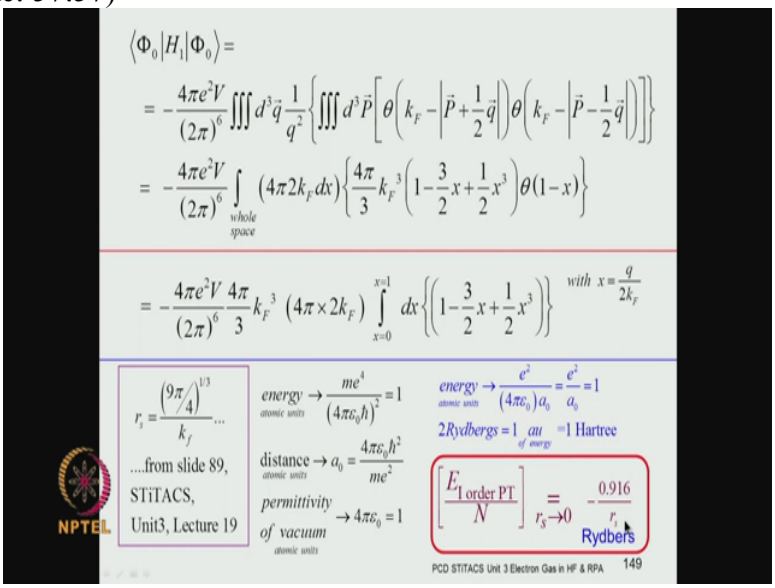

Which will correspond to integration from you can find the corresponding limits on the variable x and those limits are x going from 0 to 1, you have got the twice kF coming over here, the 4pi is coming from here okay. So, here you will now have the result having some perturbation theory this is the first order perturbation correction to the unperturbed energy which you got from the kinetic energy part of the Hamiltonian alone.

Interestingly we were actually able to use perturbation theory despite the fact that the electron-electron interaction is quite strong and that is because we took the high density limit okay. In the high density limit this is perfectly valid and now we can rewrite this result in terms; so you carry out this integration this is just integration over x.

From between limits x = 0 to 1 of 1 - 3 by 2x + half 3x cube and if you put in these values use the appropriate atomic units okay. So, you carry out the transformation write the result in atomic units or which is the Hartree or you can write this result in with Rydberg's and write this value of energy correction to the first-order perturbation energy coming from the kinetic energy part alone and this turns out to be 0.916 upon rs.

And we have seen this result earlier it came from the Hartree Fock self-consistent field method and now we get it from perturbation theory. So, this is a very happy coincidence that Hartree Fock self-consistent field method and the perturbation theory gives you essentially the same result.

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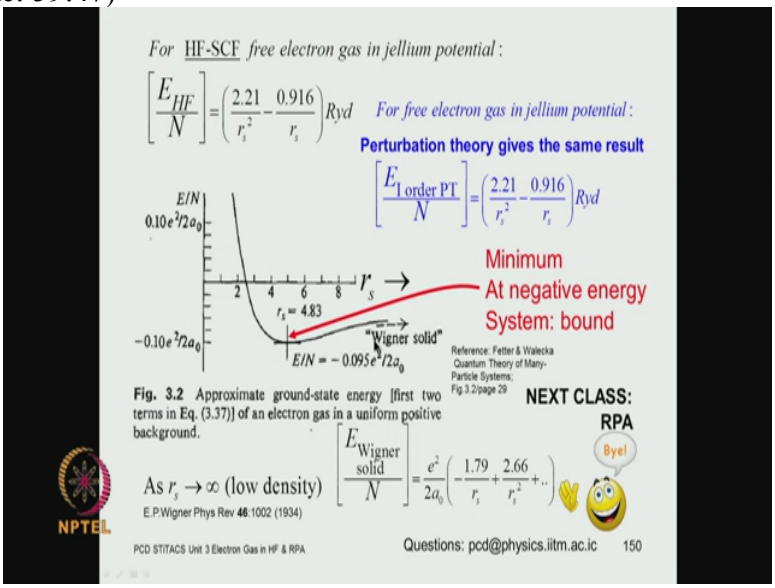

So, this is the result from the Hartree Fock self-consistent field method which we had obtained in our previous classes this is the result from perturbation theory both are exactly identical okay. If you plot energy of course it goes as a function of rs, this term is positive, this term is negative. So, you can when the first term is equal to the second term you will get a 0, which come happens at this value of rs.

You can find the derivative and find at what value of rs will this have a minimum by determining de by dr = 0. So, you find the minimum and then after this minimum this rises again and as are the value of rs increases okay. So, then it becomes a very thinly populated gas right. So, what a high density limit which is as rs tends to 0 and a low density limit that rs becomes very large.

So in the high density limit you get what is called as a Wigner solid which I will not discuss because that is not the region of interest. We are, we will deal with the, this limit and in this

limit you can go through Wigner's article in Physics review 46 which was out long back. And you get what is called as a Wigner solid.

But this is how the energy behaves as a function of rs by and large and we have found that the self-consistent field method of Hartree Fock and the perturbation theory gives exactly the same result. But our worry is going to be that the second and higher-order terms do not give you convergence that is where we will introduce RPA the random phase approximation in the next class.