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

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

## Lecture 24
## Bohm-Pines approach to Random Phase Approximation

Greetings, this is the last lecture of unit 3 in which we are discussing the electron gas in the random phase approximation. Specifically we are using the Bohm Pines approach there are various alternative ways of arriving at the random phase approximation. In the next unit in unit 4 we will be discussing the logramatic perturbation theory.

But today we will conclude the discussion on the Bohm Pines formalism of the random phase approximation.

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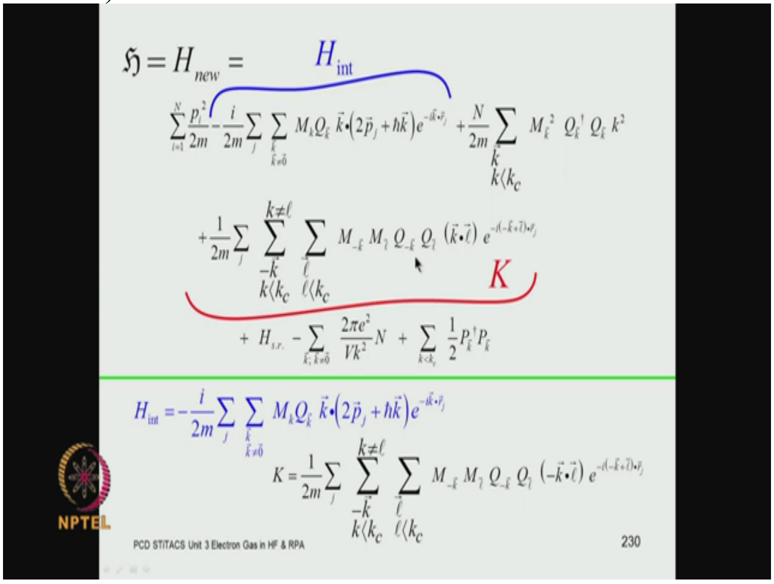

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N}\frac{p_i^2}{2m} \overbrace{-\frac{i}{2m}\sum_j \sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}} M_k Q_{\vec{k}}\, \vec{k}\bullet\left(2\vec{p}_j + \hbar\vec{k}\right)e^{-i\vec{k}\bullet\vec{r}_j}}^{H_{\text{int}}} + \frac{N}{2m}\sum_{\substack{\vec{k}\\ k\langle k_c}} M_{\vec{k}}^2\, Q_{\vec{k}}^{\dagger}\, Q_{\vec{k}}\, k^2$$

$$\underbrace{+\frac{1}{2m}\sum_j \sum_{\substack{-\vec{k}\\ k\langle k_c}}^{k\neq\ell} \sum_{\substack{\vec{\ell}\\ \ell\langle k_c}} M_{-\vec{k}}\, M_{\vec{\ell}}\, Q_{-\vec{k}}\, Q_{\vec{\ell}}\, (\vec{k}\bullet\vec{\ell})\, e^{-i(-\vec{k}+\vec{\ell})\bullet\vec{r}_j}}_{K}$$

$$+ H_{s.r.} - \sum_{\vec{k};\,\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2}N + \sum_{k<k_c}\frac{1}{2}P_{\vec{k}}^{\dagger}P_{\vec{k}}$$

$$H_{\text{int}} = -\frac{i}{2m}\sum_j \sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}} M_k Q_{\vec{k}}\, \vec{k}\bullet\left(2\vec{p}_j + \hbar\vec{k}\right)e^{-i\vec{k}\bullet\vec{r}_j}$$

$$K = \frac{1}{2m}\sum_j \sum_{\substack{-\vec{k}\\ k\langle k_c}}^{k\neq\ell} \sum_{\substack{\vec{\ell}\\ \ell\langle k_c}} M_{-\vec{k}}\, M_{\vec{\ell}}\, Q_{-\vec{k}}\, Q_{\vec{\ell}}\, (-\vec{k}\bullet\vec{\ell})\, e^{-i(-\vec{k}+\vec{\ell})\bullet\vec{r}_j}$$

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Now in our previous class we rewrote the transformed Hamiltonian in a certain number of terms. Now here just for the sake of our discussion and for book keeping this we recognize already is a kinetic energy term. This is what I will write as a certain interaction. This is an interaction which is part of the new Hamiltonian.

In the; under the unitary transformation we have arrived at a new representation of the Hamiltonian. So, this term is what we will write as H interaction and this term over here as K okay. So, these are just some book keeping devices, so that we can discuss these terms separately.

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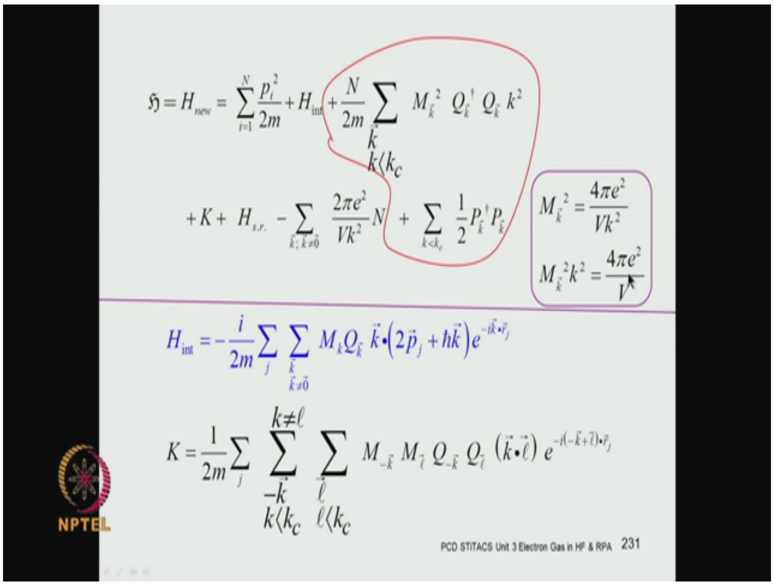

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + H_{int} + \frac{N}{2m} \sum_{\substack{\vec{k} \\ k \langle k_c}} M_{\vec{k}}^{2}\, Q_{\vec{k}}^{\dagger}\, Q_{\vec{k}}\, k^2$$

$$+ K + H_{s.r.} - \sum_{\vec{k};\, \vec{k} \neq \vec{0}} \frac{2\pi e^2}{Vk^2} N + \sum_{k<k_c} \frac{1}{2} P_{\vec{k}}^{\dagger} P_{\vec{k}}$$

$$\boxed{\begin{aligned} M_{\vec{k}}^{2} &= \frac{4\pi e^2}{Vk^2} \\ M_{\vec{k}}^{2} k^2 &= \frac{4\pi e^2}{V} \end{aligned}}$$

$$H_{int} = -\frac{i}{2m} \sum_{j} \sum_{\substack{\vec{k} \\ \vec{k} \neq \vec{0}}} M_k Q_{\vec{k}}\, \vec{k} \bullet \left(2\vec{p}_j + \hbar \vec{k}\right) e^{-i\vec{k} \bullet \vec{r}_j}$$

$$K = \frac{1}{2m} \sum_{j} \sum_{\substack{-\vec{k} \\ k \langle k_c}}^{k \neq \ell} \sum_{\substack{\vec{\ell} \\ \ell \langle k_c}} M_{-\vec{k}} M_{\vec{\ell}}\, Q_{-\vec{k}}\, Q_{\vec{\ell}} \left(\vec{k} \bullet \vec{\ell}\right) e^{-i(-\vec{k}+\vec{\ell}) \bullet \vec{r}_j}$$

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So, now you have H interaction here and K here and these are the complete expressions for H and K. Now the Hamiltonian looks more compact that does not mean that we have solved the problem it only looks a little more compact. Now look at this part we are and some of you are beginning to recognize this term this term is beginning to look like the Hamiltonian for a harmonic oscillator okay.

It is looking like that already. Here we have used Mk square, so this is Mk square there is also a k square here. So, Mk square k square is nothing but 4pi e square by V, so together they will give you the plasma frequency which is a frequency of oscillations but of course there are other terms.

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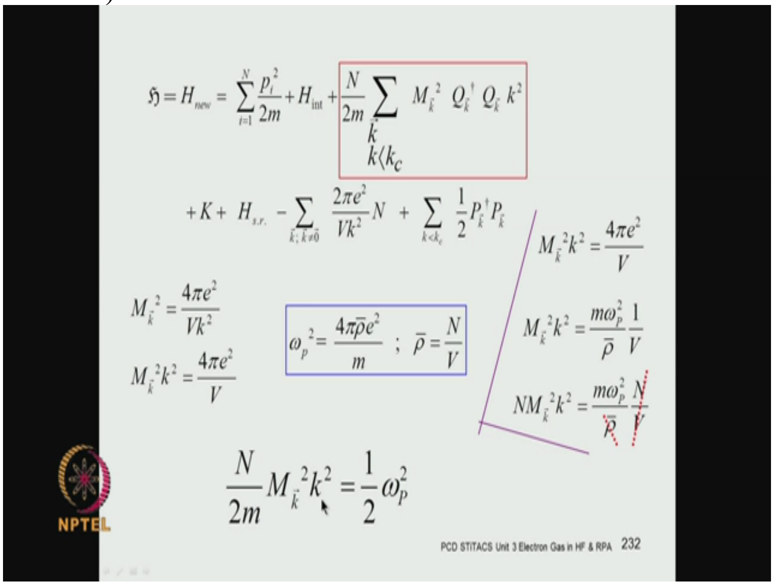

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + H_{int} + \boxed{\frac{N}{2m} \sum_{\substack{\vec{k} \\ k \langle k_c}} M_{\vec{k}}^{2}\, Q_{\vec{k}}^{\dagger}\, Q_{\vec{k}}\, k^2}$$

$$+ K + H_{s.r.} - \sum_{\vec{k};\, \vec{k} \neq \vec{0}} \frac{2\pi e^2}{Vk^2} N + \sum_{k<k_c} \frac{1}{2} P_{\vec{k}}^{\dagger} P_{\vec{k}}$$

$$M_{\vec{k}}^{2} = \frac{4\pi e^2}{Vk^2}$$

$$M_{\vec{k}}^{2} k^2 = \frac{4\pi e^2}{V}$$

$$\boxed{\omega_p^{\,2} = \frac{4\pi \bar{\rho} e^2}{m} \;;\; \bar{\rho} = \frac{N}{V}}$$

$$M_{\vec{k}}^{2} k^2 = \frac{4\pi e^2}{V}$$

$$M_{\vec{k}}^{2} k^2 = \frac{m\omega_p^2}{\bar{\rho}} \frac{1}{V}$$

$$N M_{\vec{k}}^{2} k^2 = \frac{m\omega_p^2}{\cancel{\bar{\rho}}} \frac{\cancel{N}}{\cancel{V}}$$

$$\frac{N}{2m} M_{\vec{k}}^{2} k^2 = \frac{1}{2} \omega_p^2$$

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So, let us look at these terms now, let us first have a good look at this term. So, here Mk square k square is 4pi e square by V which means that the plasma frequency omega square will be which we know is 4pi Rho V square by  m because Rho bar is nothing but this N by

V. So, this N is coming here, 1 over V is coming from here, so 4pi Rho bar e square by m gives you the square of the plasma frequency okay.

So, N over V which gives you the average static charge density is here, this is N and the 1 over V is an Mk square. So, Mk square k square is 4pi e square by V and that is what we have used okay. So, this gives you the plasma frequency and you can just rewrite this instead of in terms of M square k square you can now write it in terms of the plasma frequency. Here N over V will cancel this 1 over Rho bar in the denominator.

So, that will give us some further simplification, so N over 2m M square k square because if you divide this term by 2 then you get half of omega square. So, that is the half omega square written here. So, we have rewritten this term now it looks a little more familiar and much more like the harmonic oscillator term.

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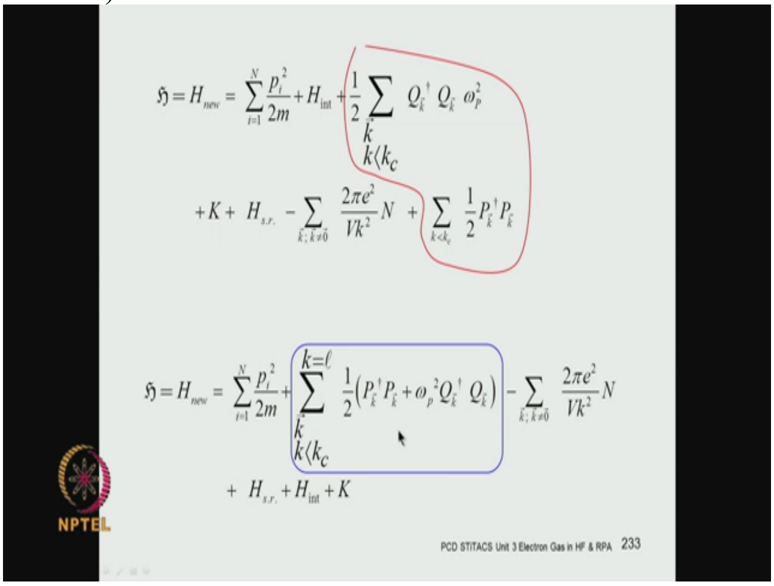

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + H_{int} + \frac{1}{2} \sum_{\substack{\vec{k} \\ k\langle k_c}} Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\, \omega_p^2$$

$$+ K + H_{s.r.} - \sum_{\vec{k};\,\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N + \sum_{k<k_c} \frac{1}{2} P_{\vec{k}}^{\dagger} P_{\vec{k}}$$

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\substack{\vec{k} \\ k\langle k_c}}^{k=\ell} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right) - \sum_{\vec{k};\,\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N$$

$$+ H_{s.r.} + H_{int} + K$$

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Here it is if you combine these two terms you have k less than kc okay. And these two terms together there is a half common to both the terms there is a P dagger P which is here. Then you have got omega square Q dagger Q which is here these operators P and Q are not hermitian but does not matter okay. But they do represent a harmonic oscillator this is the harmonic oscillator Hamiltonian.

Then you have this term which is here, you have the interaction Hamiltonian which is here, you have got a short range term which is here and you have got k which is here and you also have this minus of 2pi e square Vk square N which is here. So, all the terms everything is there.

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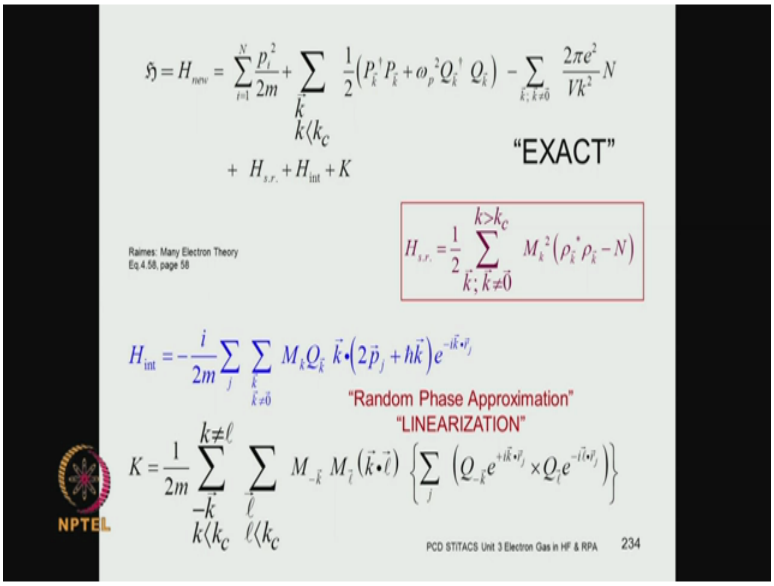

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\substack{\vec{k} \\ k \langle k_c}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right) - \sum_{\vec{k};\, \vec{k} \neq \vec{0}} \frac{2\pi e^2}{Vk^2} N$$

$$+ H_{s.r.} + H_{\text{int}} + K$$

"EXACT"

Raimes: Many Electron Theory
Eq.4.58, page 58

$$\boxed{H_{s.r.} = \frac{1}{2} \sum_{\vec{k};\, \vec{k} \neq \vec{0}}^{k > k_c} M_k^2 \left(\rho_{\vec{k}}^{*} \rho_{\vec{k}} - N\right)}$$

$$H_{\text{int}} = -\frac{i}{2m} \sum_{j} \sum_{\substack{\vec{k} \\ \vec{k} \neq \vec{0}}} M_k Q_{\vec{k}}\, \vec{k} \cdot \left(2\vec{p}_j + \hbar \vec{k}\right) e^{-i\vec{k} \cdot \vec{r}_j}$$

"Random Phase Approximation"
"LINEARIZATION"

$$K = \frac{1}{2m} \sum_{\substack{-\vec{k} \\ k \langle k_c}}^{k \neq \ell} \sum_{\substack{\vec{\ell} \\ \ell \langle k_c}} M_{-\vec{k}} M_{\vec{\ell}} (\vec{k} \cdot \vec{\ell}) \left\{ \sum_j \left( Q_{-\vec{k}} e^{+i\vec{k} \cdot \vec{r}_j} \times Q_{\vec{\ell}} e^{-i\vec{\ell} \cdot \vec{r}_j} \right) \right\}$$

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The whole expression is exact the short range part of the Hamiltonian is what we had identified earlier. This was the part corresponding to k less than kc. So, these are the exact expressions, there is no approximation anywhere as yet its exact okay. Now it perhaps occurs to some of you looking at these terms because we have done this earlier, when we dealt with the classical model.

We dealt with the electron gas in the classical model or what did we do we use the random phase approximation, we did the linearization, we threw off the quadratic terms and it is because of certain terms which were coming in. There were phase terms cos theta sine theta they were coming from this e to the i theta expressions right. We recognize that they are like vectors in a two-dimensional surface.

And when they are randomly oriented the sum total of all these vectors will vanish okay the cos theta sine theta terms and you have them in the term K. The interaction represented by the term K is here this is the complete form of K. And here you have got terms which are quadratic in Q and you have got these phases you are summing over k and you are also summing over l.

But these are random phases and you expect them to cancel each other which is what gives you the random phase approximation. If you ignore the term K completely which is to go ahead and linearise ignore the quadratic term in Q okay. Ignore this term do the linearization keep track of these phases and these phases being random. They allow a cancellation of vectors on a two-dimensional surface.

Because these complex numbers are can any complex number can be represented as a vector. So, the vector sum of all of these would vanish. This is exactly the same argument as we did in the previous case. So, in the land of phase approximation K can be ignored. This term can be thrown off. Yes (Question time: 08:39- not audible) it is the same argument as we did in the classical model. In the previous class we had exponential functions.

We had each of the theta e to the Phi which is cos theta + i sine theta and cos Phi + i sine Phi and you had a cos theta + i sine theta multiplied a cos Phi + i sine Phi. All of these cosine and sine terms are of modulus 1, the maximum value is 1. The value of the products is less than 1 okay and when you sum over all of that all of these sine and cosine waves in random phases they will cancel each other.

You can think of it as a vector diagram because a complex number A + iB can be written as Rho e to the i theta, the phase theta is sine inverse of the ratio of x over y right. So, you can write it as a vector and these vectors on a plane are randomly oriented. So, there is sum of all these randomly oriented for every vector which is in this direction there is a vector in the opposite direction, the sum of these two vectors will 0, will give you 0.

So, all of these vectors in pairs will cancel each other which is why it seems like such a good approximation. So, you are certainly throwing out the term K certainly the motivation to do it is I am sure that it is such a complicated term. But the justification for doing it is the fact that all of these vectors will cancel each other which is the random phase approximation. So, the name random phase approximation is extreme be appropriate.

It is completely justified because it is coming from the cancellation of these oscillations which are in random phases they all cancel each other. So, in the random phase approximation you have a linearization process you are ignoring these quadratic terms and this is then cancelled. So, the term K which contributes to this transformed Hamiltonian can now be thrown off okay. So, this is the random phase approximation.
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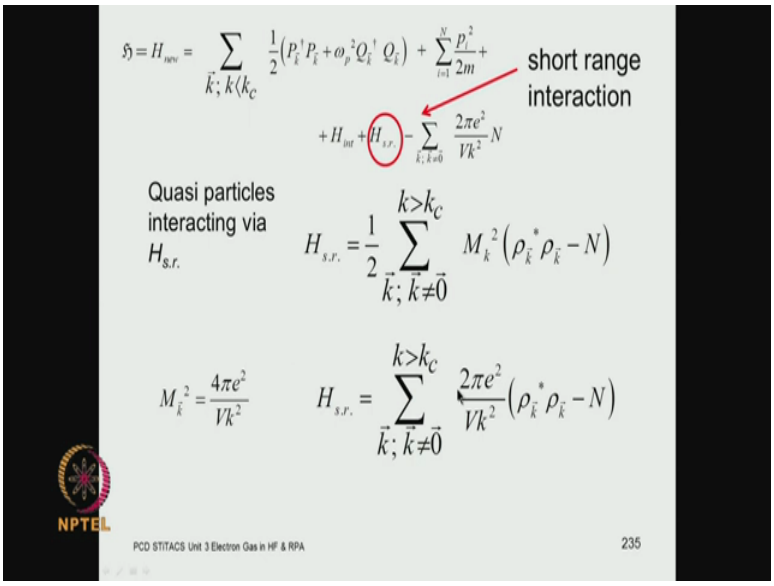

$$\mathfrak{H} = H_{new} = \sum_{\vec{k};\, k\langle k_c} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^{\,2} Q_{\vec{k}}^{\dagger}\, Q_{\vec{k}}\right) + \sum_{i=1}^{N} \frac{p_i^{\,2}}{2m} +$$

$$+ H_{int} + \boxed{H_{s.r.}} - \sum_{\vec{k};\, \vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N$$

short range
interaction

Quasi particles
interacting via
$H_{s.r.}$

$$H_{s.r.} = \frac{1}{2} \sum_{\vec{k};\, \vec{k}\neq\vec{0}}^{k>k_c} M_k^{\,2}\left(\rho_{\vec{k}}^{\,*}\rho_{\vec{k}} - N\right)$$

$$M_{\vec{k}}^{\,2} = \frac{4\pi e^2}{Vk^2} \qquad H_{s.r.} = \sum_{\vec{k};\, \vec{k}\neq\vec{0}}^{k>k_c} \frac{2\pi e^2}{Vk^2}\left(\rho_{\vec{k}}^{\,*}\rho_{\vec{k}} - N\right)$$

Now let us write the Hamiltonian, the rest of the Hamiltonian and we do not have K anymore in this okay. What is this short range interaction term, now let us see what kind of a system does this Hamiltonian represent what is the physical system? What is the meaning of this physical system? We have cancelled a term namely the term K, the net Hamiltonian you have now has got these pieces and we will interpret them.

First let us have a look at this short range term what is it? What is it telling us? The explicit form of the short range part of the Hamiltonian is this. This is the; you remember this was the term T2. In the previous class we discussed the term T2 in the original Hamiltonian. We recognized that when you transform the Hamiltonian you transform the term T2 which is actually invariant.

But the invariant T2, we wrote in two parts and this is the short range part of T2. This is essentially the short range part of T2 and what it represents is a set of quasi particles which are interacting via a short range. These are not the real electrons, these are quasi particles. Now let us have a look at these terms a little closely Mk square is this term okay.

So, you write instead of Mk square you have a factor of half here. So, you have a half here and a 4pi here, so that gives you a 2pi, so this is 2pi e square over Vk square. This is your short range Hamiltonian,
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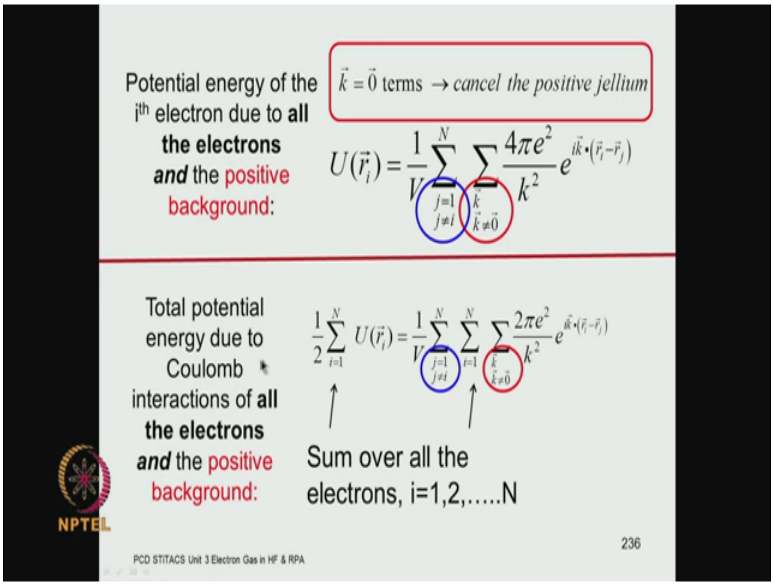

Potential energy of the i<sup>th</sup> electron due to **all the electrons** ***and*** the positive background:

$\vec{k} = \vec{0}$ terms → *cancel the positive jellium*

$$U(\vec{r}_i) = \frac{1}{V}\sum_{\substack{j=1\\ j\neq i}}^{N}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{4\pi e^2}{k^2}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}$$

Total potential energy due to Coulomb interactions of **all the electrons** ***and*** the positive background:

$$\frac{1}{2}\sum_{i=1}^{N} U(\vec{r}_i) = \frac{1}{V}\sum_{\substack{j=1\\ j\neq i}}^{N}\sum_{i=1}^{N}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}$$

$\uparrow$ $\uparrow$

Sum over all the electrons, i=1,2,.....N

Now let me remind you that the potential energy of the ith electron due to all the electrons and the positive background is given by this term. We have discussed this explicitly in one of the previous classes may be just one or two or three classes earlier right. So, this is the potential energy of the ith electron.

What is it energy due to it is because of all the other electrons, all the electrons and the positive background. What about this? If you now add, U ri sum over i going from 1 through N. So, that you sum over all the electrons. Now all the electrons are summed over. So, there is no single electron which is separated out. So, you are counting the all the energy.

But the energy potential energy between one electron and the other is the same as a potential energy between this electron and the first. So, that is the reason you must take a factor of half over here. So, that you do not do any double counting. So, this is the total potential energy due to the Coulomb interactions of all the electrons and the positive background.

Why is a positive background involved because you have dropped the k = 0 term. That is the term which cancels the background effects okay and the background terms are of two fold one is the background-background interaction in the original Hamiltonian and the other is the electron background interaction. So, that is also taken care of.

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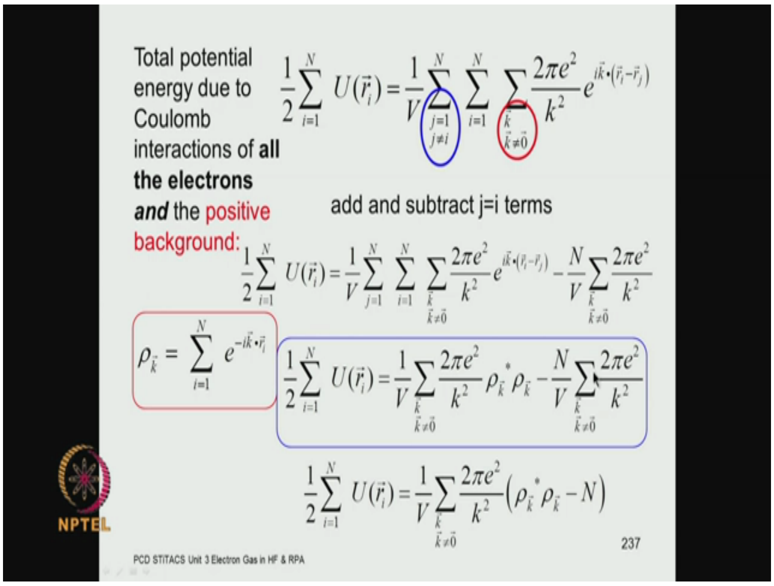

Total potential energy due to Coulomb interactions of **all the electrons** ***and*** the positive background:

$$\frac{1}{2}\sum_{i=1}^{N} U(\vec{r}_i) = \frac{1}{V}\sum_{\substack{j=1\\ j\neq i}}^{N}\sum_{i=1}^{N}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}$$

add and subtract j=i terms

$$\frac{1}{2}\sum_{i=1}^{N} U(\vec{r}_i) = \frac{1}{V}\sum_{j=1}^{N}\sum_{i=1}^{N}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)} - \frac{N}{V}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}$$

$$\boxed{\rho_{\vec{k}} = \sum_{i=1}^{N} e^{-i\vec{k}\cdot\vec{r}_i}}$$

$$\boxed{\frac{1}{2}\sum_{i=1}^{N} U(\vec{r}_i) = \frac{1}{V}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}\rho_{\vec{k}}^{*}\rho_{\vec{k}} - \frac{N}{V}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}}$$

$$\frac{1}{2}\sum_{i=1}^{N} U(\vec{r}_i) = \frac{1}{V}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}}\frac{2\pi e^2}{k^2}\left(\rho_{\vec{k}}^{*}\rho_{\vec{k}} - N\right)$$

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So, this is the total potential energy due to the Coulomb interactions of all the electrons and the positive background. Now if you add and subtract the j = i term because here j = i was eliminated. Now if you add and subtract the j = i term. So, now j = 1 through N is included here. But j = i has been added, it was not there in the original some right. Then you must subtract the corresponding extra term that you are mathematically added.

What you have to subtract is this term, we have discussed this earlier right. Because for j = i, you get ri = rj, so you get e to the 0, so you get 2pi e square over k square which you must add to itself N times right. So, you get N there is a 1 over V here so that gives you N over V times this summation k not equal to 0 2pi e square by k square. What is this? This is coming from the self energy because for j = i you have essentially the self energy right.

So, what you have added is what you are subtracted and what you have subtracted is the self energy. So, this is the term that you have to subtract and here you have got the components of the Fourier components of the charge density. So, you can rewrite this expression in terms of Rho k star okay. This is k e to the ik dot ri times e to the i k dot rj but the exponent is with a minus sign here.

So, you get Rho k star Rho K you are summing over i and j both from 1 through N nothing is missed out on because the j = i term is included in this summation and the corresponding effect of self energy is subtracted over here. So, if you now combine these two terms you have 2 pi e square by k square summed k common in both the terms. So, you have 1 over V which is common to both the terms.

You have got 2 pi e square by k square which is common to both the terms and you must subtract Rho k star Rho k - this N to get the net result. So, this is the total potential energy

due to the Coulomb interactions of all the electrons on the positive background the self energy term is here okay. This is the self energy term, so that is taken care of all right.
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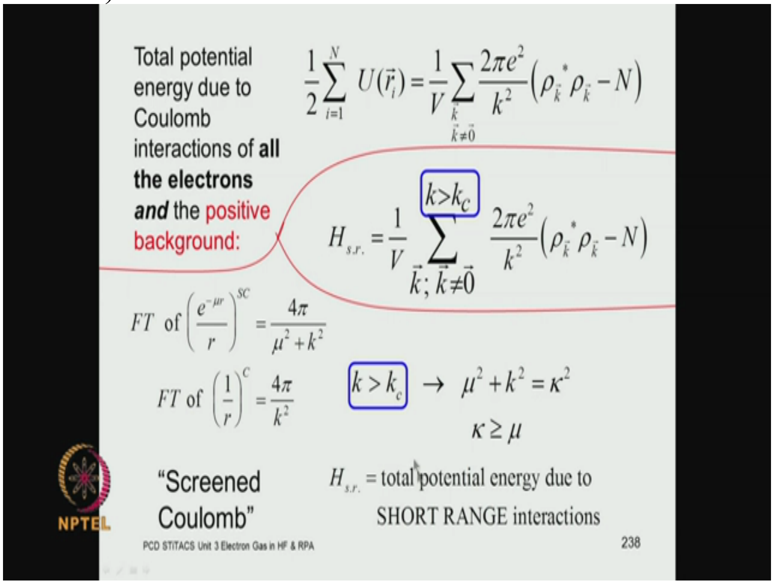

Total potential energy due to Coulomb interactions of **all the electrons** ***and*** the positive background:

$$\frac{1}{2}\sum_{i=1}^{N} U(\vec{r}_i) = \frac{1}{V}\sum_{\substack{\vec{k}\\ \vec{k}\neq\vec{0}}} \frac{2\pi e^2}{k^2}\left(\rho_{\vec{k}}^{*}\rho_{\vec{k}} - N\right)$$

$$H_{s.r.} = \frac{1}{V}\sum_{\vec{k};\,\vec{k}\neq\vec{0}}^{\boxed{k>k_c}} \frac{2\pi e^2}{k^2}\left(\rho_{\vec{k}}^{*}\rho_{\vec{k}} - N\right)$$

$$FT \text{ of } \left(\frac{e^{-\mu r}}{r}\right)^{SC} = \frac{4\pi}{\mu^2+k^2}$$

$$FT \text{ of } \left(\frac{1}{r}\right)^{C} = \frac{4\pi}{k^2}$$

$$\boxed{k>k_c} \rightarrow \mu^2+k^2=\kappa^2$$

$$\kappa \geq \mu$$

"Screened Coulomb"

$H_{s.r.}$ = total potential energy due to SHORT RANGE interactions

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Now this is our result which is the total potential energy due to Coulomb interactions of all the electrons all the pair interactions are taken care of, the background is taken care of. What was our expression for the short-range Hamiltonian? We had separated the term corresponding to k greater than kc which is the short range part of the Hamiltonian. And look at these two relations they look so much the same right.

But there is some difference, the difference is here that in this k must be greater than kc right. So, this is the difference and this if you remember the Fourier transforms of the Coulomb interaction and the screened Coulomb interaction, the difference is here because if you write mu square + k square as kappa square if you okay, this is where I have written then whenever k is greater than kc it amounts to having a kappa which is greater than or equal to mu.

So, you can write this as 4pi over kappa square which is similar to the Coulomb interaction itself. So, the difference is the same as that you have between the Coulomb interaction and the screened Coulomb interaction. So the short range part of the Hamiltonian the HSR what it represents is the total potential energy due to short range interactions.
This is the screened Coulomb interaction not between the electrons but between these quasi particles. So, that is the term corresponding to the screened Coulomb potential.
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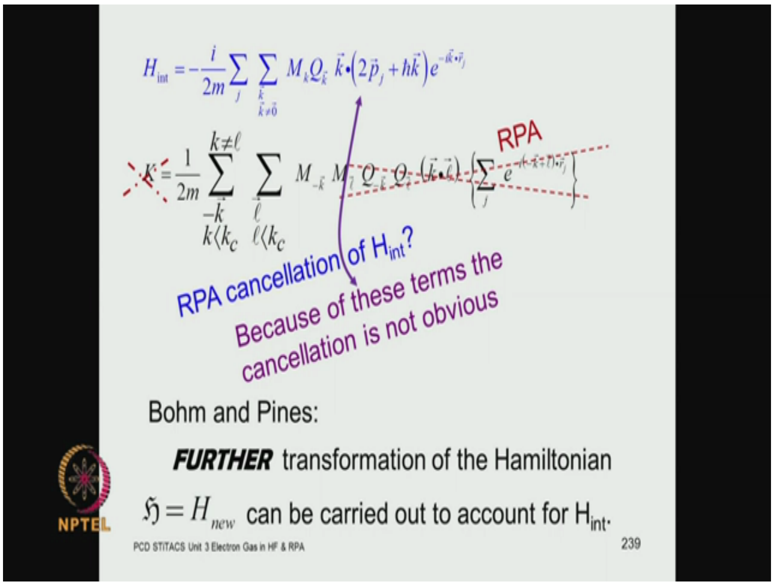

$$H_{\text{int}} = -\frac{i}{2m}\sum_{j}\sum_{\substack{\vec{k} \\ \vec{k}\neq\vec{0}}} M_{k} Q_{\vec{k}}\, \vec{k}\bullet\left(2\vec{p}_{j} + \hbar\vec{k}\right) e^{-i\vec{k}\bullet\vec{r}_{j}}$$

$$\cancel{K} = \frac{1}{2m}\sum_{\substack{-\vec{k} \\ k\langle k_{c}}}^{k\neq\ell}\sum_{\substack{\vec{\ell} \\ \ell\langle k_{c}}} M_{-\vec{k}} M_{\vec{\ell}} Q_{-\vec{k}} Q_{\vec{\ell}} \left(\vec{k}\bullet\vec{\ell}\right)\left\{\sum_{j} e^{-i(-\vec{k}+\vec{\ell})\bullet\vec{r}_{j}}\right\}$$

RPA cancellation of $H_{\text{int}}$?

Because of these terms the cancellation is not obvious

Bohm and Pines:

***FURTHER*** transformation of the Hamiltonian

$\mathfrak{H} = H_{new}$ can be carried out to account for $H_{\text{int}}$.

So, now you have got the short range identified the term K is ignored in the random phase approximation but you still have to worry about the H interaction term. Now can you do something like RPA to get rid of this term okay and because of the presence of these terms it is not obvious that you will be led to cancellations but in fact it can be done.

And that is a little more detailed involved algebra which I am not going to do in this class or in this course. I will only mention the result that it is not obvious that this gets cancelled. But what you can do is to carry out a further transformation and we have used these tricks earlier on in interpreting the Dirac equation. We did the Foldio Dyson transformation then we did another Foldio Dyson and transformation.

So, a cascade of transformations leads you to certain terms which become amenable to easy physical interpretation. And in this case you need to carry out another canonical transformation okay. So, obviously there will be more terms to keep track off and you know a little more cumbersome mathematics not difficult just a little bit cumbersome.

So, if you do a further transformation and this was carried out by Bohm Pines which enables you to take into account major effects of the H interaction term by ignoring certain terms again there will be a linearization process. There will be some more auxiliary coordinates and momenta which are introduced in the second transformation right. And in that you will have new quadratic terms which you could ignore just the way you did over here.

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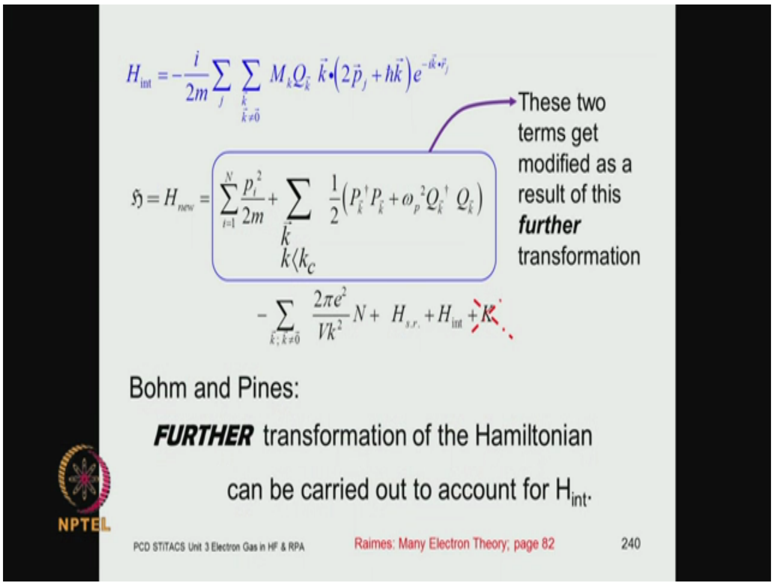

$$H_{\text{int}} = -\frac{i}{2m}\sum_{j}\sum_{\substack{\vec{k} \\ \vec{k}\neq\vec{0}}} M_k Q_{\vec{k}}\, \vec{k}\cdot\left(2\vec{p}_j + \hbar\vec{k}\right)e^{-i\vec{k}\cdot\vec{r}_j}$$

$$\mathfrak{H} = H_{new} = \boxed{\sum_{i=1}^{N}\frac{p_i^2}{2m} + \sum_{\substack{\vec{k} \\ k\langle k_c}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger}P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger}\, Q_{\vec{k}}\right)}$$

$$-\sum_{\vec{k};\,\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2}N + H_{s.r.} + H_{\text{int}} \cancel{+K}$$

These two terms get modified as a result of this ***further*** transformation

Bohm and Pines:

***FURTHER*** transformation of the Hamiltonian

can be carried out to account for $H_{\text{int}}$.

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Raimes: Many Electron Theory; page 82

So, you can carry out this process of RPA to another level which we will not do in this course. But when you do that what happens is in the first RPA you can already ignore K and in the second RPA you can carry out this transformation of the full Hamiltonian once again after K is dropped.

This is not the original Hamiltonian this is the transformed Hamiltonian not even the exact transformed Hamiltonian. But the transformed Hamiltonian from which K is dropped. So, you drop K and then carry out this transformation and the result is that these two terms get modified.

This is the thing which looked like an oscillator. But you cannot live with it anymore because it is going to get modified. If you want to ignore H interaction term the price that you will have to pay is that these terms get modified. These two terms get modified and what is that result what is the modification

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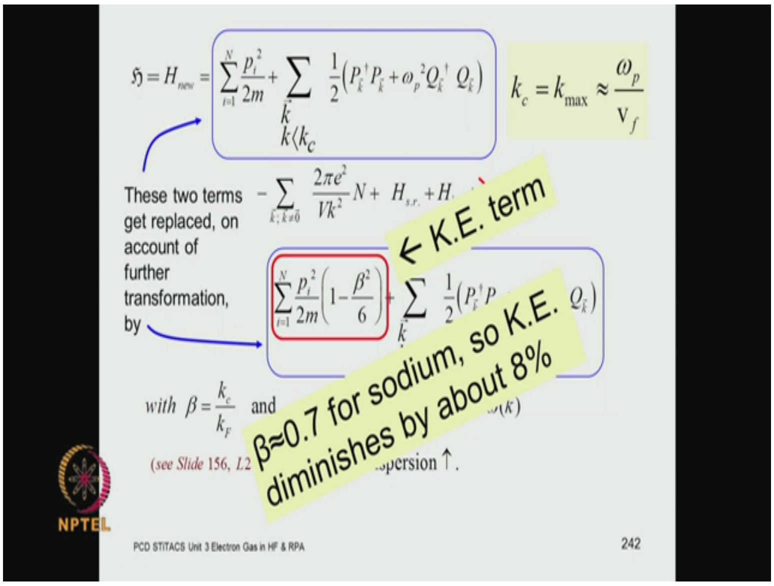

$$\mathfrak{H} = H_{new} = \sum_{i=1}^{N}\frac{p_i^2}{2m} + \sum_{\substack{\vec{k} \\ k\langle k_c}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger}P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger}Q_{\vec{k}}\right)$$

$$k_c = k_{\max} \approx \frac{\omega_p}{v_f}$$

These two terms get replaced, on account of further transformation, by

$$-\sum_{\vec{k};\, k\neq\vec{0}} \frac{2\pi e^2}{Vk^2}N + H_{s.r.} + H$$

← K.E. term

$$\sum_{i=1}^{N}\frac{p_i^2}{2m}\left(1-\frac{\beta^2}{6}\right) + \sum_{\vec{k}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger}P \quad Q_{\vec{k}}\right)$$

with $\beta = \frac{k_c}{k_F}$ and $(k)$

(see Slide 156, L2 persion ↑.

β≈0.7 for sodium, so K.E. diminishes by about 8%

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the modification is this that the sum of the first two terms has to be rewritten as a result of this second Bohm Pines canonical transformation of the Hamiltonian and instead of this P squared over 2m you get P squared over 2m which is scaled by the factor of 1 - beta square by 6 where beta is a new parameter which is a ratio.

Which is defined by this kc over kf and you get another a different Hamiltonian over here which again happily looks like a harmonic oscillator. But with a slightly different frequency which is not omega p square. But omega p square + a function a quadratic function of k. So, this becomes dispersal, so it is weakly dispersal. But you get a harmonic oscillator again okay.

So, this is the transformation which is useful this is the second canonical transformation carried out by Bohm Pines it includes slight dispersion. So that the frequency of oscillations of the electron plasma, now becomes k dependent, so it becomes dispersive and the kinetic energy term is no longer just this p squared over 2m. But it is scaled by a factor of 1 minus beta square by 6.

And then detailed calculations can be done, so I will just quote a result for one of the metals like for sodium atom beta turns out to be nearly equal to .7 and the kinetic energy because you have to subtract the kinetic energy from this 1 you have to diminish this term beta square by 6. So, the kinetic energy is diminished by about 8 percent.

So, there is a certain small correction that you are led to because of this second canonical transformation. So, the first canonical transformation already gives you a handle on the system and now you carry out a second transformation and you get an 8 percent reduction of the energy.

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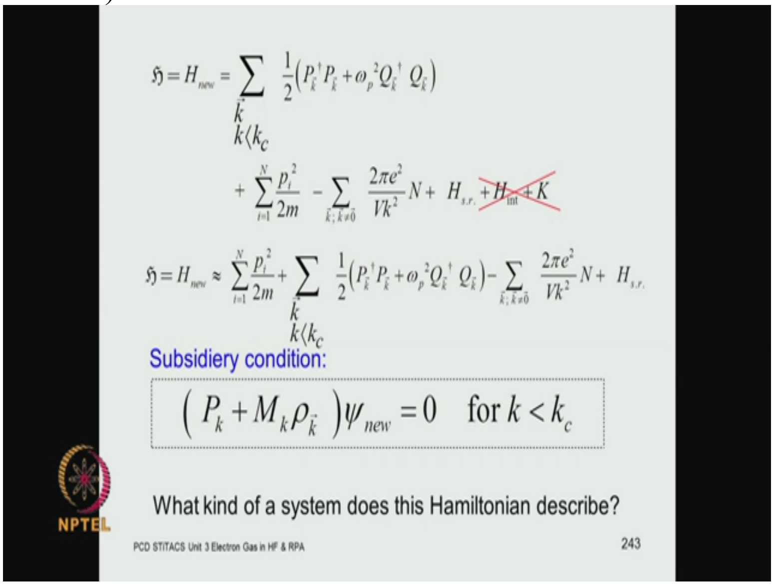

$$\mathfrak{H} = H_{new} = \sum_{\substack{\vec{k} \\ k\langle k_c}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right) + \sum_{i=1}^{N} \frac{p_i^2}{2m} - \sum_{\vec{k};\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N + H_{s.r.} \cancel{+ H_{int} + K}$$

$$\mathfrak{H} = H_{new} \approx \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\substack{\vec{k} \\ k\langle k_c}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right) - \sum_{\vec{k};\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N + H_{s.r.}$$

Subsidiery condition:

$$\boxed{\left(P_k + M_k \rho_{\vec{k}}\right) \psi_{new} = 0 \quad \text{for } k < k_c}$$

What kind of a system does this Hamiltonian describe?

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So, now with having discussed how we account for all the terms. How we account for the H interaction term? How we can deal with it using an additional canonical transformation? We can now throw these two terms okay. And interpret the rest of the Hamiltonian. So, this is what we have the new Hamiltonian then has this term the P squared over 2m the kinetic energy term. This is a harmonic oscillator kind of term.

Then you have got this 2 pi e square over Vk square which is here and you have got the short range interaction term, which we have identified as the short range interaction between particles or quasi particles which are interacting through this screened Coulomb interaction well. Now we can answer this question what kind of a physical system does this Hamiltonian describe.

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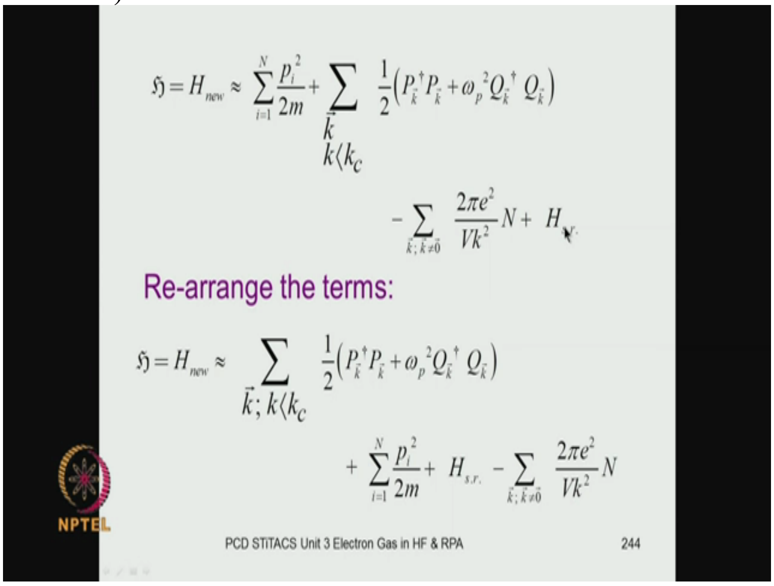

$$\mathfrak{H} = H_{new} \approx \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\substack{\vec{k} \\ k\langle k_c}} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right) - \sum_{\vec{k};\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N + H_{s.r.}$$

Re-arrange the terms:

$$\mathfrak{H} = H_{new} \approx \sum_{\vec{k};\, k\langle k_c} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right) + \sum_{i=1}^{N} \frac{p_i^2}{2m} + H_{s.r.} - \sum_{\vec{k};\vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N$$

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So, let us first of all rearrange the terms a little bit I combine this term with Hsr okay. So, I can look at these two terms together okay. So, these two terms were written in the same summation. So, we are not doing any approximation or anything we are only interpreting this term and this term together. This we already know what it is? This is coming from the self-energy right.

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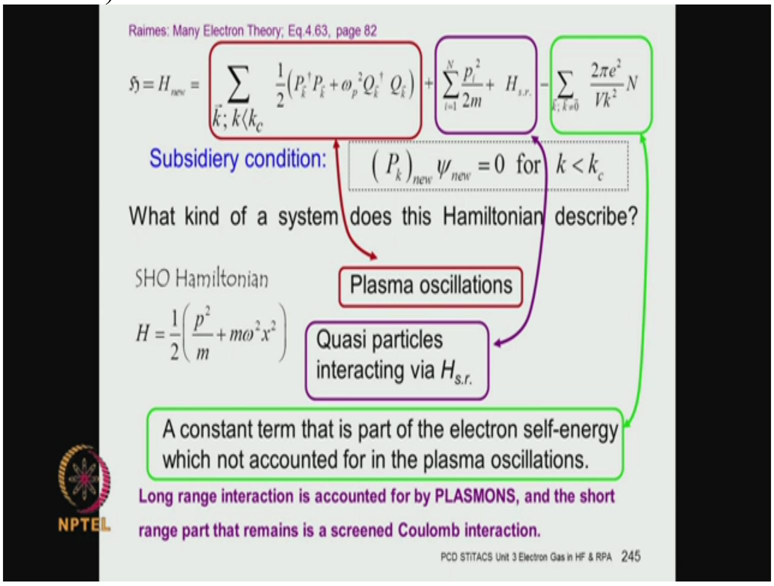

Raimes: Many Electron Theory; Eq.4.63, page 82

$$\mathfrak{H} = H_{new} = \boxed{\sum_{\vec{k};\, k \langle k_c} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right)} + \boxed{\sum_{i=1}^{N} \frac{p_i^2}{2m} + H_{s.r.}} - \boxed{\sum_{\vec{k};\, \vec{k} \neq \vec{0}} \frac{2\pi e^2}{V k^2} N}$$

Subsidiery condition: $(P_k)_{new}\, \psi_{new} = 0$ for $k < k_c$

What kind of a system does this Hamiltonian describe?

SHO Hamiltonian

$$H = \frac{1}{2}\left(\frac{p^2}{m} + m\omega^2 x^2\right)$$

Plasma oscillations

Quasi particles interacting via $H_{s.r.}$

A constant term that is part of the electron self-energy which not accounted for in the plasma oscillations.

Long range interaction is accounted for by PLASMONS, and the short range part that remains is a screened Coulomb interaction.

So, let us have a look at the transformed Hamiltonian. We have now ignored K, we have ignored H interaction ignored in the sense yes and no ignored because we are not going to discuss it here. But not ignored because we have mentioned if not analyzed in details how that term can be handled. It can be handled by carrying out a further Bohm Pine transformation of further canonical transformation okay.

We know that its effect is to lead to a slight reduction of the kinetic energy term. We know that it will involve a further approximation which is again a random phase approximation which will involve linearization. It will involve ignoring certain quadratic terms of new auxiliary coordinates which have to be introduced in the transformation right.

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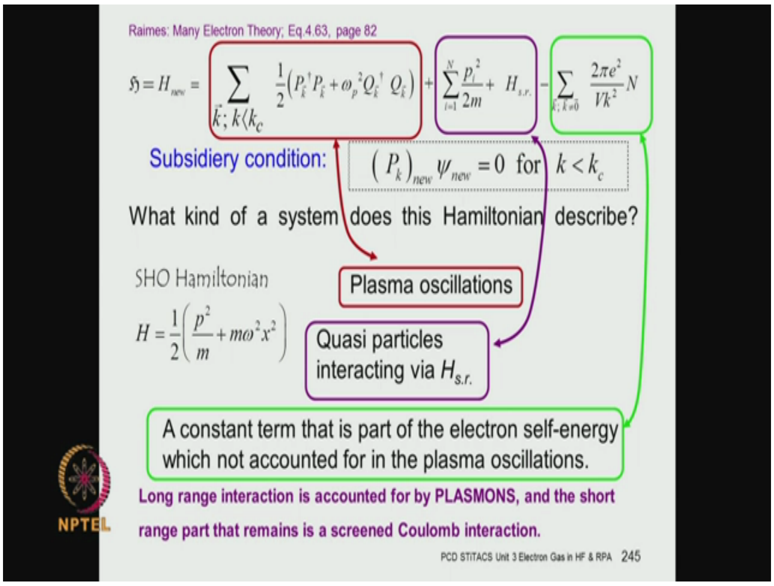

Raimes: Many Electron Theory; Eq.4.63, page 82

$$\mathfrak{H} = H_{new} = \boxed{\sum_{\vec{k};\, k\langle k_c} \frac{1}{2}\left(P_{\vec{k}}^{\dagger} P_{\vec{k}} + \omega_p^2 Q_{\vec{k}}^{\dagger} Q_{\vec{k}}\right)} + \boxed{\sum_{i=1}^{N} \frac{p_i^2}{2m} + H_{s.r.}} - \boxed{\sum_{\vec{k};\, \vec{k}\neq\vec{0}} \frac{2\pi e^2}{Vk^2} N}$$

Subsidiery condition: $\left(P_k\right)_{new} \psi_{new} = 0$ for $k < k_c$

What kind of a system does this Hamiltonian describe?

SHO Hamiltonian

$$H = \frac{1}{2}\left(\frac{p^2}{m} + m\omega^2 x^2\right)$$

Plasma oscillations

Quasi particles interacting via $H_{s.r.}$

A constant term that is part of the electron self-energy which not accounted for in the plasma oscillations.

Long range interaction is accounted for by PLASMONS, and the short range part that remains is a screened Coulomb interaction.

And everything is reference to a subsidiary condition that the new momenta which change under the transformations. They do not when they act upon the wave function you get a zero and now we can really describe this system. So, you have got an oscillator which looks like the simple harmonic oscillator over here. This is the typical expression for the simple harmonic oscillator and this represents essentially the plasma oscillations.

So, their quanta are the plasmons that we talked about okay. Then you have the short range interaction between these quasi particles okay. So, this is like any other Hamiltonian you have got a kinetic energy part plus a potential energy part okay. It is of certain interaction so this is; what is the interaction now? This is the short-range interaction this is not the Coulomb interaction.

The Coulomb interaction we these transformations enable us to separate the Coulomb interaction into a short range part which is sitting in this box here in the Hsr. And a long-range part whose effect has been taken care of, it is buried in the plasma oscillations okay. It goes into these terms, so the long-range part of the Coulomb interaction has been handled separately.

The short range part of the interaction is what you are left with. This is the interaction between quasi particles which are interacting with each other only through short range terms like a screen Coulomb potential. And then you have got a term over here which is just a constant term which has to be added because it is corresponding to the self energy part which is not accounted for in the plasma oscillations.

So, there is a certain self energy part which is in this last term. So, all the terms are now taken care of and we know exactly what this new Hamiltonian tells us. Notice that we had a mess, we had so many terms and we needed to take a break, we had lots of terms and they looked so terribly messy.

But then it requires somebody like Bohm and Pines to think of these transformations carrying them out effectively to a new set of auxiliary coordinates and momenta. In terms of which you can get to address those terms that you had left out in the Hartree Fock theory. These are coming from density fluctuations okay. These are the density fluctuations of the electron gas Hartree Fock theory does not deal with it.

It is as if you have got a static electron density in a Hatree Fock gas okay we does not change. So, if a particle if one of the electron is going to move rapidly from one point to another what happens to the remaining charge density. We pretend in the Hartree Fock approximation that it does not change. So, that is the frozen orbital approximation which is underscored in the Hartree Fock.

Those would generate density fluctuations what was ignored in the Hartree Fock, other density fluctuations because you feel have got a rapid transit of a charged particle over there in the medium. Then of course it will change the local density and that will then generate a wave these are the waves which we are now talking about. These are the collective oscillations of the electron gas.

This is coming from the electron correlation which was missing in the Hartree Fock model or in the first order perturbation theory model. The second and higher order perturbation theory does not converge. So, perturbative approach does not work but these methods work. There are alternative ways of doing quantum theory. One is method of canonical transformations as was done by Bohm Pines.

There are some other ways also but this is one of the very powerful ways of doing quantum theory which so carry out canonical transformations. And this one is a particularly useful one because the resulting Hamiltonian now looks so neat okay. You have got the harmonic oscillators over here, so you have got the collective oscillations of the electron gas. You have got a Hamiltonian for a set of particles.

But these are not the original particles, so these are called as quasi particles these are like the elementary excitations which interact through a short range interaction and then you have got a self energy correction. And the long range part of the interaction is accounted for in the plasmons and the short range terms are over here. So, it is not that there is a new interaction there is no external perturbation that we have added to the system.

These are all interactions which are internal intrinsic to the system, it is intrinsic to nature. But what the mathematical model has enabled us to do is to interpret these interactions by going beyond the single particle model, the Hartree Fock model is a single particle model it expresses the solution as a Slater determinant made up of these N particles. But there is a single Slater determinant.

The product wave functions are, you know the anti symmetrised wave function is made up of products of these one particle wave functions but there is only one set that you use. Of course you can deal with these correlations in some other way also. You can do a multi configurational Hartree Fock that the Hartree Fock wave function which is a single Slater determinant does not give you the correct solution.

Because it has left out electron correlations, so you can write to the system wave function as a linear superposition of a number of wave functions and that is one way of taking into account correlation. So, there are various alternative paths to doing many-body theory. There is no unique path but this is one of the very promising paths. This is the method of canonical transformations; this is the method of Bohm and Pines.
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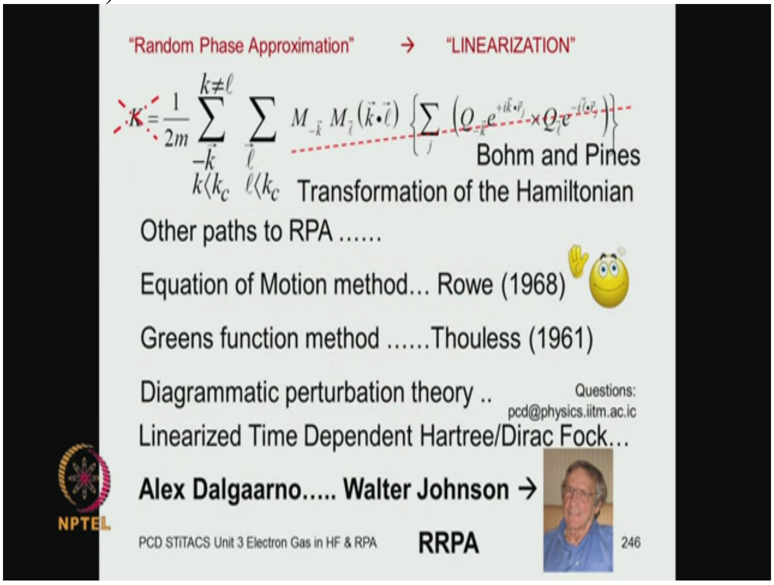

"Random Phase Approximation" → "LINEARIZATION"

$$\cancel{K} = \frac{1}{2m} \sum_{\substack{-\vec{k} \\ k<k_c}}^{k\neq\ell} \sum_{\substack{\vec{\ell} \\ \ell<k_c}} M_{-\vec{k}} M_{\vec{\ell}} (\vec{k}\cdot\vec{\ell}) \left\{ \sum_j \left( Q_{-\vec{k}} e^{+i\vec{k}\cdot\vec{r}_j} \times Q_{\vec{\ell}} e^{-i\vec{\ell}\cdot\vec{r}_j} \right) \right\}$$

Bohm and Pines

Transformation of the Hamiltonian

Other paths to RPA ......

Equation of Motion method... Rowe (1968)

Greens function method ......Thouless (1961)

Diagrammatic perturbation theory ..

Questions:
pcd@physics.iitm.ac.ic

Linearized Time Dependent Hartree/Dirac Fock...

**Alex Dalgaarno..... Walter Johnson →**

PCD STiTACS Unit 3 Electron Gas in HF & RPA

**RRPA**

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And what it is based on is a linearization process and this is the heart of the RPA, of course there are other things which go into the RPA. This is not the only thing but this is the heart of the approximation that the quadratic terms are ignored because these terms which have got random phases they represent a vector addition of a large number of vectors of equal and opposite which are equal and opposite so their sum total goes to 0.

There are other paths to RPA there is a method known as the equation of motion method, there is a greens function method, there is diagrammatic perturbation theory. So, there are various alternative ways of arriving at this. Why are the equivalent, because they all involve the heart of the RPA which is the linearization process.

The tools are different the details are different but all of them involve one common feature which is the process of linearization. There is also the Hartree Fock method but you have to go beyond the Hartree Fock. But follow the Hartree Fock approach and this is done in the time-dependent Hartree Fock.

This was developed by Delgaarno and Victor and there is the time-dependent Hartree Fock which also you can use. But there again you will have to do some linearization. So, this was done by Delgaarno and Victor. And relativistic version was developed by Walter Johnson which is a relativistic random phase approximation.

So, this is an alternative way of doing a linearization approximation which is also therefore call as a random phase approximation. But the approach is different and in this unit I discussed the Bohm Pines method specifically because this method explains the term random phase approximation.

Why what are these phases but when you are dealing with other methods like time-dependent Hartree Fock or the equation of motion method right. You are not going to meet terms of this kind okay. You will have some linearization process, so you will have a process which is mathematically equivalent to this.

So, which is why many books and research papers refer to the to these approximations as RPA but they simply say that the term RPA only has a historical importance and it is not because you need to look for what phases are cancelling each other because they are random. So, the terminology comes from the Bohm Pines method of canonical transformation.

And we have discussed that in unit 3 in considerable detail. We spent many classes to develop this only to explain this term random phase approximation. And in the next unit I will introduce the diagrammatic perturbation theory the Feynman diagrams and there also we will develop the Feynman diagrams.

And we will see that a certain class of diagrams correspond to the RPA. So, the Feynman diagrams have got various shapes and there are diagrams which we will write as what are known as ring diagrams. And these are the diagrams which we can retain ignore some of the other diagrams. We do that also in the linearized time-dependent Hartree Fock.

In the non relativistic RPA or you do the same thing in a linearized time-dependent Dirac Fock, when your starting point is a Dirac equation rather than the Schrodinger equation. So, that is approach which was taken by Walter Johnson. And you have the linearized time-dependent Dirac Fock formalism which is also the random phase approximation. But when it is based on the relativistic equation it is a relativistic RPA.

So, thank you very much if there is any question I will be happy to take otherwise we will go over to the next core, next unit which is the diagrammatic perturbation theory. Yes (Question time: 39:54-not audible) yes Jobin; I have question when you factorise this Hamiltonian is it okay to say that the gas one oscillation is a correlation thing and the other, the second term is it okay to say that or it is not so.

Well it is like a Hartree Fock the second term corresponding to you are referring to the short range part of the Hamiltonian right. Yeah that quasi particles in a short range yeah you are referring to this term, yes, you can think of this as interaction between single particles just as you do in the Hartree Fock. The difference is that these single particles are no longer the physical elementary particles of nature.

These are dressed particles these are pseudo particles these are quasi particles they are not particles of nature the sum i going from 1 through N is over a certain number of particles which are like quasi particles and they interact with each other. So, if there is any further correlation between them that is not included so in that sense you can think of it as a Hatree Fock system of quasi particles okay.

So, they are treated as single particles but these are not the original particles. So, one has to be careful, so they are interacting particles but they are not correlated, so, any further correlations between these quasi particles is not contained in the Hamiltonian which is Hsr. So, if there is any residual correlation between these quasi particles it is not included over here.

So, in that sense you can think of them as a Hatree Fock gas of pseudo particles. This is the collective oscillations of the electron gas. So, any residual correlation of these particles is not included in this Hamiltonian. So, this is the transformed Hamiltonian in which the term K is dropped because of the random phases. The term H interaction is dropped in how we have written it, where it does not mean that it has to be completely ignored.

Because some part of it can be accounted for by carrying out a further canonical transformation. So, that is a matter of detail and one of the consequences that we mentioned was the reduction of the kinetic energy by about 8 percent in the case of sodium atom. Any other question (Question time: 43:28- not audible) what is the physical reduction of kinetic energy for sodium;

That it is just a net result; then how physically like kinetic energy is reduced yeah your no more and you are not talking about the particles, these are pseudo particles. So, that it is just a mathematical reorganization of the total energy. So, you have got the total energy of the system. But it is like having plenty of food in this hall right. And there is that much of energy which is available in this hall and if some of us eat some of it the energy gets reorganized.

The total energy remaining the same, so because you have carried out a transformation of the Hamiltonian you interpret certain terms to have a kinetic energy which is reduced in relation to the earlier one it is not that the energy is lost because it is taken care of in some of the other terms. So, there is some energy which goes into the plasma oscillations okay. These are simple harmonic oscillator excitations.

So, what is excitation spectrum of a simple harmonic oscillator it is N plus half h cross omega. This omega is a plasmon and frequency it is either omega P or the one with dispersion which is a different frequency. So, there is some energy over there, there is some energy in the self energy term right. So all of this put together, so what is reduced over here, is not lost it goes into some of the other terms.

Otherwise where will the energy form the other things come from. So, it is just a redistribution of the energy but you interpret the physical system not in terms of the original electron gas but in terms of collective behaviour of the electron gas. So, though you do not say that this is electron A,B,C,D electron1, electron2, electron3.You do not do that in Hatree Fock as well.

But there you do not do it only to the extent that the statistical correlations are taken care of. You do not do it because of the identity of the particles because of the Fermi Dirac statistics. So, there is a certain correlation because of the Fermi Dirac statistics that is taken care of in the Hartree Fock. But over and above that there is additional correlation this is what we call as the Coulomb correlation okay.

Very often when we discuss the Hartree Fock in our earlier course on atomic physics there also we mentioned that we make a technical difference in the term in the usage of the expression Coulomb interaction and Coulomb correlation. So, Coulomb interaction of course is taken care of in the Hartree Fock along with the exchange.

But the Coulomb correlation is what are left out of the Hartree Fock that over and above this there is a certain correlated dynamics. Because if you create any disturbance in the charge density you got an electron gas and you remove a certain charge density or you add some charge density over here you are pretending as if nothing is happening to the environment. How is it possible if you create a hole over here right.

Then another electron part of the electron gas which is around it, will tend to move in you are not allowing that movement in a frozen orbital approximation. Which is why this is a method which allows you to take into account the electron correlations. So, this is the fully many-body method which allows you to address the electron correlations all right.

Any other question yes Moorthy (Question time: 48:07- not audible) how to call that random phases are leading to cancellation or random phases leading to linearization. It is same, it is same linearization involves; the ignoring cancellation of the random phases, ignoring the quadratic terms you cannot do linearization without the cancellation of the phases or vice versa they are part of the same term okay.

The quadratic part under phase terms which kill each other because of their random nature is the same term okay. So, thank you very much and in the next unit we will do diagrammatic perturbation theory.