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

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Lecture 22
Bohm-Pines approach to Random Phase Approximation

Greetings, so today we are about to introduce the Random Phase Approximation and what we are discussing is the classical model. We had the oscillations of the electron gas set by some spurious thermal motion it is not that we are taking explicit account of thermal motion at this point. But we had this electron gas in oscillations and that is a classical model our interest of courses in the quantum treatment.

So we will be introducing the quantum treatment as well in today's class but before that let me introduce the RPA in the classical model.

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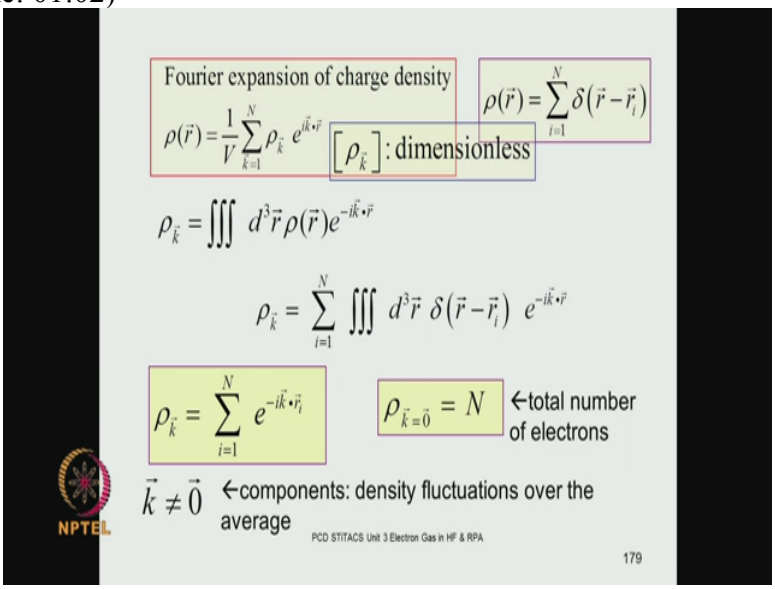

So, I will begin by recapitulating the results that we had in the towards the end of the last class. So, we had the Fourier expansion of the charge density. And we had the explicit expression for the Fourier components which we know can be written as an integral over the delta functions.

Because its charge density is a delta function, so this is the expression for the Fourier components inclusive of the impact of the delta function. And we know that the expression for k = 0 gives you the total number of particles because you will just add one n number of times.

So, the components the Fourier components k which do not correspond to the null vector in the momentum space they will correspond to density fluctuations over the average. Now for this these Fourier components we proceeded to set up the equation of motion okay. This is a classical equation of motion that we set up for the kth Fourier component which is given by its second derivative with respect to time.

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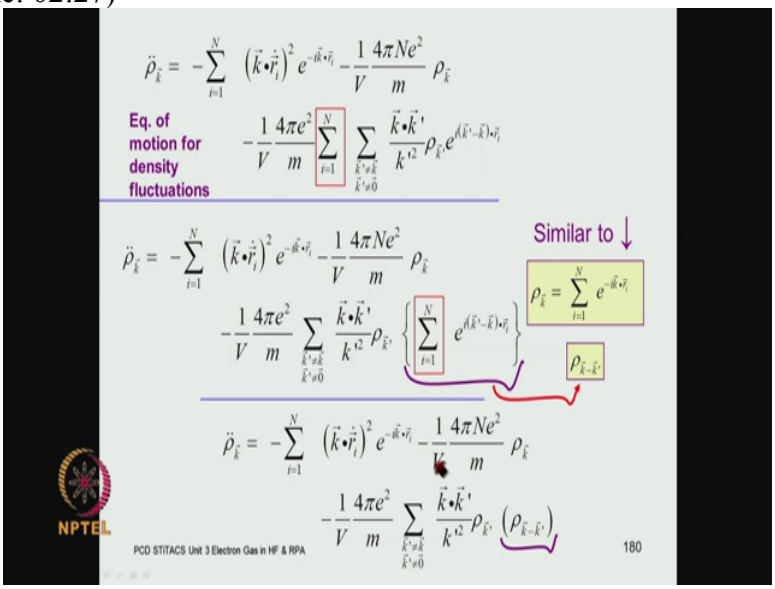

And we have a number of terms over here. We rewrote this term by identifying what is affected by the summation over i, so this is collected in this beautiful brackets in this term. So, this function what you find is just the same as the Fourier component Rho k except that the value of k this time is referred to k prime.

So, it is k prime - k okay. So, this is nothing but the Fourier component corresponding to the index k - k prime. And combining this result we write the second time derivative of Rho k to be given by this expression in which we have now used this Rho k - k prime over here. So, you have got one term which is linear in Rho k and this term is quadratic in the Fourier component one with the index k prime and this is with the index k - k prime.

Now the point I had made toward the end of the last class is that if you had only this term and none of the others. Then you would have the second time derivative equal to minus a certain coefficient times Rho k and that would be an expression very similar to what we have for a classical harmonic oscillator but we have these additional terms.

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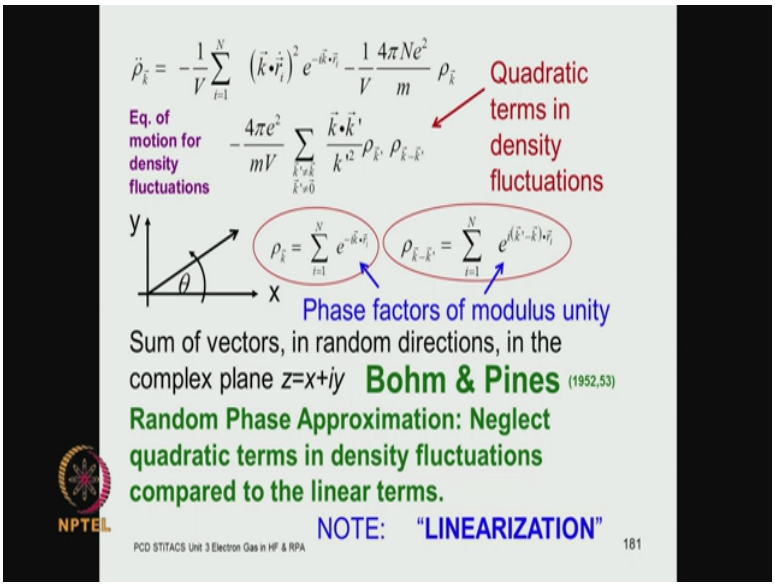

So, let us inquire if we can interpret these terms in some clever manner such that we can reduce this equation because when you have got a complicated differential equation which you cannot solve right away. Then the best thing to do is to try and make some approximation to it or find out what terms really matter if there are ignoring okay. So, that is how theoretical models are always developed.

And what you find is that you have got quadratic terms in density fluctuations in the last term. Now these quadratic terms in the density fluctuations let us write these Fourier components explicitly and you have got these cosine and sine functions. These are basically sinusoidal functions cosine and sine functions. So, this is the superposition of all these cosine and sine functions.

So, e to the i theta or e to the -i theta it does not matter it is cos theta plus or minus i sine theta right. So, now you have got these complex numbers which you are adding and these complex numbers you can also represent another way of looking at it these different phases expressed by the angle theta can also be thought of in terms of an equivalent plane vector diagram.

Because complex numbers can be plotted on a two dimensional surface and you have complete one-to-one mapping between complex numbers and vectors in a plane right. Because the vector is expressed by two components x and y a complex number is also represented by two real numbers which is x plus iy by essentially the same and there is a direct correspondence between a complex number and components of a vector.

So, you can think of this also in terms of vectors but what are these vectors. You have got sum over all the k prime and this is; these are vectors in the momentum space. So, in the Fermi surface in the momentum space for every vector in one direction there will be a vector

in the opposite direction. And there are large number of these vectors in all random directions okay.

So, what you are really doing is adding these phase factors of modulus unity when you multiply any sinusoidal function by another sinusoidal function like a sine theta and a cosine Phi both have got values less than or equal to 1 the maximum value of the sinusoidal or cosine function is 1.

So, that product is small right, so by enlarge these code these terms when you are multiplying these two terms Rho k with Rho k - k prime you will have these product terms which become ignorable they become small okay. And you can think of it also as a summation of vectors in a complex plane where these vectors in random directions okay because a random theta will correspond to a random direction in the vector space in the two dimensional vector space.

So, what Bohm and Pines model uses that they propose that the quadratic term which are here, these quadratic terms are dense these can be neglected in comparison to the linear terms. So, the linear term is here in linear in the Fourier component Rho k and these are quadratic terms. And the Bohm Pine thinking is that the quadratic terms can be ignored in comparison with the linear terms.

And this is because of the phases which are random in these two terms. So, this is why this approximation is called as random phase approximation and the essential point over here is that the quadratic terms are ignored with respect to the linear term. So, it is the linearization process which is intrinsically fundamental to the random phase approximation.

Now this is done in a variety of different alternative approaches to developing tools to deal with electronic correlations beyond the Hartree Fock or beyond the first order perturbation Theory those two are equivalent as we have seen earlier. And these are there are various alternative tools to go beyond the single particle model, to go beyond the Hartree Fock.

To take into account the electron correlations and when you do that many of the alternative schemes also employ a linearization process. So, they all give relations which are mathematically completely equivalent to each other and they are all called as the random phase approximation. But the origin of the term RPA comes from this model and other than that it is only of historical importance.

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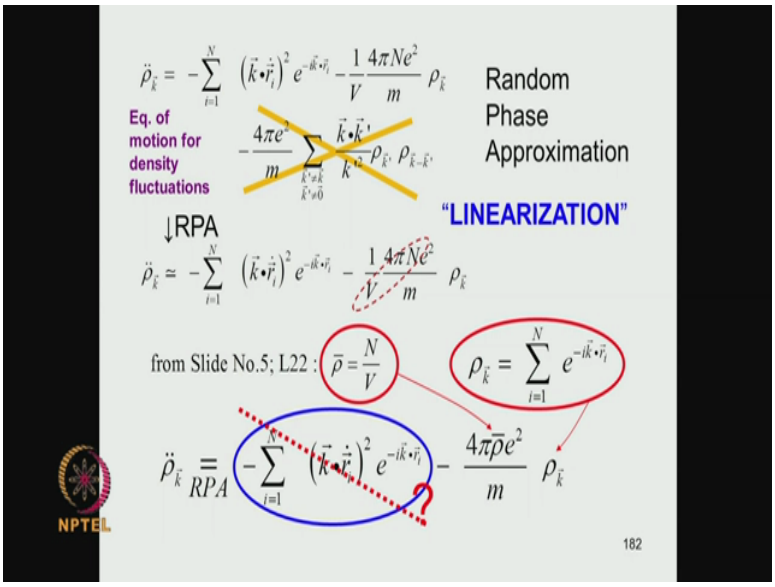

So, in the RPA you ignore these quadratic terms, so you strike it out. Now you are left with these two terms and you still do not have an equation of motion for a simple harmonic oscillator because you have got the second derivative over here on the left hand side. On the right hand side if you had only the second term which is minus a certain coefficient times the displacement Rho right.

Then you would have an equation of motion for the linear harmonic oscillator and we are still left with this term. But then under certain circumstances could you then ignore the first term. Now the first term is quadratic in k, so if the value of k is small then k square becomes smallest term okay. So, for small values of k you can throw the first term also. So, you have already done the linearization.

You have already done the random phase approximation but you need to do something more but all of this belongs to the family of approximation which are called as the RPA. So, this is the RPA, you now have as a result of RPA we now ignore this term and the left-hand side is now nearly equal to the sum of only the first two terms. The third term is neglected not that we claim that it is 0.

But we have given a reason why it is ignorable small. So, now you have got the RPA equation. So, you have got these two terms and then over here this N over V is nothing but the charge density. So, you can write this as Rho bar, so there are two Rho which are going to be used one is the Rho bar which is N over V and the other is Rho k which is this Fourier component of the charge density.

So, it is an anticipation of this that I used the symbol Rho bar over here. So, now your RPA equation is a sum of these two terms in which n over V has been written as Rho bar, so let us

take this to the top of the next equation next slide and we still have to worry about the first term okay.

This is the question we are going to ask can we ignore the first term under some circumstances can we ignore. We already know that its value should be small but we have to ask how small should it be okay. We have to put some sort of a limit some sort of an upper bound of that. So, let us ask this question under what circumstances and we ignore the first term.

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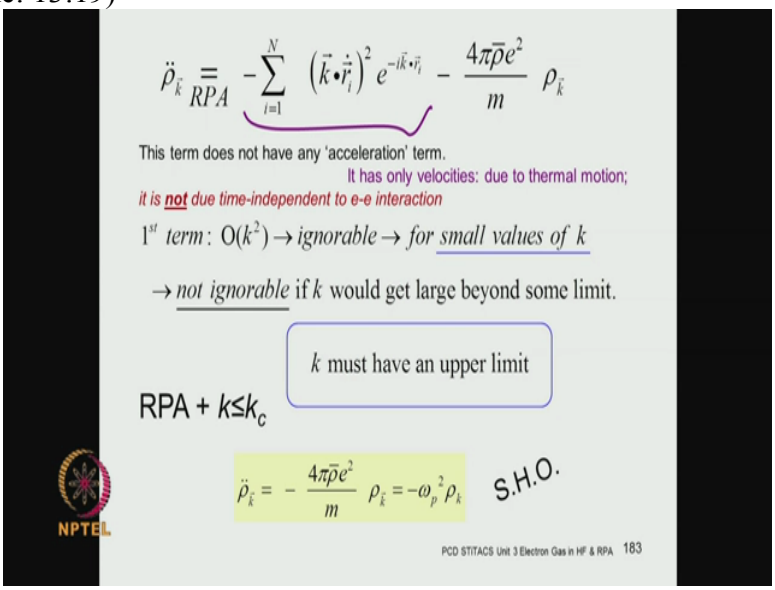

So, let us rewrite this Rho k, this is the first term now, this has got the velocity does not have any acceleration and this is coming as we have seen when we develop the equation of motion for the kth component of the Fourier component of the charge density. And there is no explicit time independent the electron-electron interaction which is being referred to over here, it is not due to that.

So, the first term which is of order k square will be ignorable for small values of k and if we do that there must be a certain upper limit okay. So, k would not; k would get large beyond some limit then you will not be able to ignore these terms. So, there has to be some upper bound and this is a certain cut off on the wavelength. Because k is just the inverse wavelength right, k is just the inverse wavelength.

So, it gives you a certain cut off on the wavelength and that cut off is that this k must have an upper limit in other words it must be less than or equal to a certain bound which I have indicated by kc. So, RPA has been made already by throwing the quadratic terms in the linearization process.

And we are now enquiring under what circumstances can you ignore the first term. And if k is less than or equal to a certain upper bound then you have got an equation of motion to the linear harmonic oscillator. So, the collective behaviour of the electron gas is now described by electron; you know these are some quasi particles if you like and this collectively oscillates.

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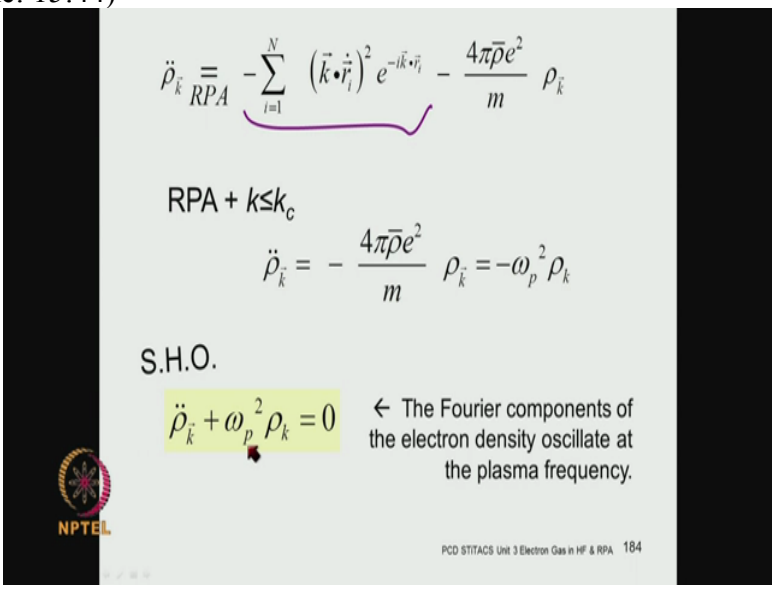

So, these are not the oscillations of individual electrons but the collective oscillations of the whole electron gas. So, this is an equation of motion for the simple harmonic oscillator. So, this is the expression that we have okay. This will give you the natural frequency of the collective oscillations right because this proportionality is nothing but the square of the natural frequency right.

This is the 2pi nu actually the frequency is nu, so this is the circular frequency as we might call it. Now with this circular frequency given by omega p, p stands for plasmas because that is the term which is used for the collective oscillations of the electron gas. So, this gives you an equation of motion for the simple harmonic oscillator.

And it is an equation for how the Fourier components of the electron density oscillate at a certain frequency which is called as the plasma frequency because this is the frequency of oscillation of the entire electronic plasma okay.

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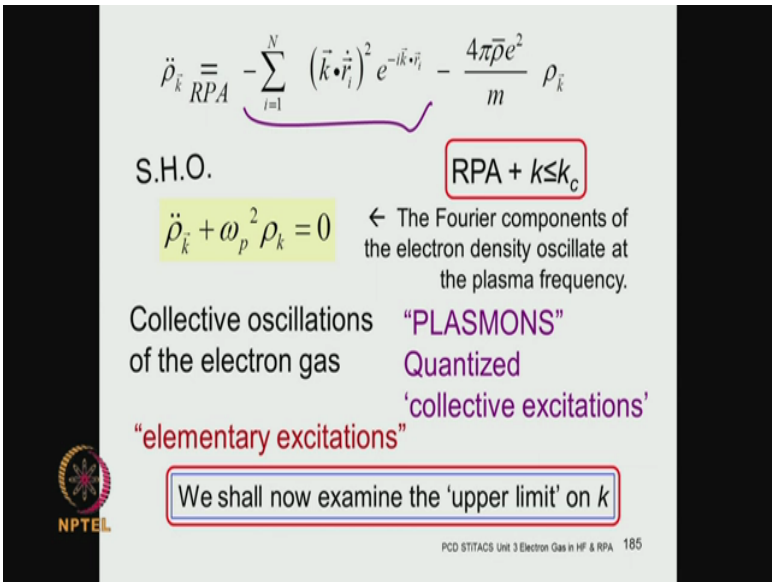

So, so far so good these are these are collective oscillations as such. If you quantize these oscillations then you have what are called as Plasmon's or these are actually pseudo particles. So, these are sometimes also called as elementary excitations of the electron gas okay. And elementary excitation means it is a collective behaviour of the many particle system.

The fundamental particles of nature of course are electrons Plasmon's are not fundamental particles of nature okay. So, plasmas are quantum particles, these are quantization of the collective excitations of the electron gas. These are not real physical particles like electrons, positrons, protons and so on which are fundamental particles.

But they are elementary excitations because you can describe the behaviour of the collective behaviour of the electron gas in terms of these collective excitations which you can go further than what we have just done. Develop a quantum model quantize this and then you get the plasmas which are the elementary excitations of the electron gas.

Now let us inquire what this upper limit should be. We have agreed that there has to be a certain upper limit on k, so that this approximation can be developed.

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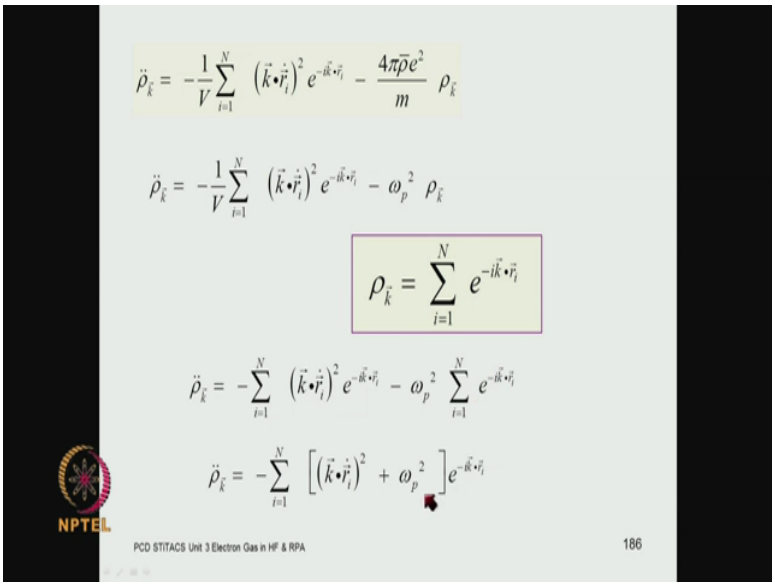

So, we write this expression here okay. This proportionality is written now in terms of the plasma frequency, frequency of plasma oscillations, Rho k we know is given by this expression so you can plug it over here and then extract this e to the minus ik dot ri common in both the terms okay.

When you do that see now you have e to the minus ik dot ri explicitly in both the terms. And you can factor it out as a common term and now inside this rectangular bracket you have got two terms. So, if you want to ignore the first term compared to the other now we know exactly what the conduction will be okay.

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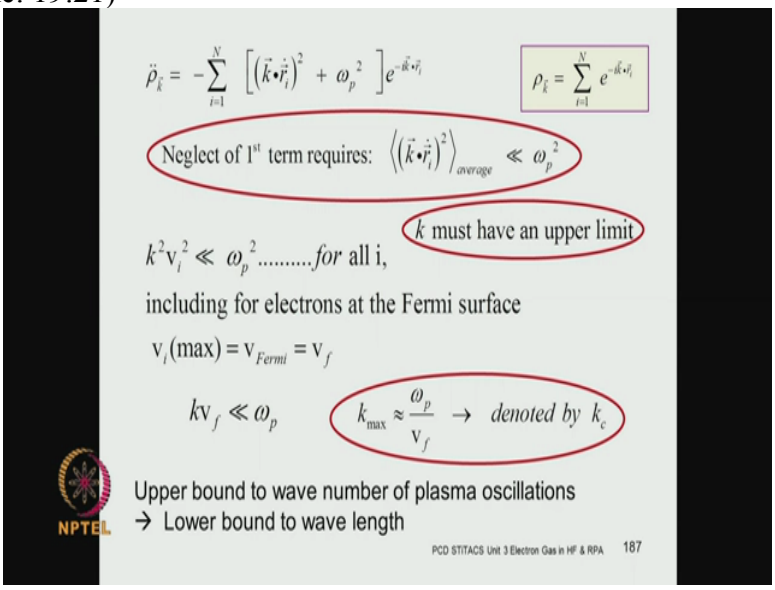

So we you want the first term to be ignored in relation to the second the first term over here is of the order of the magnitude of the wave vector k times the velocity. So, this average value of the first term must be much smaller than the second term which is the square of the plasma

frequency. So, this is the condition, so k has this upper limit which is given by this and this is quadratic in kv.

So, k square v square must be less than or equal to actually it should be much less than the square of the plasma frequency for all values of i. And the maximum value of the velocity of any particle is what it would have at the Fermi surface because that is where the momentum is the largest right. So, that sets the upper limit, so if you choose k, v, f to be much less than omega p then you can throw the first term in relation to the second.

So, that gives us a very simple condition on the maximum value of k. So, this is the k max which must be which is approximately omega p over vf where v is the velocity of the particle, velocity of the individual electrons and the Fermi surface. So, this is the upper bound to the wave number of plasma oscillations. Corresponding to this upper bound to the wave number there is a lower bound to wave length because the wave length and k are just inverse of each other.

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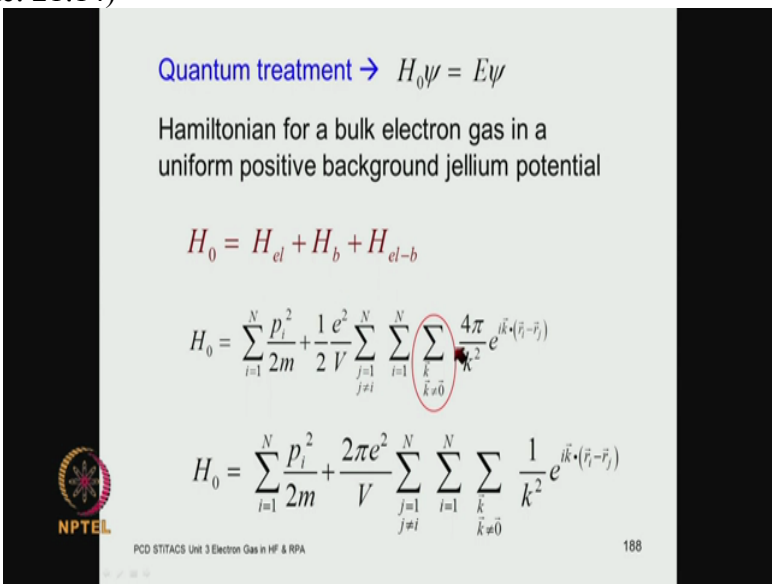

Now we will proceed to develop the quantum treatment because our treatment thus far has been predominantly classical it was at best semi classical. And in quantum theory what you will have to develop is look for the solutions of the Schrodinger equation our Hamiltonian here is what you have already discussed. It is the Hamiltonian for a bulk electron gas in a uniform positive background Jellium potential.

Now we have developed this Hamiltonian in great detail where spend a lot of time in getting the explicit form of this. So, it had these electron terms, it had the terms from background and it had the terms from the electron background interaction. And we have shown that this, some of these three terms is equal to the Hamiltonian for a bulk electron gas.

In which you have got the kinetic energy of the electrons plus the electron-electron term expressed in these for your components of the Coulomb interaction except for k = 0, because it is the k = 0, term which cancel the background terms Hb + these two terms right that we have discussed in our previous classes.

So, this is now our complete expression for the Hamiltonian for the bulk electron gas in a uniform positive background Jellium potential. Remember that k = 0 is removed from this because that is the one which cancels the background terms. So, here I have simply obtained this 4pi over 2 gives me 2pi, so you have got 2pi e square by V and this is the form I will be using okay.

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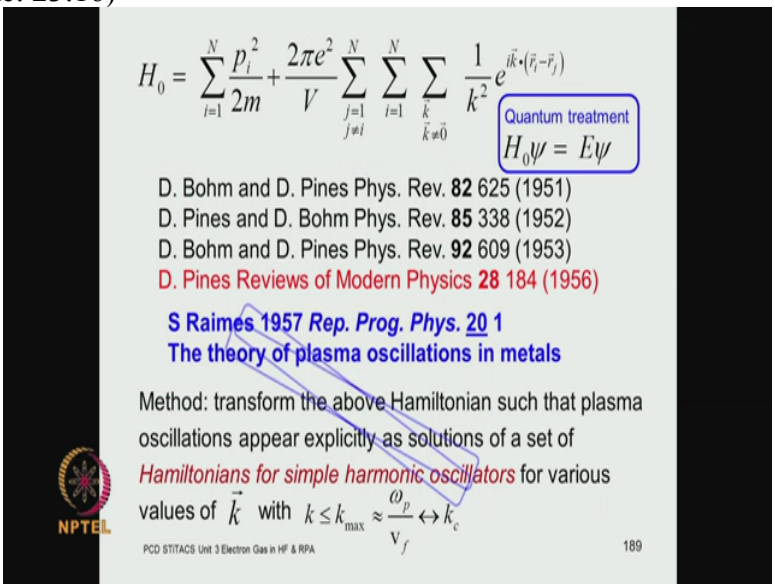

Now this is the problem we have to solve with this Hamiltonian and the treatment is based on a good number of papers which Bohm and Pines wrote in the early 1950's there is a very good review by Pines in reviews of modern physics in the 1956 but then Pines also has got a book and this is very nicely collected in that book.

So, you will also find a good discussion in reports on progression and physics and article written by Raimes, other than the books by Raimes which I have been referring to. What does this method involve the quantum method in the quantum method you are looking at a quantum equation with this Hamiltonian? This is the Hamiltonian for the electron gas in the Jellium potential, background potential.

You expect it to correspond to the classical model that we just discussed; there will be some correspondence right because the classical model is some approximation to the quantum

theory. And we saw that in the classical model we ended up with an equation of motion for the simple harmonic oscillator for the collective excitations of the electron gas.

So, intuitively we expect that the quantum model will lead us to a Hamiltonian for a linear harmonic oscillator and we are well conversant with the Hamiltonian for a simple harmonic oscillator in quantum theory. It is one of the first problems one does in the first course in quantum mechanics. Now this certainly does not look anywhere like a Hamiltonian for a linear harmonic oscillator right.

But then can we carry out certain transformations on the Hamiltonian and then make the transform problem look like a simple harmonic oscillator which will correspond to the collective excitations of the electron gas. Which are described by the plasma, by the plasmons okay?

The quantum of those collective excitations will be the plasmons. So, the method that we are going to follow which was developed by Bohm and Pines is to transform this Hamiltonian. So, this is the, what is called as a method of canonical transformations. Method of canonical transformations of the Hamiltonian to new set of coordinates, new generalized coordinates and new momentum okay.

And can we carry out, can we affect certain canonical transformations of the Hamiltonian which will be so effective that it will finally give us a new Hamiltonian which will have the terms corresponding to the Hamiltonian for a linear harmonic oscillator whose solutions whose Eigen states will describe the collective oscillations of the electron gas.

And because it will come as a solution to the quantum simple harmonic oscillator the quanta of those oscillations will be the Plasmon's. So, this is what we are looking for.

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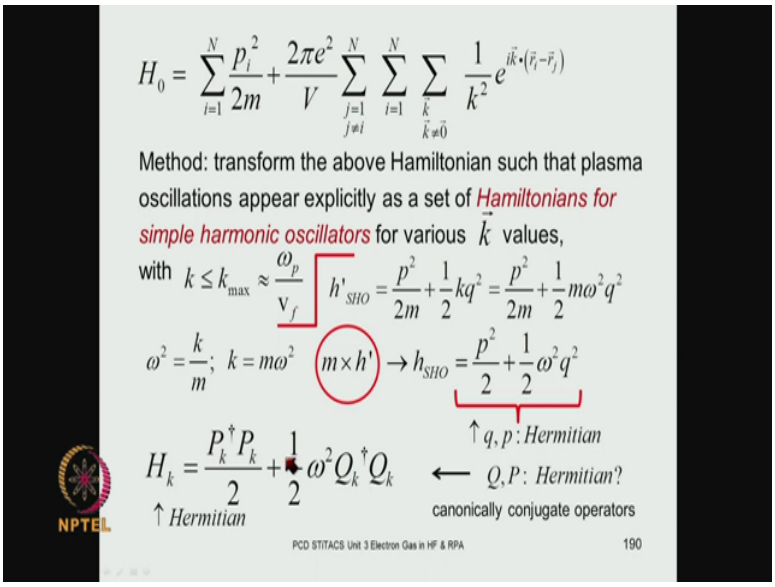

So, the method rests on the transformation of this Hamiltonian and some of you will be reminded of the method of transforming the Hamiltonian that we discussed in a completely different context. Which was in relativistic quantum mechanics when we did the Dirac equation, we did the Foldio Dyson transformations and what the transformed Hamiltonian we carried out a series of Foldio Dyson and transformations.

And we found that when you do carry out the Foldio Dyson transformations once twice and thrice then you are led to a form from which you can recognize the terms that you are really looking for like the spin-orbit interaction okay. This is sitting in the Dirac equation but it manifests itself when you carry out these transformations.

So, to that extent the method that we are now discussing has got a little bit of parallel although it is different in details but so the similarity is always limited, the scope of the similarity should never be taken beyond certain limits. But then what these canonical transformations will enable us to do is to carry out the transformations of the Hamiltonian to a new form.

From which certain terms will become manifest just the way the spin-orbit interaction became manifest after you carried out the Foldio Dyson transformations. So, we have to exercise those series of transformations and finally we are expecting to find a form of a Hamiltonian which looks like the Hamiltonian for the simple harmonic oscillator. This is the Hamiltonian for the simple harmonic oscillator right.

q and p are the; this is a position operator this is the momentum operator and this is the Hamiltonian for a simple harmonic oscillator. Now this certainly does not look anything like this, but we are expecting to be able to carry out certain transformations. And then find these

terms for the simple harmonic oscillator in the transformed Hamiltonian that will pop out as we carry out these transformations.

Now the frequency over here is nothing but the square of the frequency is given by the spring constant divided by the inertia. So, we can write this Hamiltonian in which you remove the mass. So, that in the right hand side in the explicit form of the Hamiltonian you do not have the term in mass. So, it becomes independent of mass so this is the form of the Hamiltonian for the simple harmonic oscillator.

In this the position and momentum operators are hermitian. So, what we are going to look for is, think of a certain Hamiltonian which has got a similar form. Now Hk is a hermitian operator which has got the same kind of form as this. It is made up of new momentum operators P and new coordinate operators Q okay. So, this is the canonical transformation from small q small p to capital Q capital P okay.

So, there are new coordinates and coordinate and momentum operators such that you have an expression for a harmonic oscillator this is the kind of thing that you are looking for. And since this is going to be a transformation, this is a mathematical transformation it is not mandatory that we look for hermitian operators.

We can even deal with non hermitian operators as the mathematical intermediate steps. Because our interest is in the Hamiltonian not in actual measurements of coordinates or momenta okay. So, if you are dealing with measurements then of course you need real Eigen values and you will need to look for affirmation operators but not in this context.

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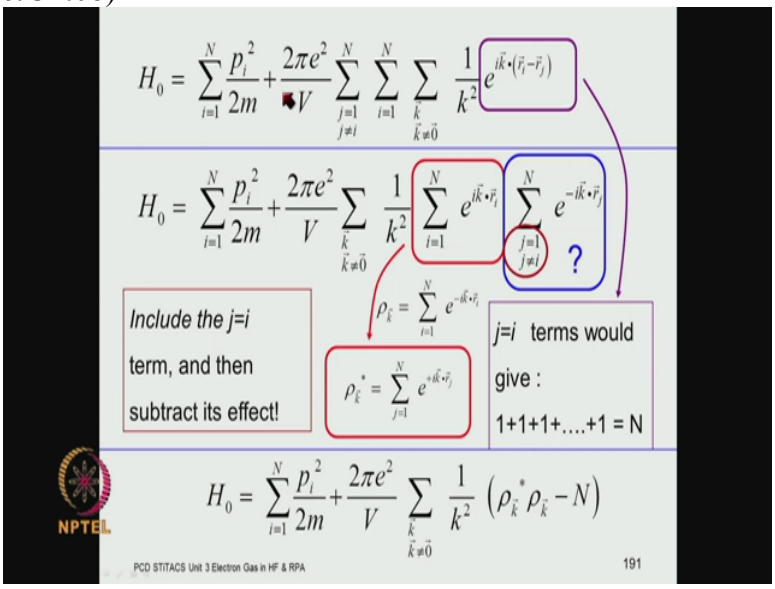

So, let us examine this possibility now. So, the first thing to do is to rewrite this term in a form which is convenient for our analysis. So, we have written this term which is the Hamiltonian for the electron gas of the interacting electron gas the Coulomb interactions are taken care of. And then you have also taken care of the background-background interaction and the electron background interaction by removing the k equal to the null vector term.

So, this is the same expression rewritten but I have factored out these two exponential terms of which you recognize this term immediately because this is very similar to the Fourier component for k except that over here you have got a minus sign but we have got a plus sign over here right. So, essentially you have got the complex conjugate of the Fourier term okay. So, far so good what about here is it also similar.

To a large extent, yes but not exactly because you have removed the j = i term. If j = i were included it would be the Fourier component of the charge density right. But you have excluded j = i, so what do you do, if you want to find and a term corresponding to the charge density over here. Then put in the value for j = i which will make it look like the Fourier component of the charge density.

But having put it, subtract it as well, so it is like adding and subtracting at all okay. So, we have to take care of the fact that the summation excludes j = i. So, we first include the term j = i and then subtract its effect that is a very simple technique that we always use in carrying out analysis. And what is it that we will have to subtract; we already know that when you add it you will get the Fourier component of the charge density.

What will you have to subtract? You will have to subtract whatever you have added and what you have added is by putting j = i. Now when you put j = i over here this ri minus rj goes to zero okay, j = i gives you each to the power 0, so you end up adding 1 + 1 because e to the power 0 is 1 you keep adding one to itself n times and you get the total number of electrons. So, what you are doing is you can rewrite this Hamiltonian.

The first term is the kinetic energy term the second term 2pi square by V is here you have got the sum over k, 1 over k square is here and from here you have got Rho k star Rho k – N. So, this is the explicit equivalent form in which the Hamiltonian for the electron gas in the Jellium potential is described in terms of the Fourier components okay.

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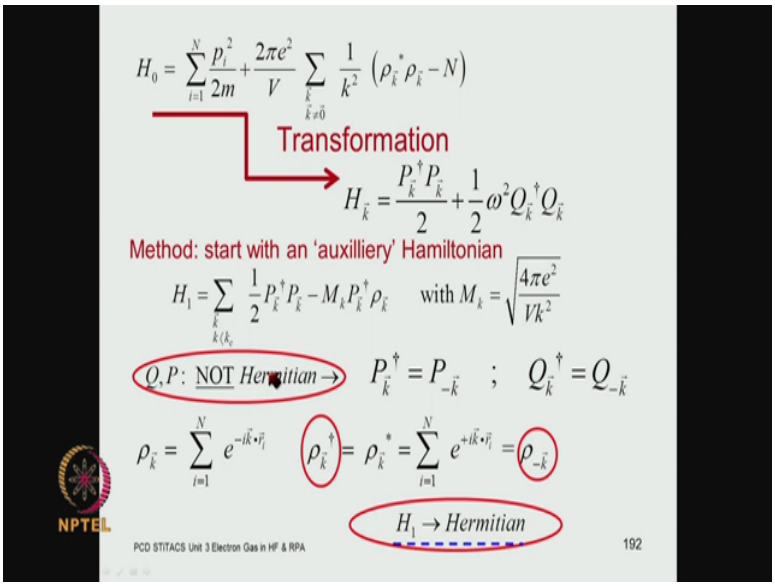

So, here you are and now we have to find if there is some way in which we carry out transformations and make this whole thing look like simple harmonic oscillators okay. What we do is begin with an auxiliary Hamiltonian okay. It is the mathematical device, so introduce an auxiliary Hamiltonian which is composed of this term.

In which Mk is defined as root of 4pi e square by Vk square. Q and P are not hermitian. They do not have to be, instead we choose the P dagger for the component k to be equal to P not of k but a -k and the Q dagger of k not equal to Q of k but Q of - k okay. So, these are not hermitian, so this is your Rho k, what about Rho k adjoint? What happens to this adjoint?

This is adjoint is nothing but the complex conjugate of the Fourier component of the charge density which becomes this summation. But now you have got e to the +ik dot ri and this will now be equal to root of -k okay. So, Q and P are not hermitian. H1 however is hermitian okay.

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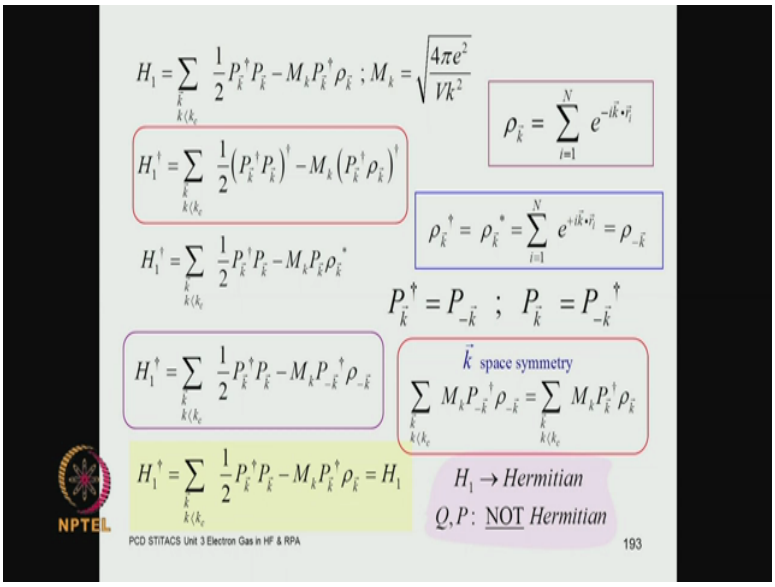

You can see that quite easily by carrying out the; by finding out what is the adjoint of the operator H1. So, this is a adjoint of the operator H1, you take the adjoint of all the terms. So, you take the adjoint of the first term which is P dagger P and then you take the adjoint of this MP dagger Rho. So, you take the adjoint of this and what is it you get P dagger Pk over here right, over here you get Mk, Pk and Rho k star.

Now this is Rho k, this is Rho k star we have these relations which we pointed out on the previous slide that our operators are not self adjoint they are not hermitian and we take advantage this and we now write this adjoint Hamiltonian as half P dagger P which is coming from this term. Here you have -Mk that is fine. Pk becomes P - k dagger and Rho k star becomes Rho of – k.

Now that still does not look like H1 does it, but actually it is because you are summing over these momentum vectors okay. And there are as many vectors in one direction as there are in the other. In other words when you look; when you add up all the terms it does not matter whether you are adding over + k or you are adding over –k. So, that summation is completely the same, it gives you essentially the same result.

So, this is because of the symmetry in the momentum space, so this summation over the -k index is completely equivalent to the summation over the + k index. And now you have a form which is this which is nothing but the same as the H1 that you started out with. So, you see that H+1 is self adjoint even if Q and P are not okay.

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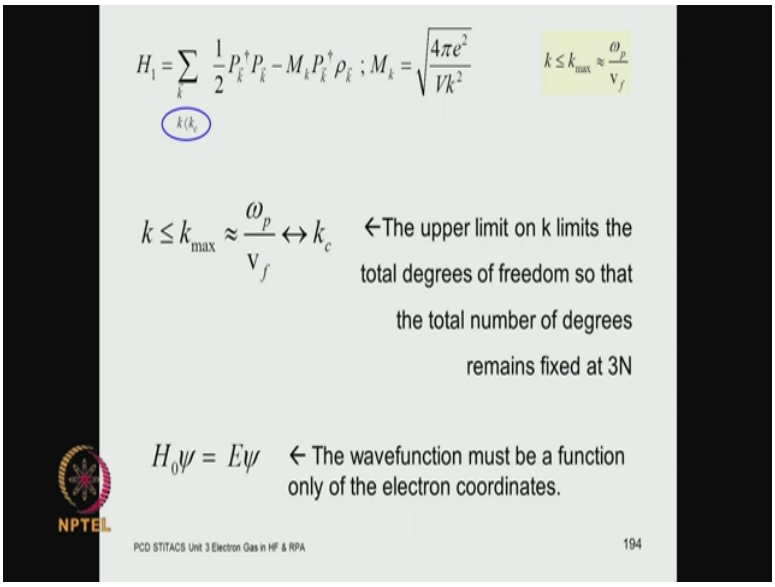

So, so far so good we have to remind ourselves that we are expecting an upper limit on k we showed how it comes in classical mechanics. We knew that it has this value, so the total degrees of freedom will be limited because of this upper limit on k. So, the wave function must be a function only of the electron coordinates and now these you have introduced these new coordinates which are the capital Qk.

The wave function cannot begin to depend on these new additional coordinates right. Because you cannot introduce any additional degrees of freedom just because you are carrying out the transformation does not mean that you are adding to the number of degrees of freedom, so one has to remember that.

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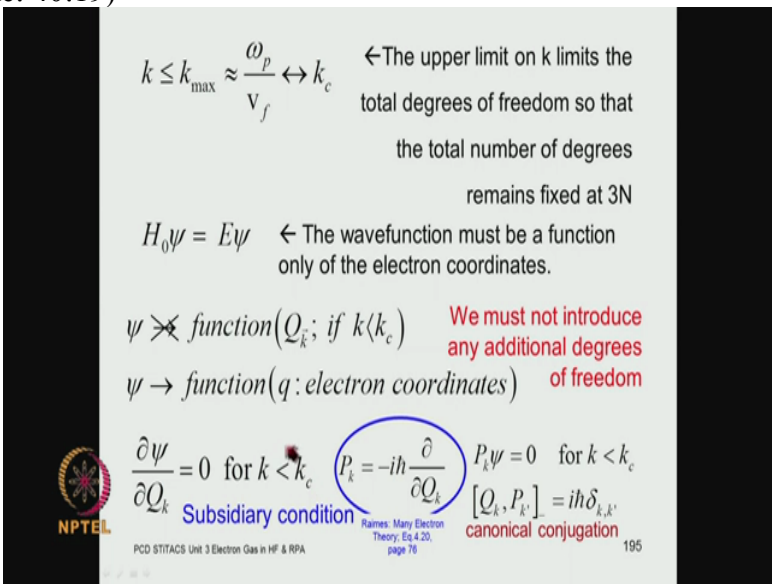

So, we have to remember this and this will give us certain auxiliary and subsidiary conditions. It means that the wave function is not a function of Qk if k is less than kc okay.

Because for k less than kc the wave function is a function only of the original electron coordinates and you are not adding any additional degrees of freedom.

So, this is our requirement which means that the derivative of the function with respect to Qk, if k is less than kc would vanish, it cannot depend on that, so its derivative vanishes. And what is the operator del over del Q it is the gradient operator right. It is the derivative operator, the derivative operator is the momentum operator, momentum is -ih cross gradient right.

So, it is the same thing over here except that we are using a new set of coordinates. So, if del by del Q of Psi is 0, which it must be because you are not allowing any additional degrees of freedom. The momentum operator which is given by -ih cross derivative operator then this momentum operator operates on the wave function you will get a 0, because this momentum operator is nothing but the derivative operator.

So, for k less than kc this equation holds, now we are going to use this result. But when the momentum operator operates on the wave you get 0. Q and P canonically conjugate okay, so they satisfy the uncertainty principle. And this is the subsidiary condition that we are getting that the momentum operator operating on the wave function would go to 0 for k less than kc all right.

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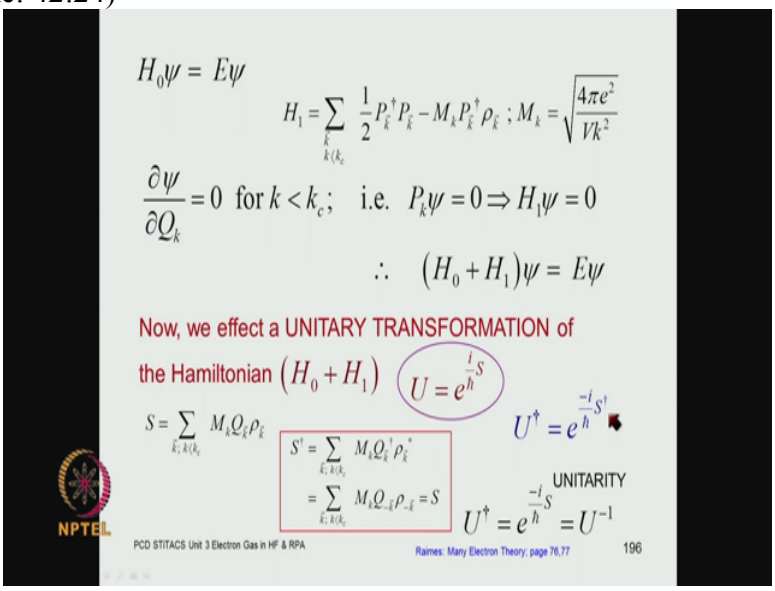

So, this is our auxiliary Hamiltonian which we have introduced, we have learned that it is self adjoint. We have learnt that the momentum operator operating on Psi goes to 0 and if the momentum operator goes up to applying when it is applied to a wave function goes to 0 then H1 operating on Psi will also go to 0 because H1 is made up of this momentum operator to the right.

So, it will kill the wave function right it will give you a 0. So, now we have got these two results a H0 Psi equal to E Psi which is an original Schrodinger equation H1 Psi = 0. So, you can add this relation to this equation what does it give you that H0 + H1 Psi =E Psi. So, in as much as H0 Psi = E Psi was the Schrodinger equation you are working with your reasonably safe okay with reference to whatever approximation we are made so far.

To deal with another Hamiltonian which is not the original H0 but H0 + H1 because it gives you essentially the same quantum mechanics, it gives you exactly the same Schrodinger equation that H0 + H1 Psi = E Psi after all the system in classical mechanics is described by position and momentum right. That is the definition of a state of a system in classical mechanics.

You can represent it not just by position and momentum but also by a function of position and momentum. So, you can describe the state of the system by the Hamiltonian and you can describe it in quantum theory by quantizing this Hamiltonian by choosing appropriate quantum operators for the position and momentum.

It is very straightforward. So, this is now the description of the system in terms of this H0 + H1. And now we will seek a unitary transformation of the Hamiltonian. The Hamiltonian that we are now working with is not just a H0 but to that we have added an auxiliary Hamiltonian which retains the form of the Schrodinger equation intact.

So, what kind of unitary transformation are we searching for? So, this is a typical expression for a unitary transformation okay. We choose this operator s to be given by this sum over k with k less than kc which is this upper limit on k of product of these three terms. What is s dagger, s dagger find out what is the adjoint of this?

So, you have got Mk Qk dagger Rho k star and this s dagger because Qk dagger is the same as Q - k, Rho k star is the same as Rho - k and Mk and M - k are the same because notice that Mk depends on k in the quadratic term in the denominator. So, this denominator k square is the same irrespective of the direction of the vector being + k or – k.

So, only the square of its magnitude is coming here in the denominator. So, Mk is remains the same. In other words this operator s is hermitian it is self adjoint, so if you now take the adjoint of this operator U since s is self-adjoint, this operator is unitary. So, that is the unitary transformation that we are seeking okay.

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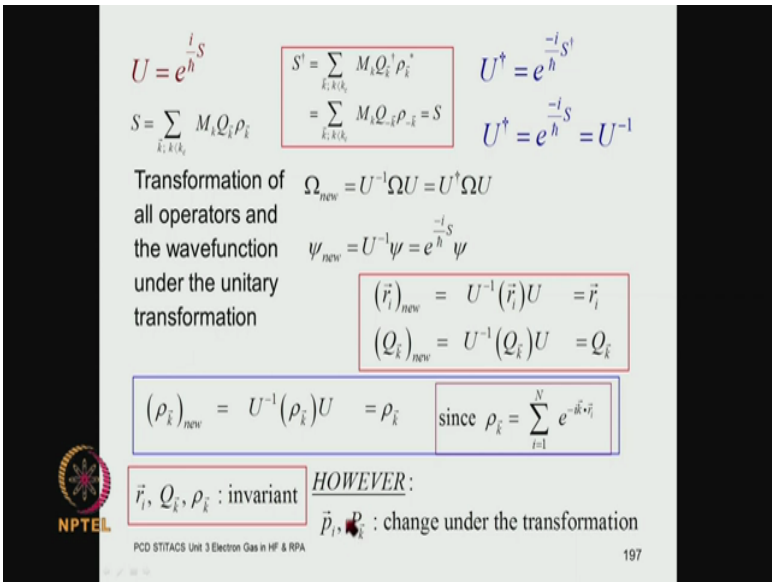

So, we have got the unitary transformation we have identified the operator s. Having chosen s to be given by this summation we get an appropriate unitary transformation. So, these results we bring from our previous slide. And we will now subject various operators and the wave functions to a unitary transformation which is described by this operator U.

So, the new operators will be given by U inverse omega U or U dagger omega U which is the same thing U inverse and U dagger are equal and the new wave function will be given by U inverse operating on Psi which is e to the minus i over h cross s operating on Psi okay. This is the U inverse; U is with the plus sign, U inverses with the minus sign.

What about the operators the operators that we are working with are the position operators and the new position operators it up with Q okay. So, the new position operator this ri you can see immediately commutes with U because what is U made up of, U is made up of these operators made up of S and what is S made up of, S is made up of Rho and this is made up of the terms ri the position vectors right they are sitting over here.

And the position vector of course commutes with any function of a position operator. So, this operator ri commutes with this. So, U inverse U ri will give you ri itself. So, the new coordinate remains invariant, the coordinate Q operators also remain invariant because after all the transformed Q requires you to examine the commutation of Q with these operators but Q will not commute with the momenta but with other coordinates it certainly commutes.

So, this Q is also invariant and it remains the same under the unitary transformation. The charge density components will of course remain invariant because the position operator is invariant. Position operator is made up of these ri's, so this is invariant. So, these three

operators remain invariant, what about the momenta the lower case momenta which are the moment are corresponding to the electrons that we began with.

And these are the operators that we introduced in the auxiliary term. So, these as we will see actually do undergo a transformation they do not remain invariant under the canonical transformation. If everything remains the same it would not be of much use, much interest. So the momenta are actually change under these transformations.

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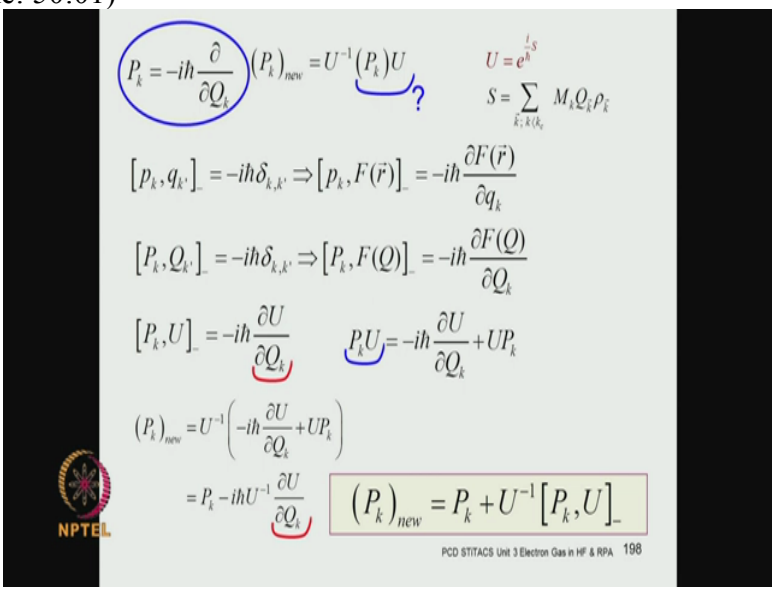

So, let us look at the momentum operators. So, the new momentum operator will be U inverse P U we ask what is P U because if P U were equal to U P then of course it would be invariant but it does not commute so we must ask what is the commutator of P with U, now that is quite easy.

Because we certainly know that you have the basic uncertainty relation between position and momentum operators which gives you which is nothing but the expression of the uncertainty principle and if you begin with this your first course in quantum mechanics you would have done this problem that any function any operator which is a function of the position operator does not commute with the momentum operator.

But the commutator is equal to - ih cross the derivative of this operator with respect to the corresponding component p will have three components corresponding to xyz right. So, depending on which component you are considering you will have the partial derivative of this operator with respect to qk. So, this result is known from first course in quantum mechanics.

And now instead of the lower case p and the lower case q, we have the upper case P and the upper case Q operator. So, we have exactly the same result and this tells us how to get this because the commutator of P and U will now be - ih cross del U by del QK okay. What does it mean thatPk U will be this right-hand side + U Pk right.

So, now you can write the transformed momentum operator as U inverse, this U inverse and Pk U which is given by these two terms which is - ih cross del U by del Qk + U Pk and the second term would give you just Pk because U inverse with this U will give you Pk which is what I write first. And then I write the result of this which is -ih cross coming from here, you have U inverse coming over here and del U by del Qk.

So, this is the new momentum operator it is not the same as Pk it is not invariant but you must subtract from this another operator which is - ih cross U inverse del U by del Qk right. So, the new momentum operator you can write it in terms of del U by del Qk or also in terms of this commutator Pk U. But you had a -ih cross here. You have got a - ih cross which will go in the denominator here. So, you write it independent of the ih cross factor.

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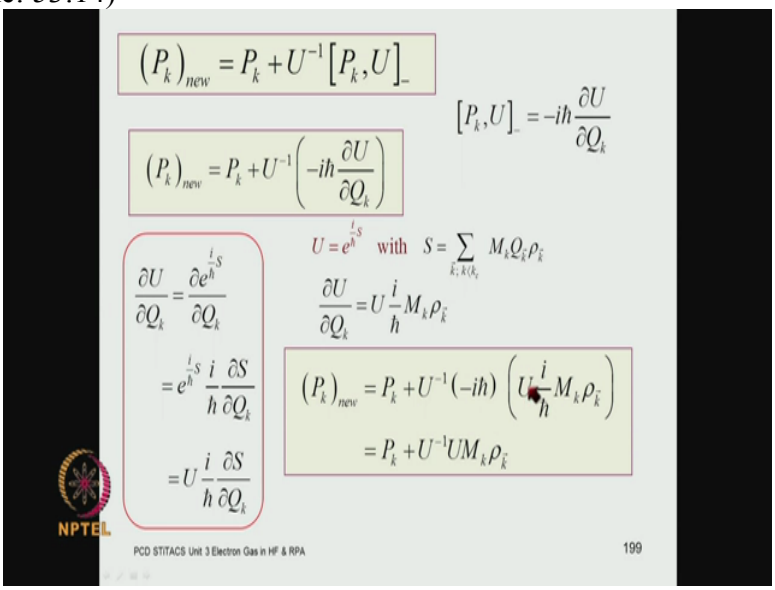

So, this is our result, the new momentum operator is not invariant okay. You can write it in these equivalent alternate forms. This is the unitary transformation we have made use of. Now let us ask what this del U by del Qk is, so del U by del Qk we find explicitly which is del by del Qk of this unitary transformation which is e to the i over h cross s which is this. So, now we have to find e over i, e to the power i over h cross s.

And then we must find the derivative of S with respect to Qk but we know S explicitly in terms of Qk, so the partial derivative of S with respect to Qk you will get the corresponding term over here. So this is the del S by del Qk right. And this is nothing but U this is nothing

but the unitary transformation itself and you can determine this derivative. What is this derivative with respect to k it is Mk Rho k right.

Derivative of this summation with respect to k will give you Mk Rho k. So, this is del U by del Qk which is U I over h cross times del S by del Qk is now this Mk Rho k and now the new momentum operator is Pk + U inverse which is coming from here - ih cross is coming from here and then you have the del U by del Qk which is this term over here. And if you now take care of the 1 over h cross cancel this.

You have got a -i square which is + 1, so you get P + U inverse U which is a unit operator. So, this is the new result for the momentum operator okay.

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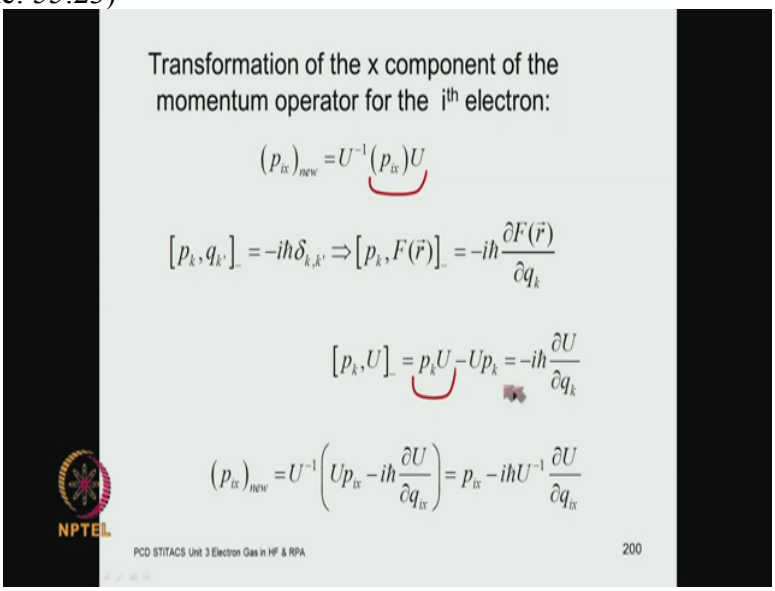

Now let us consider the transformation of the lower case momentum operator. We will do it component by component okay. We will find how the x component transforms and then we know that similarly the y and z will also transform. And we will have the expression further how the momentum operator transforms.

Again we make use of the same result which means that pk U will be given by minus ih cross del U by del Qk it is exactly the same thing that we are doing now and we; this is the term that we need here p U okay. It is coming over here, so you will now write this transformed momentum operator but now you have got this –ih cross del U by del Q and then this term goes to the right with a plus sign.

So, it is U p - ih cross del U by del Q, so there are these two terms from the first term U inverse U will give you 1 and then over here you have got this U inverse – ih cross is coming

here and the del U by del qk alright, which you can again write in terms of the commutator just as we did in the previous step.

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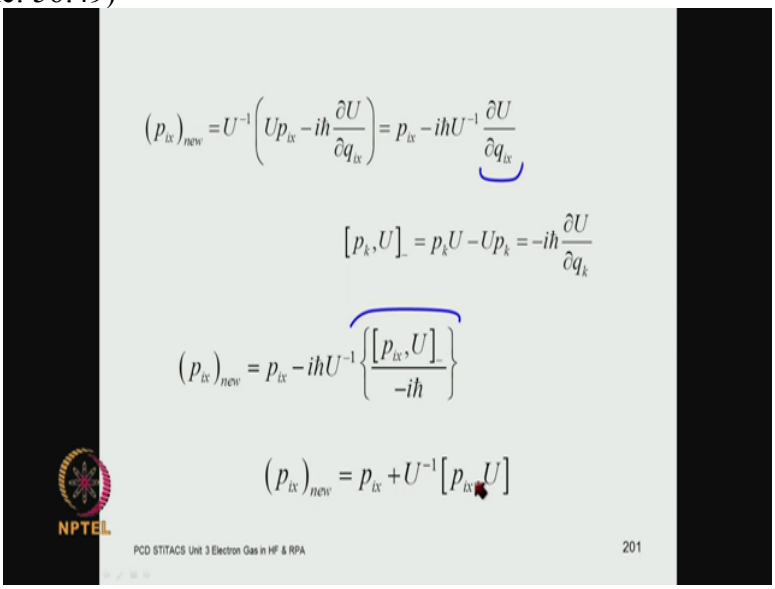

So, we can write it in terms of the commutator which is over here and now again you can cancel this -ih cross and you have got the new transformed momentum operator all right.

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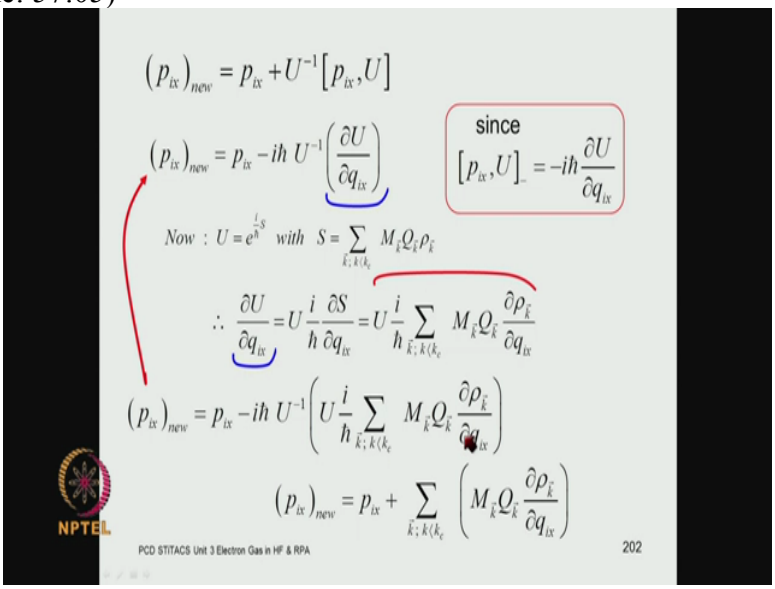

Now these are the transformations we have made use of del U by del q again we can determine explicitly. Because now you are taking the partial derivative this time not with respect to the upper case Q but with respect to the lower case q and where is the lower case q sitting in the operator S it is sitting here because Rho k is a function of the position vector ri which is actually xi, yi, zi right.

So, each component is involved over there and you must take the partial derivative of del Rho by del qi corresponding to the x component because now we are dealing only with the x

component one at a time. So, this is the result that we get and we can now write this transformed momentum in terms of the first term is p ix.

Then you have got -ih cross over here, you have got U inverse coming over here and this del U by del q is what has been determined over here and this whole thing comes in this bracket. So, this is our result now again the h cross cancels the -i square gives you +1 and this expression is a little more complicated than what we had seen earlier but simple enough.

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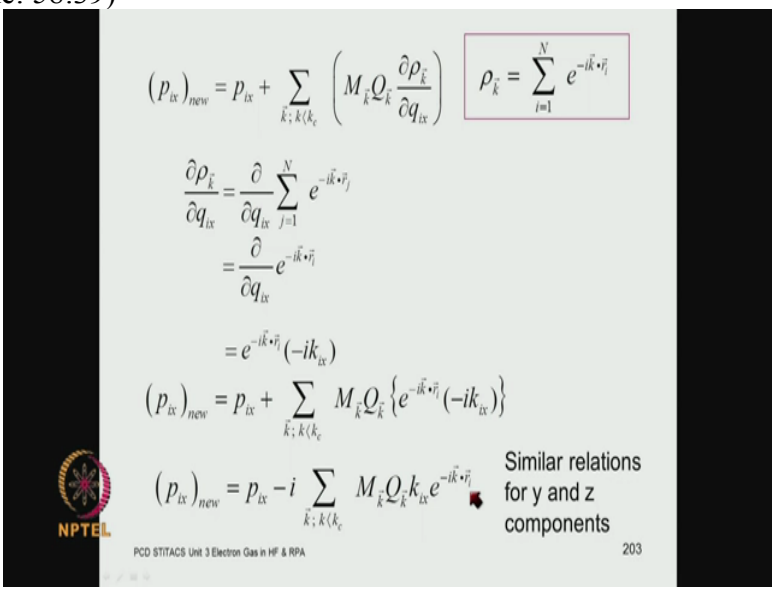

So, this is how the new transform momentum operator looks. You need del Rho by del q you have explicit form for the Fourier component of the charge density which is so; here you have got the position vectors. And you have to take the derivative with respect to del q corresponding to the i component, so you will have; when you take the derivative you will get -ik and you will have the x component here okay.

Because a dot b is like ax bx + ay by + az bz, so only the x component will come in over here okay. This is the result for the x component of the momentum operator. I have only brought this - i over here. The ki x is sitting here and all these terms have been written. Similar relations will hold for the y, z components right.

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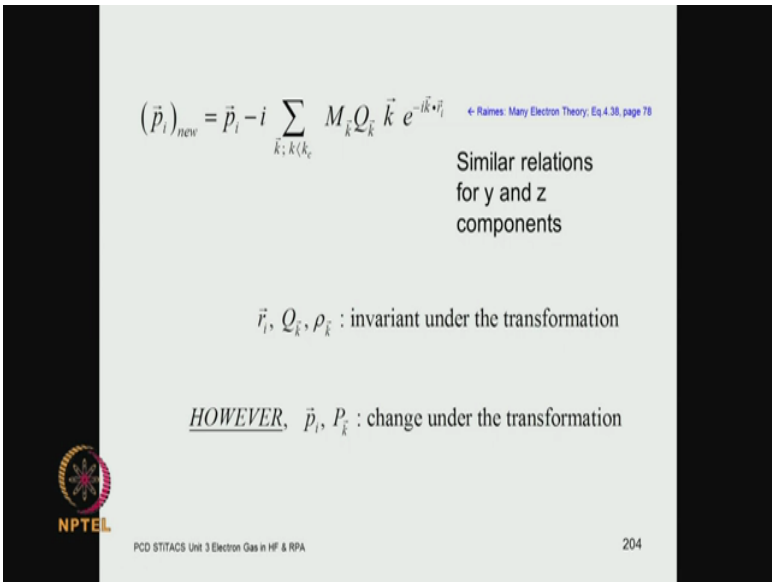

So, now what we have learned is that the coordinate operators and also the charge density in the Fourier components of the charge density operators, these do not change under the unitary transformation that we are considering. But the momentum operators they do change and we have got an explicit form for the transformation of this momentum operator for the electron for the ith electron and also for the auxiliary momentum vectors which we have inserted.

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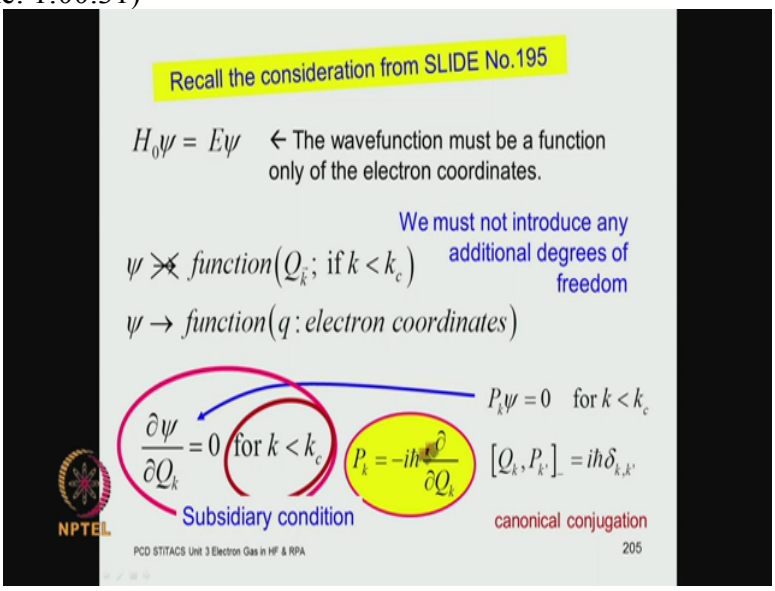

Now I would like to recapitulate quickly one consideration that we have discussed already but it is a good point to remind ourselves of that, that this is the original wave function that we wanted to; we were interested in, we agreed that when we carry out these canonical transformations. We must not introduce any additional degrees of freedom;

We therefore concluded that this wave function would not be a function of Q if k is less than kc right. Because no additional degrees of freedom are to be introduced and that gave us the

subsidiary conditions that Pk operating on Psi gives a 0 and this was something that we have really exploited.

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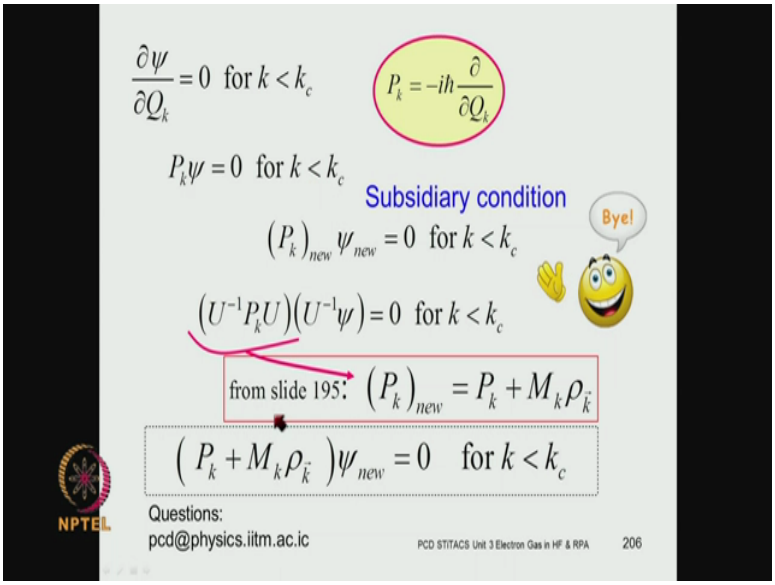

Which means that the derivative of the wave function with respect to the auxiliary coordinates Q vanish, the momentum operator operating on the wave function vanishes. And this relation will hold good in the new transform system as well. So, you have got Pk Psi under transformation Pk new and Psi new when the wave function is transformed by the same unitary transformation.

So, this relation will remain invariant for k less than kc. So, let us write Pk new as U inverse Pk U and Psi U as U inverse Psi. So, this is our result that we get. Now this is a very useful result, this is nothing but Pk new, we have obtained an explicit form for this right. So, this is where I will take a break today and we will continue from this point in the next class. Essentially this is a very useful result.

Because this will enable us to complete the transformation of the Schrodinger equation or the Hamiltonian that we started out with which is the canonical transformation of the Hamiltonian to new set of degrees of new set of collective excitations of the electron gas. So, you are still dealing your physical system is the same as the electron gas.

But the mathematical system that you will be working with is not the system of electrons anymore but this collective manifestation of the electron-electron interactions. Now this is where we go beyond the Hartree Fock okay. Because of the Hartree Fock you had the charge densities which were invariant. There was no time dependence you had complete time independent. So, that is the time independent Hartree Fock theory.

But one can do similar things using a similar approach with the Hartree Fock self-consistent field method which is to make use of the time-dependent Hartree Fock. And when you do that again you can develop a set of approximations and what is the heart of the approximations that we are working with over here, it is the random phase approximations in which the focal theme was a linearization.

So, this can be done using these alternative ways of arriving at the random phase approximation but that is something that we will discuss in the next class. If there is any question now I will be happy to take and we shall begin the discussion from this point in the next class.