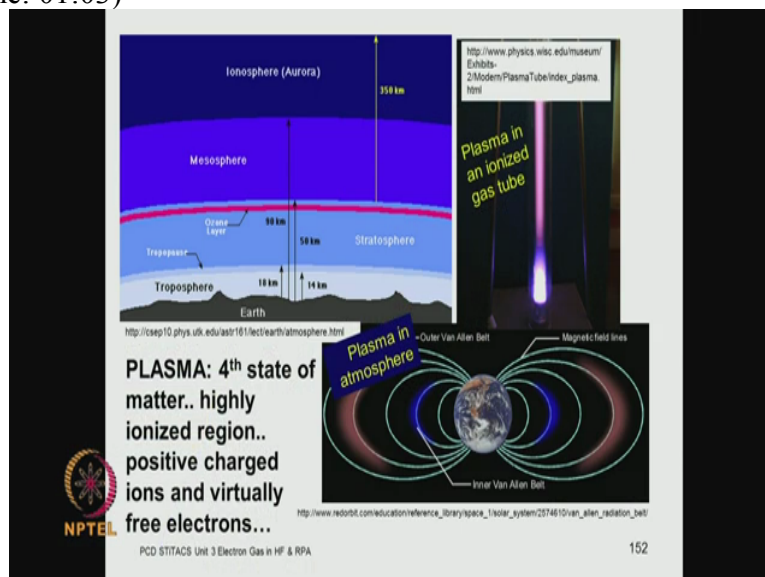


Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
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Lecture 21
Density fluctuations in an electron gas

Greetings, we will discuss the electron gas in the Jellium potential we did it at the Hartree Fock approximation, we did it using perturbative methods and we found that the result in perturbation theory is the same as what you get in the self-consistent field Hartree Fock method. But then we need to go beyond this approximation and the approximation that we are going to introduce today is the Random Phase Approximation.

And the main references for this again are from the article by Raimes and reports on Progression in Physics 1957 and his book Many Electron Theory.
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And what is done in this model is to treat the electron gas as a plasma okay. So, these are the plasma oscillations that you are going to look at the plasma is often described as a fourth state of matter it is a highly ionized region as such there are plasmas in ionized tubes in gas discharge tubes.

As one knows there is plasma in that atmosphere in the Valan, Alan, Bell's and in various bells of the atmosphere, so the plasma has a place in many places in nature and even in laboratory. It is a very highly ionized region as such you have positively charged ions in the plasma and you also have virtually free electrons in the plasma. The whole system is typically electrically neutral.

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Ignore motion of the ions... as if they are frozen....

Ions: relatively far more massive and have large inertia....

Metal \rightarrow plasma

Whole system: electrically neutral.

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Now our picture of the electrons in metal is similar to that of plasma because you have got an assembly of positive and negative charges the whole system is electrically neutral. The positive charges are sort of frozen in physical spaces so their vibrations we do not consider at this point they have far more inertia than the electrons.

So, to the first approximation we can consider them to be frozen in space their oscillations are not involved. Although when you consider lattice dynamics and so on you can always make subsequent corrections. But we begin with the model that the positive ions are frozen in space.

But beyond that we also make the Jellium potential approximation and so on, so that is something that we have done in the previous considerations. What we are going to do today is to consider oscillations of the electron gas.

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Displacement of all the electrons to the right ξ

net positive charge per unit area = $+e\bar{\rho}_p\xi$

net negative charge per unit area = $-e\bar{\rho}_e\xi$

surface charge density: $\sigma = e\bar{\rho}_e\xi$

Positive and Negative charge in balance

net field in-between $\vec{E} = \frac{1}{\epsilon_0} e\bar{\rho}_e\xi \hat{u}$

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And I had referred to this picture earlier that you have not positive and negative charge in balance. You consider a small displacement of the electron gas to the right. So, that you have

a net negative charge on the right side of the figure and the net positive charge on the left side.

So, there is a net negative charge per unit area which is $-e \bar{\rho} \xi$ if $\bar{\rho}$ is the volume charge density. And then you have got a net positive charge per unit area on the left side which is got the same magnitude but it has got a positive sign. The surface charge density is $e \bar{\rho} \xi$.

This is the; I am using $\bar{\rho}$ to represent the average charge density because we are going to very soon introduce density fluctuations okay. So, I am using the symbol $\bar{\rho}$ to represent this charge density and the net electric field will be the surface charge density divided by epsilon zero. So, that is coming straight from classical electrostatics. (Refer Slide Time: 04:42)

net field in-between

$$\vec{E} = \frac{1}{\epsilon_0} e \bar{\rho} \xi \hat{u}$$

Eq. of motion

$$m \frac{d^2 \xi}{dt^2} = \left(\frac{1}{\epsilon_0} e \bar{\rho} \xi \right) (-e) \quad \omega_p = \sqrt{\frac{\bar{\rho} e^2}{m \epsilon_0}} \quad \text{SI units}$$

CGS units

$$\frac{1}{4\pi \epsilon_0} \rightarrow 1 \quad ; \quad \frac{1}{\epsilon_0} \rightarrow 4\pi \quad \frac{d^2 \xi}{dt^2} = -\frac{\bar{\rho} e^2}{m \epsilon_0} \xi \quad \text{S.H.O.} \quad \omega_p = \sqrt{\frac{4\pi \bar{\rho} e^2}{m}} \quad \text{CGS units}$$

Frequency of plasma oscillations

Thermal motion of electrons: ignored

except that implicitly we assumed that thermal fluctuations would have caused departure from equilibrium in plasma density and thereby cause an onset of plasma oscillations.

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This is the net field and the equation of motion is just mass times acceleration is equal to the force, so the forces which are you know force per unit area which is the intensity times the charge which is $-e$. And essentially you have a simple harmonic motion over here. You have got an equation of motion for the simple harmonic oscillator.

Which oscillates at a frequency which is given by the square root of this proportionality which is the spring constant in our usual vocabulary and this is the frequency of oscillations in CGS units you will find this relation written more commonly as in terms of the natural frequency ω_p , so instead of this $\bar{\rho} e^2$ by $m \epsilon_0$, you get $4\pi \bar{\rho} e^2$ by m .

Now what we have done is we are going to ignore thermal motions at this point except that we assume that some thermal motion would have caused the initial displacement. Because

you need a region some origin it is not that you have applied an external field to displace the electron gas okay. So, this is something which happens internally but other than that we are going to ignore any thermal motion. So, that is our model.
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net field in-between

$$\vec{E} = \frac{1}{\epsilon_0} e \bar{\rho} \xi \hat{u}$$

Eq. of motion

$$m \frac{d^2 \xi}{dt^2} = \left(\frac{1}{\epsilon_0} e \bar{\rho} \xi \right) (-e)$$

$$\frac{d^2 \xi}{dt^2} = - \frac{\bar{\rho} e^2}{m \epsilon_0} \xi \quad \text{S.H.O.}$$

CGS units

$$\omega_p = \sqrt{\frac{4\pi \bar{\rho} e^2}{m}}$$

$$\bar{\rho} = \frac{N}{\frac{4}{3} \pi r_s^3} = \frac{3}{4\pi r_s^3}$$

Frequency of plasma oscillations

$$\omega_p = \sqrt{\frac{4\pi \left(\frac{3}{4\pi r_s^3} \right) e^2}{m}}$$

Thermal motion \rightarrow dispersion

when dispersion is present:

$$\omega^2 = \omega_p^2 - \frac{2E_F}{m} k^2$$

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So, in this model you have got the equation of motion for a linear harmonic oscillator a simple harmonic oscillator you have the natural frequency of the plasma oscillations given in CGS units. Rho bar is the number of electrons per unit volume, so this is the number of electrons N, this is the total volume which is the number of electron times the average volume of each electron expressed in terms of the average radius of the volume occupied by each electron.

So, the N's cancel and you have 3 over 4pi r cube, rs cube, So, that is the expression for Rho bar which is the average density and you can put this in the expression for the frequency coming from the solution to this differential equation for the simple harmonic oscillator and you have this relation you can see that the 4pi will cancel.

And you have got your plasma frequency given by this relation root of 3 e square by mr cube right, rs cube, rs is the average radius of the average volume occupied by every electron. So we have an expression for the frequency of oscillations. We are ignoring dispersion and when you have dispersion you can make corrections to this term but that is not the main interest in today's discussion.

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For free electron gas in jellium potential : Bohm & Pines: mid-fifties

$\left[\frac{E_{PT}^{HF}}{N} \right] = \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} \right) R_{Yd}$ D.Pines (1963)
Elementary excitations in solids (Benjamin, NY)


$E_{BP} = \frac{2.21}{r_s^2} + \frac{\sqrt{3}}{2r_s^{3/2}} \beta^2 - \frac{0.916}{r_s} \left(1 + \frac{\beta^2}{2} - \frac{\beta^4}{48} \right)$

$\beta = \frac{k_c}{k_f}$; k_c : upper bound to the wave number

oscillations get damped by random thermal motion of the electrons

$\omega_p = \left(\sqrt{\frac{3}{m}} \right) \left(\frac{e}{r_s^{3/2}} \right)$ zero point energy of the plasma oscillations
 $\frac{1}{2} \hbar \omega_p$ where $\hbar \omega_p = \frac{2\sqrt{3}}{r_s^{3/2}} R_{Yd}$

Random Phase Approximation

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What we found is the solution to the problem in two approximations one is the Hartree Fock which I write as a superscript here and in the Hartree Fock self-consistent field method we found the energy per unit electron to be given by 2.21 by r square - 0.916 by rs in units of Rydberg. And we got the same solution in using perturbation theory which I write as a subscript over here. So, both of these gave us essentially the same solution.

What we are going to discuss today is go beyond the Hartree Fock method, go beyond the perturbative method okay and introduce an approximation which is known as the Random Phase Approximation this was introduced by Bohm and Pines in the mid 50's but I am not going to attempt to give an exhaustive review of the historical development of the Random Phase Approximation.

Because there many alternative paths to RPA you know it was developed in nuclear physics, it was also; there is a green function method, there are other methods and I am not getting into the historical development of this method from various different points of view. But I will specifically concentrate on the method of Bohm and Pines.

Because it is this method which explains best, the term random phase which goes into this approximation okay. So, I am going to discuss the Bohm Pines's approach to some extent. And in Bohm Pines's approach you get an improvement over the expression you get either from Hartree Fock or from perturbative methods.

You get additional parameters in terms of beta which is actually a ratio and this ratio is kc over kf, kf is our old friend which is the Fermi momentum in units of h cross right. And kc is a certain upper bound to the wave number because oscillations get damped by random thermal motion above it, so I will explain why you have this upper bound.

So, you will have an electron gas in certain state of oscillations of the plasma. So, these are the collective oscillations of the electron gas, these are not the individual oscillations about an electron around a certain equilibrium point. But the collective oscillations of the electron gas and you will also have a zero point energy of the plasma oscillations just the way you have it for a simple harmonic oscillator.
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Field Operators Reference:
 $\hat{\psi}(q) = \sum_i \psi_i(q) c_i$ STITACS / Unit 3 / lecture 19 /
 $\hat{\psi}^\dagger(q) = \sum_i \psi_i^*(q) c_i^\dagger$

$$H = \int \hat{\psi}^\dagger(q) f(q) \hat{\psi}(q) dq + \frac{1}{2} \int \int \hat{\psi}^\dagger(q) \hat{\psi}^\dagger(q') v(q, q') \hat{\psi}(q) \hat{\psi}(q') dq dq'$$

equivalent

$$H = \sum_i \sum_j c_i^\dagger \langle i | f | j \rangle c_j + \frac{1}{2} \sum_i \sum_j \sum_k \sum_l c_i^\dagger c_j^\dagger \langle ij | v | lk \rangle c_l c_k$$

Complete expressions for the operators,
inclusive of spin labels →



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So, let us develop this model now you have the quantum field operator's Psi and Psi dagger. These are expressed in terms of the electron creation and destruction operators which we introduced in an earlier class. Using these you can write the Hamiltonian the electron electronic Hamiltonian in two equivalent forms one in terms of the field operator's Psi and Psi dagger or equivalently in terms of the creation and the destruction operators.

The C_i dagger and the C_j and you have the same over here. You have the two center integral, so we are have dealt with these terms earlier. So you can express the Hamiltonian in these two equivalent forms. However we did not specify the spin label explicitly in this okay. It is already sitting over here because q is a set of four variables the three spin coordinates and one spin variable.
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Complete expressions for the operators, inclusive of spin labels

$$[c_{\alpha\sigma_1}, c_{\alpha_2\sigma_2}]_{\pm} = \delta_{\alpha\alpha_2} \delta_{\sigma_1\sigma_2} \quad [c_{\alpha\sigma_1}, c_{\alpha_2\sigma_2}]_{\pm} = 0 \quad [c_{\alpha\sigma_1}, c_{\alpha_2\sigma_2}]_{\pm} = 0$$

$$\hat{\psi}_{\alpha}(q) = \sum_{\sigma} \sum_i \psi_{i\alpha}(q) c_{i\sigma} \quad \hat{\psi}_{\beta}^{\dagger}(q) = \sum_{\sigma} \sum_j \psi_{j\beta}^*(q) c_{j\sigma}^{\dagger}$$

$$H = \int \hat{\psi}_{\alpha}^{\dagger}(q) f(q) \hat{\psi}_{\beta}(q) dq + \frac{1}{2} \int \int \hat{\psi}_{\alpha}^{\dagger}(q) \hat{\psi}_{\beta}^{\dagger}(q) v(q, q') \hat{\psi}_{\gamma}(q) \hat{\psi}_{\delta}(q) dq dq'$$

becomes, inclusive of the explicit spin labels:

$$H = \sum_i \sum_{\sigma} \sum_j \sum_{\sigma'} c_{i\sigma}^{\dagger} \psi_{i\sigma}^*(q) f(q) \psi_{j\sigma'}(q) dq c_{j\sigma'} +$$

$$+ \frac{1}{2} \sum_i \sum_{\sigma} \sum_j \sum_{\sigma'} \sum_k \sum_{\sigma''} c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} \int \int \psi_{i\sigma}^*(q) \psi_{j\sigma'}^*(q) v(q, q') \psi_{k\sigma''}(q) \psi_{l\sigma''}(q) dq dq' c_{k\sigma''} c_{l\sigma''}$$

$$H = \sum_i \sum_{\sigma} \sum_j \sum_{\sigma'} c_{i\sigma}^{\dagger} \langle i\alpha | f | j\beta \rangle c_{j\sigma'} + \frac{1}{2} \sum_i \sum_{\sigma} \sum_j \sum_{\sigma'} \sum_k \sum_{\sigma''} c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} \langle i\alpha, j\beta | v | l\delta, k\gamma \rangle c_{k\sigma''} c_{l\sigma''}$$

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 Ramesh / p.42 / Eq.2.117 → inclusive of spin labels
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So, we will now write these operators explicitly inclusive of the spin labels. So, let us do that so having spelled out the spin label as sigma so you have got two operators over here a1 and a2 correspondingly you have got sigma1 and sigma2 and these are then the commutation or anti commutation relations appropriately for bosons and fermions.

For fermions you have gone to anti commutation relations for the creation and destruction operators for bosons these are the commutation relations. And we will be dealing with the anti commutator because the particles of our interest are electrons and the field operator now must be written explicitly in terms of a summation over the spin index alpha.

So, Ci alpha is the destruction operator for the state i and the spin Eigen value alpha okay. So, these are the good quantum numbers inclusive of spin and you can write the Hamiltonian which we have written without explicit indication of the spin label. But now inclusive of spin labels, we can write this Hamiltonian so this summation over ij is over the one electron states and then there is an explicit summation over the spin levels alpha, beta.

So, Ci alpha dagger and Cj beta are the corresponding creation and destruction operators. So, it is the same Hamiltonian but now we have written it fully explicitly inclusive of the spin labels. We can also write it equivalently in terms of not just the field operators but only in terms of the creation and destruction operators, so these are completely equivalent forms which we saw in the previous slide as well.
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$q \equiv \vec{r}, \zeta \rightarrow \text{space + spin coordinate}$

$\psi^\dagger(q)\psi(q) = \rho(q) \leftarrow \text{particle density operator}$

$$\sum_{\zeta} \iiint d^3\vec{r} \rho(q) = \sum_{\zeta} \iiint d^3\vec{r} \psi^\dagger(q)\psi(q) = N$$


N : number of electrons in the region

$$\int \psi^\dagger(q) \delta(q-q') \psi(q) dq' =$$

$$= \sum_{\zeta'} \int \psi^\dagger(\vec{r}') \chi^\dagger(\zeta') \delta(\vec{r}-\vec{r}') \delta_{\zeta, \zeta'} \psi(\vec{r}) \chi(\zeta) d^3\vec{r}'$$

$$= \sum_{\zeta'} \chi^\dagger(\zeta') \delta_{\zeta, \zeta'} \chi(\zeta) \int \psi^\dagger(\vec{r}) \delta(\vec{r}-\vec{r}') \psi(\vec{r}) d^3\vec{r}'$$

$$= \chi^\dagger(\zeta) \chi(\zeta) \psi^\dagger(\vec{r}) \psi(\vec{r}) = \psi^\dagger(q) \psi(q) = \rho(q)$$


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So, our notation is well understood that the label q is a set of 4 coordinates' 3 space coordinates and 1 spin coordinate okay. This is the same notation that we used in the Hartree Fock theory also. Then you have got the particle density operator which is $\Psi^\dagger \Psi$ right. And when you integrate this particle density operator you will get the total number of electrons.

But you must integrate over all the space coordinates and also sum over all the spin levels because now we have chosen to indicate that explicitly. And you can easily see that these expressions and this notation is appropriate because if you now insert a delta function and carry out this integration. This delta function is the product of the delta function for the space arguments and the Kronecker delta for the spin.

Because the spin coordinates are discrete so you can now separate the summation over the spin over here followed by integration over the space coordinates right. And if you contract these summations you get essentially the particle density. So, this is a particle density which we began with right.

So, this is the notation that I will be using okay. So, this is our particle density operator what we are going to do is to develop an equation of motion for the particle density operator because we will essentially be led to density fluctuations in the electron gas.

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$\psi^\dagger(q)\psi(q) = \rho(q) \leftarrow$ particle density operator

$$\rho(\vec{r}) = \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i)$$

$$\begin{aligned} \iiint d^3\vec{r} \rho(\vec{r}) &= \iiint d^3\vec{r} \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i) \\ &= \sum_{i=1}^N \iiint d^3\vec{r} \delta(\vec{r} - \vec{r}_i) = N \end{aligned}$$

Fourier expansion:

$$\rho(\vec{r}) = \frac{1}{V} \sum_{\vec{k}=1}^N \rho_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

$[\rho_{\vec{k}}]$: dimensionless

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So, you can see that this particle density operator is essentially a sum of the Dirac delta's is because if you integrate this, if you integrate this, then on the right hand side you will get essentially the total number of particles. So, the particle density operator is essentially a summation of the Dirac delta r okay. You can also use a Fourier expansion of the density and then this Rho k is a Fourier transform.

And this is the Fourier expansion of the particle density operator notice that 1 over volume comes explicitly over here, so this Rho, Rho k the Fourier transforms will be a dimensionless quantity in our notation okay. So, this is our, you know particle density expansion in terms of its Fourier components.

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Positive charge density $e\rho$ smeared out uniformly.

N electrons per unit volume: $\rho = N/V$

Fourier expansion of the electron-electron Coulomb interaction

$$\frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)}$$

$[c_{\vec{k}}] = [\text{charge}]^2 L^2$

The above sum is a triple sum, over the three components of \vec{k} .

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What we have done is to smear the positive charge throughout this box at a uniform density. So, now you also have the electron-electron interaction which we have expressed earlier in terms of all of these this complete set of basis of the momentum vectors in the reciprocal

space right. Notice here that the coefficient c will have dimensions of charge square over length square okay.

Because this will have a dimension of charge square over length, so this is charge square over length square and then there is a volume over here, so this is charge square into L square divided by L cube, so you will get charge square over length. So, those are the dimensions of the coefficient c_k , this is actually a triple sum because every k has got three components the k_x, k_y, k_z . So, you must sum over all the components okay.
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$$\frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$

multiplying both sides by $e^{i\vec{k}' \cdot (\vec{r}_j - \vec{r}_i)}$

$$e^{i\vec{k}' \cdot (\vec{r}_j - \vec{r}_i)} \frac{e^2}{r_{ij}} = e^{i\vec{k}' \cdot (\vec{r}_j - \vec{r}_i)} \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$

Note the sign

$$e^{i\vec{k}' \cdot (\vec{r}_j - \vec{r}_i)} \frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} e^{i(\vec{k} - \vec{k}') \cdot (\vec{r}_i - \vec{r}_j)}$$

Integrating:


$$\iiint d^3 \vec{r}_j \left[e^{i\vec{k} \cdot (\vec{r}_j - \vec{r}_i)} \right] \frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} \iiint d^3 \vec{r}_j \left[e^{i(\vec{k} - \vec{k}') \cdot (\vec{r}_i - \vec{r}_j)} \right]$$

The Wave Mechanics of Electrons in Metals - by Stanley Raimel, page 289

So, this is our expression for the Coulomb expansion we first consider the case when the momentum vector k is not equal to 0. Now when this is the case if you multiply both sides by this term e to the ik prime. So, the dummy index over here is k that is the reason I choose a different wave vector over here which is k prime and I multiply both sides by this term.

So, let us do that I multiplied e squared over r_{ij} by this exponential function on both sides okay. And now you see that the right hand side I can move this is; these two arguments are very similar except for the fact that this is k and this is k prime. On the other hand this is $r_i - r_j$ this is $r_j - r_i$.

So, if you take the dot product of $k - k$ prime with $r_i - r_j$ you get an equivalent correspondence over here okay. So, this is your expression that we will now note that there is a - sign over here and if you integrate this result. So this term is now integrated over volume, you carry out a volume integration, so you have a volume integration of the right-hand side.
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$$\iiint d^3\vec{r}_j \frac{e^{i\vec{k}\cdot(\vec{r}_j-\vec{r})}}{r_{ij}} = \frac{1}{V} \sum_k c_k \iiint d^3\vec{r}_j e^{i(\vec{k}-\vec{k}')\cdot(\vec{r}_j-\vec{r})}$$

$$e^2 \iiint d^3\vec{r}_j \frac{e^{i\vec{k}\cdot(\vec{r}_j-\vec{r})}}{r_{ij}} = \frac{1}{V} \sum_k c_k \iiint d^3\vec{r}_j e^{i(\vec{k}-\vec{k}')\cdot(\vec{r}_j-\vec{r})}$$

from slide 117, L19:

$$FT \text{ of } \left(\frac{1}{r}\right)^c = \frac{4\pi}{k'^2} \quad \frac{4\pi e^2}{|\vec{k}'|^2} = \sum_k c_k \left(\frac{1}{V} \iiint d^3\vec{r}_j \left[e^{i(\vec{k}-\vec{k}')\cdot(\vec{r}_j-\vec{r})} \right] \right)$$

Dirac δ

$$= \sum_k c_k e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} \delta(\vec{k}-\vec{k}')$$

$$\frac{4\pi e^2}{|\vec{k}'|^2} = c_{\vec{k}'}$$

i.e. $c_{\vec{k}} = \frac{4\pi e^2}{|\vec{k}|^2} \rightarrow \text{except when } \vec{k} = \vec{0}$

$[c_k] = [\text{charge}]^2 L^2$

FOOTNOTES Slide 3: Electrostatics in HF © RPA 164

And now you can see what this volume integration is going to lead you to because all I have done here is to extract the e^2 out of the integration symbol and then this is nothing but the Fourier transform of the Coulomb potential right. So you get $4\pi e^2$ into 4π over k prime square k prime because you have a k prime over here okay. So, this is the Fourier transform of the Coulomb potential.

And our result is that $4\pi e^2$ over k prime square is equal to this integral but when you look at this volume integral along with the $1/V$ you are essentially looking at the Dirac delta which we have used in the previous class okay. We have used this explicit form of the Dirac delta. So now you have got a Dirac delta and you have to sum over all values of k . So, the only term under the summation k that will survive is the one corresponding to k prime.

So, that is your result. So, on the right hand side only $c_{k'}$ will survive because of the Dirac delta and $c_{k'}$ is $4\pi e^2$ by k square k prime square and you can drop the prime now. So, this is your general expression for the coefficient c_k which is $4\pi e^2$ over k square except when $k = 0$ okay. Because when $k = 0$ this term seems to blow up, so that we will deal with separately.

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$$\frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$


$$c_{\vec{k}} = \frac{4\pi e^2}{|\vec{k}|^2} \rightarrow \text{except when } \vec{k} = \vec{0}$$

Integrating ↓ What is $c_{\vec{k}}$ when $\vec{k} = \vec{0}$?

$$e^2 \iiint d^3\vec{r}_j \frac{1}{r_{ij}} = \sum_{\vec{k}} c_{\vec{k}} \left\{ \frac{1}{V} \iiint d^3\vec{r}_j e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} \right\}$$

now, $\frac{1}{V} \iiint d^3\vec{r}_j [e^{i(\vec{k} - \vec{k}') \cdot (\vec{r}_i - \vec{r}_j)}] = \delta(\vec{k} - \vec{k}') \quad \text{Eq 3.11, page 23, F&W}$

i.e. for $\vec{k}' = \vec{0}$: $\frac{1}{V} \iiint d^3\vec{r}_j e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} = \delta(\vec{k} - \vec{0}) = \delta(\vec{k})$



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So, this is our expansion for the Coulomb potential okay. So, this is a Coulomb potential of the i th electron in the field of the j th electron. What is the value of c_k when $k = 0$ okay. We once determine the values of C_k in general but we have to find out what is its value when $k = 0$. So, what you do is if you integrate this expression, this is your complete result okay. We know that you have a Dirac delta on the right side.

And for whenever $k' = 0$, you have you put this $k' = 0$, so this will be $e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$ because k' is now set $= 0$, so this will be $\delta(\vec{k} - \vec{k}')$ but $k' = 0$, so this becomes a delta function again but not of $k - k'$ but $\delta(\vec{k})$ because $k' = 0$.

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$$e^2 \iiint d^3\vec{r}_j \frac{1}{r_{ij}} = \sum_{\vec{k}} c_{\vec{k}} \left\{ \frac{1}{V} \iiint d^3\vec{r}_j e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} \right\}$$

$$\vec{r}_j - \vec{r}_i = \vec{r} \quad \frac{1}{V} \iiint d^3\vec{r}_j e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} = \delta(\vec{k})$$

$$e^2 \iiint d^3\vec{r} \frac{1}{r} = \sum_{\vec{k}} c_{\vec{k}} \delta(\vec{k}) = c_{\vec{0}}$$

$$\therefore c_{\vec{0}} = e^2 \iiint d^3\vec{r} \frac{1}{r}$$

Potential energy of the j^{th} electron due to **one** electron charge uniformly smeared throughout the box.



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So, this is our result here that you have $\delta(k)$ and this means that when the only term that will survive under this summation is the term corresponding to $k = 0$ right which is C_0 . So, that is your coefficient C_0 now. What is C_0 ? What is this? This is nothing but the potential of

the i th electron in the field of the j th electron as if the j th electron is smeared over the whole box.

The j th electron is not at a particular location it is smeared the whole box. The potential energy of the i th electron due to just one electron but that one electron is smeared over the whole box at a uniform charge density, so that is what we get for C_0 .
(Refer Slide Time: 23:56)

Potential energy of the i^{th} electron due to the j^{th} : $\frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$

Potential energy of the i^{th} electron due to all the electrons:

$$P(\vec{r}_i) = \sum_{\substack{j=1 \\ j \neq i}}^N \frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{\substack{j=1 \\ j \neq i}}^N \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$c_{\vec{k}} = \frac{4\pi e^2}{|\vec{k}|^2} \rightarrow \text{except when } \vec{k} = \vec{0} \quad \left[\quad c_0 = e^2 \iiint d^3\vec{r} \frac{1}{r} \right]$$

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Now this is the expression now for the potential energy of the i th electron due to the j th okay. Now what will be the potential energy of the i th electron, how many electrons are there? There are N electrons. So, you have to sum over all the remaining electrons. The potential energy of the i th electron due to all the other electrons all the electrons not just the j th, so you must sum over j going from 1 through N except for $j = i$.

So, this is the net potential energy of the electron due to all the other electrons. You have got 1 over V this is it is this term, you have got this term which comes here and you are summing over j going from 1 through N and avoiding $j = i$ and we know what C_k values are, C_k is given by $4\pi e^2$ over k^2 whenever k is not equal to 0.

And whenever $k = 0$ it is given by this okay. So we have got everything that we need all right. So, having gotten this, this is just the potential energy of the i th electron in the field of all the remaining electrons. We have still not considered the Jellium potential. We have not considered the positive nuclei.
(Refer Slide Time: 25:26)

Potential energy of the i^{th} electron due to **all the electrons**:

$$P(\vec{r}_i) = \sum_{\substack{j=1 \\ j \neq i}}^N \frac{e^2}{r_{ij}} = \frac{1}{V} \sum_{j=1}^N \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$c_{\vec{k}} = \frac{4\pi e^2}{|\vec{k}|^2} \rightarrow \text{except when } \vec{k} = \vec{0} \quad \left[c_{\vec{0}} = e^2 \iiint d^3\vec{r} \frac{1}{r} \right]$$

Slide 130 (previous class)

Potential energy of the i^{th} electron due to **all the electrons and the positive background**:

$\vec{k} = \vec{0}$ term \rightarrow cancels the positive jellium

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

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What we do know that if you consider the positive background okay. Then you have various effects coming because of the background Hamiltonian and there is another part of the Hamiltonian which is the electron background interaction. But we have already found that the $k = 0$ term okay cancels the positive Jellium. We have discussed this in an earlier class okay. So, if you take this for all values of k but if you leave out the $k = 0$ term.

Because that is the term which is going to cancel the positive Jellium effects then you have got the potential energy of the i^{th} electron in the field of all the remaining electrons and the positive background okay. And that is then given by this expression on the right hand side inclusive of the summation over k except for the $k = 0$ term because that is the one which goes into the cancellation of the Jellium okay, all right.

(Refer Slide Time: 26:44)

Potential energy of the i^{th} electron due to **all the electrons and the positive background**:

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

Force exerted on the i^{th} electron: $m\ddot{\vec{r}}_i = m\dot{\vec{v}}_i = -\vec{\nabla}_i U(\vec{r}_i)$
weaker magnetic forces ignored

$\ddot{\vec{r}}_i = \dot{\vec{v}}_i = -\frac{1}{m} \vec{\nabla}_i U(\vec{r}_i) = -\frac{1}{V} \sum_{j=1}^N \sum_{\substack{\vec{k} \\ \vec{k} \neq \vec{0}}} \frac{4\pi e^2}{mk^2} (\vec{\nabla}_i e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)})$
acceleration of the i^{th} electron

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

$\uparrow i = \sqrt{-1}$

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So, this is our potential now which is the potential energy, energy of the i^{th} electron due to all the remaining electrons and the positive background okay. Now you have got the potential

and if you have the potential, you can find what is the force acting on it? Because force is the negative gradient of the potential, so let us write the force which is mass times acceleration which is mass times the time derivative of the velocity.


And this will be the negative gradient of the potential the potential U is given by this relation at the top. This is a net force which the electron experiences, of course if charges are in motion they will generate magnetic fields. And the magnetic field will in turn exert a force on this charge which will go as $\mathbf{v} \times \mathbf{B}$ that is the Lorentz force right. So, that is typically lot weaker than the forces we are considering.

And those weaker magnetic forces we are ignoring in this analysis. So, the expression for the acceleration because you have to divide everything by mass so you have got $1/m$ coming here, and $1/m$ coming here, so you have essentially the negative gradient of the potential. So, you have to take the gradient the negative gradient of the potential.

Now what is dependent on r because gradient will take space derivatives with respect to the coordinates i and the only thing that depends on i is sitting over here okay, the $4\pi e^2$ squared over $m k^2$ does not respond to the gradient operator. So you have got the gradient operator which I have written in a bracket along with the term for where it really matters. So, this is the acceleration of the i th electrons.

So, this is still a classical model and today I am going to discuss the classical model and then tomorrow we will get into the quantum model. So, now we have to take the gradient now what is the gradient? Gradient of this term with respect to the i th coordinate is $i k$ right. And then you have got an exponential function. This i of course is square root of -1 okay.

And this r_i which is the subscript on the position vector is referring our discussion to a particular i th electrons. I am using the symbol i for two things one is the index of the electron and the other of course is the square root of -1 , so there is.
(Refer Slide Time: 29:40)



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

Due to the symmetrical distribution of the vectors \vec{k}

the summand on the RHS for $(j=i)$ is $\sum_{\substack{\vec{k} \\ \vec{k} \neq \vec{0}}} \frac{4\pi e^2}{mk^2} (i\vec{k}) = \vec{0}$

Hence no need to exclude $j=i$ term

$$\ddot{\vec{r}}_i = \dot{\vec{v}}_i = -\frac{1}{m} \vec{\nabla}_i U(\vec{r}_i) = -\frac{1}{V} \left(\sum_{j=1}^N \right) \sum_{\substack{\vec{k} \\ \vec{k} \neq \vec{0}}} \frac{4\pi e^2}{mk^2} (i\vec{k} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)})$$

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So, this is our result for the acceleration of the i th electron which I write at the top of this right now. Now notice that this is a summation over j going from 1 through N but $j = i$ was avoided. On the other hand if you look at this term which is in the box and analyse this term and ask yourself what would happen to this box? This box is what I will call as a summand. This is something which is being summed over right.

Like the integrand is what gets integrated but summand is what gets summed up. So, what is sitting in this red box is going to be summed up for different values of j , j going from 1 through N but we are avoiding $j = i$, so j not equal to i specified explicitly over here. But what is being summed up is this term which for $j = i$ will give you a 0 here $r_i - r_j$ will go to 0 for $j = i$ because $r_j - r_i$ will go to 0. So, you get e to the power 0 over here which is 1 okay.

And you are then summing the rest of the vectors the summoned on the right hand side for $j = i$ is this. And this is of course 0 because there you are summing over all the momentum vectors and there are as many momentum vectors in one direction as there are in the opposite which are exactly equal and opposite.

You have got the entire Fermi's, Fermi surface which is a spherical surface and there are vectors in opposite directions in this Fermi surface whichever direction you look at right. So, they will all cancel each other and you have got the vector sum of k summed over k , k is not equal to 0 and this will give you a null vector. And therefore it really does not matter whether you include $j = i$ or you do not include $j = i$.

Because the term corresponding to $j = i$ gives you a zero anyway. So you are only adding a 0 coming from $j = i$ terms and it really does not matter. So, we have no real need to exclude the $j = i$ item. So, now we write this summation over j going from 1 through N but we do not

specify any further that $j = i$ has to be avoided. So, this $j \neq i$ is not written over here we are letting $j = i$ as well because it really does not matter okay. (Refer Slide Time: 32:32)

acceleration of the i^{th} electron

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

electron charge density

$$\rho(\vec{r}) = \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i)$$

$$\iiint d^3\vec{r} \rho(\vec{r}) = \sum_{i=1}^N \iiint d^3\vec{r} \delta(\vec{r} - \vec{r}_i) = N$$

Fourier expansion of charge density

$$\rho(\vec{r}) = \frac{1}{V} \sum_{\vec{k}=1}^N \rho_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \quad [\rho_{\vec{k}}]: \text{dimensionless}$$

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So, this is our expression for the acceleration. What is the electron charge density? We had this relation earlier with us. We know that when you integrate this charge density you get the total number of electrons we discuss this. We have the Fourier expansion of the charge density in terms of the Fourier components ρ_k which in our system of equations is dimensionless.

This, the left hand side has got a dimension of whatever volume it is the number per unit volume. And the inverse volume dimension is taken care of by $1/V$ over here. So, the equation is essentially balanced dimensionally.

(Refer Slide Time: 33:18)

Fourier expansion of charge density

$$\rho(\vec{r}) = \frac{1}{V} \sum_{\vec{k}=1}^N \rho_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \quad [\rho_{\vec{k}}]: \text{dimensionless}$$

$$\rho(\vec{r}) = \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i)$$

$$\rho_{\vec{k}} = \iiint d^3\vec{r} \rho(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} = \iiint d^3\vec{r} \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i) e^{-i\vec{k} \cdot \vec{r}}$$

$$\rho_{\vec{k}} = \sum_{i=1}^N \iiint d^3\vec{r} \delta(\vec{r} - \vec{r}_i) e^{-i\vec{k} \cdot \vec{r}}$$

$$\rho_{\vec{k}} = \sum_{i=1}^N e^{-i\vec{k} \cdot \vec{r}_i} \quad \rho_{\vec{k}=\vec{0}} = N \leftarrow \text{total number of electrons}$$

$\vec{k} \neq \vec{0}$ \leftarrow components: density fluctuations over the average

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So, these are our expressions for the Fourier expansion of the charge density. The Fourier components can be written in terms of the inverse transforms right. And this density is

nothing but the summation over the deltas, delta functions. And if you write this summation symbol because this is summation over i, this is the integration over space, this is a particle index, this is space integration.

So, these are completely independent operations, so you can write this behind the integration and then you carry out this integration over here. So, that essentially what you will find is that the Fourier component is given by sum over i going from 1 through N. And under this Dirac delta integration the only term that will survive is e to the -ik for r equal to ri because of this delta r must be equal to ri otherwise the integral will vanish.

So, this is the expression for the Fourier component of the charge density. For k = 0 you of course get the total number of electrons okay. So, now let us analyze these expressions further. It is the k not equal to 0 terms which will be involved in the density fluctuations over the average.

So, you have got a certain static every charged density which is smeared over the whole space but then you can have density fluctuations on top of it and these are the ones which were not included in the Hartree Fock if you remember. Because the Hartree Fock approximation is essentially a frozen orbital approximation you do not consider these density fluctuations in the Hartree Fock.

And the Hartree Fock we have also seen is completely equivalent to what you get from the first order perturbation theory. So, of the as we are going beyond the perturbative method, we are also going beyond the Hartree Fock.
(Refer Slide Time: 35:37)

The slide contains the following mathematical derivations:

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

acceleration of the i^{th} electron

$$\ddot{\vec{r}}_i = \dot{\vec{v}}_i = -\frac{4\pi e^2 i}{mV} \sum_{\substack{\vec{k} \\ \vec{k} \neq 0}} \frac{\vec{k} e^{i\vec{k} \cdot \vec{r}_i}}{k^2} \left(\sum_{j=1}^N e^{-i\vec{k} \cdot \vec{r}_j} \right)$$

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

$$\ddot{\vec{r}}_i = \dot{\vec{v}}_i = -\frac{4\pi e^2 i}{mV} \sum_{\substack{\vec{k} \\ \vec{k} \neq 0}} \frac{\vec{k}}{k^2} \rho_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i}$$

$$\dot{\rho}_{\vec{k}} = \sum_{i=1}^N e^{-i\vec{k} \cdot \vec{r}_i} \frac{d}{dt} (-i\vec{k} \cdot \vec{r}_i)$$

$$\dot{\rho}_{\vec{k}} = -i \sum_{i=1}^N e^{-i\vec{k} \cdot \vec{r}_i} (\vec{k} \cdot \dot{\vec{r}}_i)$$

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So, this is our expression for the acceleration of the i th electron. You have got sum over j we are now admitting $j = i$ it does not matter. And I have simply rewritten these terms this is just bookkeeping. But I factored this exponential function into e to the i e to the $ik \cdot r_i$ term which is here and e to the there is a $-$ sign here $- ik \cdot r_j$, so that comes over here.


So, I have separated these two terms and I have confined the summation over j over here because this is the only thing which is affected by j . So, what does it tell us that this term you have e to the $ik \cdot r_i$ when you sum over i going from 1 through N and this is exactly the same term right. This is nothing but the Fourier component ρ_k right. So, in the expression for the acceleration which is the time derivative of the velocity?

These terms remain the same, you have got i , you have got sum over k , $k \neq 0$ all that is fine, you get k over k^2 here, you have got e to the $ik \cdot r_i$ which is here and this is nothing but the Fourier component ρ_k is appearing here. Now we are developing the equation of motion look at this. Now if you want to develop an equation of motion for the Fourier components you must take the first derivative which will give you the velocity.

And then you must take the second derivative which will give you the acceleration and actually equation of motion as we know is the relationship between position, velocity and acceleration. So, we have to get up to the second time derivative. So, the first time derivative we give you the $\rho_k \cdot$. So, let us do that, so you have to take the time derivative of this summation.

So $\rho_k \cdot$ will give you the time derivative; this is just an exponential function and then you must take that the derivative of the exponent. So which is $ik \cdot r_i$ and k is time dependent so you will get $k \cdot \dot{r}$ which is $k \cdot$ velocity term. So, this is the time derivative of the Fourier component ρ_k right.

(Refer Slide Time: 38:19)



$$\ddot{\rho}_{\vec{k}} = \sum_{i=1}^N \left[-(\vec{k} \cdot \dot{\vec{r}}_i)^2 - i(\vec{k} \cdot \ddot{\vec{r}}_i) \right] e^{-i\vec{k} \cdot \vec{r}_i}$$

$$\ddot{\rho}_{\vec{k}} = - \sum_{i=1}^N (\vec{k} \cdot \dot{\vec{r}}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - i \sum_{i=1}^N (\vec{k} \cdot \ddot{\vec{r}}_i) e^{-i\vec{k} \cdot \vec{r}_i}$$

from Slide 170: $\ddot{\vec{r}}_i = \dot{\vec{v}}_i = -\frac{4\pi e^2 i}{mV} \sum_{\vec{k}' \neq 0} \frac{\vec{k}}{k^2} \rho_{\vec{k}'} e^{i\vec{k}' \cdot \vec{r}_i}$

$$\ddot{\rho}_{\vec{k}} = - \sum_{i=1}^N (\vec{k} \cdot \dot{\vec{r}}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - i \sum_{i=1}^N \left(\vec{k} \cdot \left[-\frac{4\pi e^2 i}{mV} \sum_{\vec{k}' \neq 0} \frac{\vec{k}'}{k'^2} \rho_{\vec{k}'} e^{i\vec{k}' \cdot \vec{r}_i} \right] \right) e^{-i\vec{k} \cdot \vec{r}_i}$$

$$\ddot{\rho}_{\vec{k}} = - \sum_{i=1}^N (\vec{k} \cdot \dot{\vec{r}}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - \frac{4\pi e^2}{m} \frac{1}{V} \sum_{i=1}^N \sum_{\vec{k}' \neq 0} \frac{\vec{k} \cdot \vec{k}'}{k'^2} \rho_{\vec{k}'} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}_i}$$

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Now we can take the second derivative because then we will be led to the equation of motion. This is all classical; it will be tomorrow that we will discuss the quantum treatment and the second derivative according to Newton's law which is involved in the equation of motion. So, the second derivative of the Fourier component will give you the time derivative of the velocity term which is Rho dot.

So, which is - i summation over i going from 1 through N which is coming from here then you have got the time derivative of the product of these two functions okay. There are two functions over here both have got a time dependent term, r_i is time dependent and the velocity will also be time dependent okay. Because the velocity of the i th particle depends on time its time derivative will give you the acceleration of the i th particle right.

So, both of these terms are time to dependent and you will therefore get two terms the first term times the time derivative of the second plus the time derivative of the first term times the second term, so you have these two terms now. So, you have got the time derivative of the first term which is e to the $-ik \cdot r_i$ times the time derivative of the exponent which is $-ik \cdot \dot{r}_i$ right.

And then the second term has got the first term times the time derivative of the second which gives you know acceleration of the i th coordinate. So, these are the two terms which appear in this equation of motion for the k th Fourier component in the charge density. Now you can write e to the $-ik \cdot r_i$ common in both and you have got these two terms okay. So, that is what you have got.

Now it is a very interesting kind of situation now because look at these terms do you recognize some familiar terms in this. If you look at this r_i double dot this is we already have

this result. And this was expressed in terms of the acceleration of the i th particle which we obtained just a little while ago okay. And this is from a previous slide just few slides prior to this one.


And in this one we have got the acceleration term of the i th electron for which we obtained this result and we can plug in this expression over here. Let us do that so we have got the second derivative of ρ okay. You have got the first term which is written exactly as it is over here. The second term you have got $-i \sum_{i=1}^N$ which is here then you have got $k \cdot$ and now you have this acceleration of the i th particle.

And that for that we use this right hand side over here which is put in this beautiful bracket and then of course you have this $e^{-i k \cdot r_i}$ which comes here all right okay. Notice that there is a minus sign over here and a minus sign over here, so that will give you a $+1$ factor but then notice that there is an i over here and i over here, so that will give you i^2 , so you will have a -1 popping out of it.

So, you take care of all of these signs and the i^2 , so you get a minus sign coming because of the i^2 okay. The first term is written as it is now these two minus signs have been taken care of. The i^2 is taken care of, you have got the $4\pi e^2 / mV$ over here, you have got the summation over i going from 1 through N over here. And now you have got the summation over k' , $k' \neq 0$.

You have this $k \cdot k'$ right, so that is coming over here in the numerator, you have got k'^2 in the denominator, you have got the Fourier component $\rho_{k'}$ and then you have got the product of these two exponential functions which gives you i to the power $k \cdot k' - k \cdot r_i$ okay.

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$$\ddot{\rho}_{\vec{k}} = -\sum_{i=1}^N (\vec{k} \cdot \vec{r}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - \frac{1}{V} \frac{4\pi e^2}{m} \sum_{i=1}^N \sum_{\substack{\vec{k}' \\ \vec{k}' \neq \vec{k}}} \frac{\vec{k} \cdot \vec{k}'}{k'^2} \rho_{\vec{k}'} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}_i}$$

$$\ddot{\rho}_{\vec{k}} = \left[\begin{array}{l} -\sum_{i=1}^N (\vec{k} \cdot \vec{r}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} \\ -\frac{1}{V} \frac{4\pi e^2}{m} \left[\frac{\vec{k} \cdot \vec{k}}{k^2} \rho_{\vec{k}} \sum_{i=1}^N e^{0 \cdot i} \right] \\ -\frac{1}{V} \frac{4\pi e^2}{m} \sum_{i=1}^N \sum_{\substack{\vec{k}' \\ \vec{k}' \neq \vec{k}}} \frac{\vec{k} \cdot \vec{k}'}{k'^2} \rho_{\vec{k}'} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}_i} \end{array} \right]$$

$\vec{k}' = \vec{k}$ term
 $\vec{k}' \neq \vec{k}$ terms

$$\ddot{\rho}_{\vec{k}} = -\sum_{i=1}^N (\vec{k} \cdot \vec{r}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - \frac{1}{V} \frac{4\pi N e^2}{m} \rho_{\vec{k}} - \frac{1}{V} \frac{4\pi e^2}{m} \sum_{i=1}^N \sum_{\substack{\vec{k}' \\ \vec{k}' \neq \vec{k}}} \frac{\vec{k} \cdot \vec{k}'}{k'^2} \rho_{\vec{k}'} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}_i}$$

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Now let us bring this to the top of the next slide it is the same essentially the same expression. And now this summation has; is a summation over k prime and I break this summation into two parts one corresponding to k prime = k and the remaining set of terms corresponding to k prime not equal to k. Because in some cases k prime will be equal to k, so that is the term I separate out.

So, now only these two terms are in the equation in the first row over here but the summation over k prime is written with one of the terms, the term corresponding to k prime = k separately and the other terms in which k prime is not equal to k. In both cases k prime is not equal to 0 right. So, this is the term corresponding to k prime = k and this is the term it is corresponding to k prime not equal to k.

So, now what were three terms two terms in the first expression appear as three terms because this summation is now separated to right one term explicitly for k prime = k and these are the remaining terms, so these are the three terms now. Let us take these three terms and you notice that this k dot k by k square is nothing but unity because this will give you k square by k square right. Then if you look at this sum over here e to the power 0 is 1.

So, you are adding 1 to itself N times so you will get a factor of the total number of electrons over here okay. Which means that the next time you write this result you can drop this k dot k by k square because it is just multiplying everything by 1. And instead of this factor sum over i going from 1 through N e to the power 0 you can write the total number of electrons. So, let us do that which I have written over here.

I have dropped this factor of unity and I have written N over here so this term becomes -1 over V 4pi Ne square this is the N and this is the e square and this is the m and then this is the

Rho k which is the Fourier component right. And the third term is written just the way as it is okay.
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The slide contains the following content:

$$\ddot{\rho}_{\vec{k}} = -\sum_{i=1}^N (\vec{k} \cdot \dot{\vec{r}}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - \frac{1}{V} \frac{4\pi N e^2}{m} \rho_{\vec{k}}$$

Eq. of motion for density fluctuations

$$\ddot{\rho}_{\vec{k}} = -\sum_{i=1}^N (\vec{k} \cdot \dot{\vec{r}}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - \frac{1}{V} \frac{4\pi e^2}{m} \sum_{\substack{\vec{k}' \neq \vec{k} \\ \vec{k}' \neq 0}} \frac{\vec{k} \cdot \vec{k}'}{k'^2} \rho_{\vec{k}'} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}_i}$$

Now, remember that ↓

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

$$\ddot{\rho}_{\vec{k}} = -\sum_{i=1}^N (\vec{k} \cdot \dot{\vec{r}}_i)^2 e^{-i\vec{k} \cdot \vec{r}_i} - \frac{1}{V} \frac{4\pi N e^2}{m} \rho_{\vec{k}} - \frac{1}{V} \frac{4\pi e^2}{m} \sum_{\substack{\vec{k}' \neq \vec{k} \\ \vec{k}' \neq 0}} \frac{\vec{k} \cdot \vec{k}'}{k'^2} \rho_{\vec{k}'} \left\{ \sum_{i=1}^N e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}_i} \right\}$$

Bye!

NPTEL Questions: pcd@physics.iitm.ac.in PCD STITACS Unit 3 Electron Gas in HF & RPA 177

So, let us take this term now to the top of the next slide which is here all right. What is this? This is the equation of motion for density fluctuations of the Fourier component k. Now this looks a little messy but we will see that it can be really simplified because if you now carry out this summation over i okay, where does i appear? I appear only over here. So, carry out the summation over i, i going from 1 through N.

And then you have got this summation okay, what does it give you? That looks very much like this right. What you have in this beautiful bracket is just a term similar to this except that you have got an argument which is k prime - k and that will give you the Fourier component k - k prime. So, this will Fourier component Rho k and this is the Fourier component Rho k and this will be the Rho k - k prime component right.

Now this is the equation of motion for the Fourier component. This is the second derivative of with respect to time of the Fourier component Rho k. And this has got all of these terms 1, 2, 3. Now this looks messy but we are going to develop an approximation which is the Random Phase Approximation which will help us write this equation in a very simple form. And you can already see what is the most simple form that you can extract from this.

If you were a mathematician and you were looking for what terms look familiar; you have got acceleration on the left hand side and you have got one term on the right hand side which is proportional to the displacement itself which is this term okay. The second time derivative is proportional negative to the displacement Rho right. Now that is the situation you have for a simple harmonic oscillator.

But what you have is not that just that but you have additional terms. Now what if these other terms do not matter if you can find some way of throwing them out, not just because you do not want to solve such a complicated mathematical equation but because there is some good physical reason for it. And in fact as you might begin to suspect there is in fact a good physical reason for this which I will be discussing in the next class.

But what this reason will help you do is to ignore these terms these terms you will be able to ignore because of an approximation which is the Random Phase Approximation. And you will find some additional reason to ignore this term as well and then what you will be left with is the second time derivative of ρ_k which is directly proportional to the displacement ρ_k itself and always directed inward okay.

Which is what you have in a simple harmonic oscillator, so it is just the equation of motion for a simple harmonic oscillator $F = -kx$ for one-dimensional linear harmonic oscillator k is the spring constant, so that is precisely the equation that you will get. So, Bohm Pines found a very good reason to ignore these terms and I will discuss this reason in tomorrow's in the in the next class in some details.

And they found a good reason why this term can be ignored notice that this is the quadratic term okay. There is only a one linear term in ρ over here. There are two terms in ρ , so this term that you are going to ignore is the quadratic term in ρ and the heart of this approximation is this linearization process. The nonlinear term is thrown out, so the heart of the RPA lies in this linearization process.

So, this is the approximation which gets to be known as the Random Phase Approximation and you can already see that the phases in picture are coming from these phases because you have got these exponential functions. So, $e^{i\theta}$, θ is the phase right, so it is the sum of cosine and sine terms and you have got these quadratic terms. So, they will cancel each other because of the cancellation of the random phases.

But I will discuss this in some details in the next class. There is any question on what we have done so far in today's class I will be happy to take it, questions? Essentially what we did was a classical model we have not really not done any quantum theory okay. What we did was the expression of the charge density resolved dated Fourier components.

Found out the position vector of the i th electron, found its velocity found its acceleration okay and using that we set up the equation of motion for the density fluctuations okay. So, it

is a classical model or a semi classical model if you like because we did use the Hamiltonian earlier in some part of the discussion. So, it is like semi classical but mostly classical model we are still using you know the equation of motion.

We are still using Newton's laws $F = ma$, so this is all classical argument but then in the next class we will also get into the quantum method which will also develop by Bohm and Pines. So, if there is any question I will be happy to take otherwise thank you for today and we will meet at the next class.