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DYNAMICAL EFFECTS ON ELECTRON FLUID WITH NON-LOCAL ELECTRON HOLE INTERACTION

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We have calculated the dynamic structure factor by solving the vertex integral equation with the ansatz, that the electron-hole interaction is non-local and has a separable form. Our results are not inconsistent with previous theories and also with experiment. As a further check we have also obtained the plasma dispersion relation. Our model yields reasonable agreement with experimental values of plasma dispersion parameter.

1. Introduction

An important physical observable related to the dielectric response function $\varepsilon(\vec{k}, \omega)$, is the dynamical structure factor $S(\vec{k}, \omega)$, which contains important information about elementary excitations of density fluctuations in the electron system. In recent years there has been renewed interest[1] in the study of the electron gas at metallic densities due to an experimental observation of a double peak structure by Platzman and Eisenberger[2] in the inelastic X-ray scattering experiment in metallic regions which suggests a possible breakdown in the random phase approximation for $S(\vec{k}, \omega)$. An interesting feature of this experimental observation is that there exists a double peak structure in the momentum transfer region $k_F < k < 2k_F$, which is interpreted as the continuation of plasmon excitation in the particle-hole continuum[3], whereas it disappears for $k > 2k_F$. Furthermore this feature persists in a wide range of metals, e. g. C, Be, Al, and indicate the influence of dynamical behaviour of electron gas.

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To obtain $S(\vec{k}, \omega)$, we first determine the dielectric function, $\varepsilon(\vec{k}, \omega)$, by solving the appropriate integral equation for the proper vertex function. In the next section we briefly outline a method to obtain an expression for the frequency and wave-vector dependent dielectric response function. The expression for the local field correction factor, the plasma dispersion and the dynamical structure factor are also given, in the following section. In the final section we report our numerical results and compare them with available experimental results and calculations of other theories.

2. *Evaluation of dielectric and other related functions*

The proper vertex function can be determined through the integral equation[4]

$$\tilde{\Lambda}_k(p) = 1 + \frac{1}{\mathrm{i}} \int \frac{\mathrm{d}^4 p'}{(2\pi)^4} \tilde{I}(p, p') G(p') G(p' + k) \tilde{\Lambda}_k(p')$$

and the dielectric function, $\varepsilon(k)$, in terms of the vertex function can be written as

$$\varepsilon(k) - 1 = \frac{-2V_k}{\mathrm{i}} \int \frac{\mathrm{d}^4 p'}{(2\pi)^4} \tilde{\Lambda}_k(p') G(p') G(p' + k)$$

where $k = (\vec{k}, \omega)$, $p = (\vec{p}, p_0)$, $G(p)$ is the exact propagator for an electron in the state p and $V_k = 4\pi e^2/k^2$ stands for Coulomb interaction. Assuming a static interaction $\tilde{I}(\vec{p}, \vec{p}')$ the above equations can be simplified and we obtain

$$\tilde{\Lambda}_{\vec{k}\omega}(\vec{p}) = 1 - \sum_{\vec{p}'} \tilde{I}(\vec{p}, \vec{p}') g_{\vec{k}\omega}(\vec{p}') \tilde{\Lambda}_{\vec{k}\omega}(\vec{p}') \tag{1}$$

and

$$\varepsilon(\vec{k}, \omega) = 1 + 2V_k \sum_{\vec{p}'} g_{\vec{k}\omega}(\vec{p}') \tilde{\Lambda}_{\vec{k}\omega}(\vec{p}') \tag{2}$$

where

$$g_{\vec{k}\omega}(\vec{p}) = (f_{\vec{p}+\vec{k}} - f_{\vec{p}})/(\omega + \mathrm{i}\eta + \varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{k}}),$$

$$\varepsilon_{\vec{p}} = p^2/2m + \sum_{\vec{p}'} \tilde{I}(\vec{p}, \vec{p}') f_{\vec{p}'}, \tag{3}$$

η is a positive infinitesimal quantity, $f_{\vec{p}}$ is the Fermi function and $\sum_{\vec{p}}$ is shorthand for $(2\pi)^{-3} \int \mathrm{d}^3 p$. The interaction $\tilde{I}(\vec{p}, \vec{p}')$ is chosen as the superposition of non-local separable forms namely

$$\tilde{I}(\vec{p}, \vec{p}') = -4\pi e^2 \left[\frac{\lambda_1^2}{(p^2 + \beta_1^2)(p'^2 + \beta^2)} + \frac{\lambda_2^2}{(p^2 + \beta^2)(p'^2 + \beta_1^2)} \right] \tag{4}$$

where λ_1^2, λ_2^2, β^2 and β_1^2, are the screening parameters which are suitably chosen. Such a non-local form of the interaction could result in the non-relativistic quantum theory if one assumes that in the coordinate space the free Green's function for the associated scattering problem is dominated by the contribution from two intermediate states only. Then it would yield superposition of non-local forms. The use of non-local potential in quantum mechanical systems is not new[5] and has been used in many branches in connection with scattering problems in nuclear and solid state physics[6]. An important outcome of using this non-local separable form for $\vec{I}(\vec{p}, \vec{p}')$ is to make the local field correction factor ω dependent. Using Eq. (4) in Eq. (1), the expression for the dielectric function, $\varepsilon(\vec{k}, \omega)$, becomes

$$\varepsilon(\vec{k}, \omega) = 1 + 2V_k I_1 + f(\vec{k}, \omega) \tag{5}$$

where

$$f(\vec{k}, \omega) = \frac{1}{\Delta} \{2V_k 4\pi e^2 (\lambda_1^2 + \lambda_2^2) I_2(\beta) I_4(\beta_1) +$$

$$+ 2V_k (4\pi e^2)^2 \lambda_1^2 \lambda_2^2 [I_4^2(\beta_1) I_3(\beta) + I_2^2(\beta) I_5(\beta_1)]\} + \tag{6}$$

$$+ 4V_k (4\pi e^2)^2 \frac{\lambda_1^2 \lambda_2^2}{(\beta^2 - \beta_1^2)} [I_2^2(\beta) I_4(\beta_1) - I_4^2(\beta_1) I_2(\beta)]\}$$

$$\Delta = \begin{vmatrix} 1 - \dfrac{4\pi e^2 \lambda_1^2}{(\beta^2 - \beta_1^2)} [I_4(\beta_1) - I_2(\beta)] & -4\pi e^2 \lambda_2^2 I_3(\beta) \\ -4\pi e^2 \lambda_1^2 I_5(\beta_1) & 1 - \dfrac{4\pi e^2 \lambda_2^2}{(\beta^2 - \beta_1^2)} [I_4(\beta_1) - I_2(\beta)] \end{vmatrix}$$

$$\Delta \neq 0$$

and

$$I_1 = \int \frac{d^3 p'}{(2\pi)^3} g_{\vec{k}\omega}(\vec{p}'). \tag{7}$$

The Lindhard polarizability $Q_0(\vec{k}, \omega)$ can be identified in terms of I_1 as

$$Q_0(\vec{k}, \omega) = 2V_k I_1. \tag{8}$$

The expression for $I_2(\beta)$ and $I_4(\beta_1)$ have the following form:

$$I(x) = \int \frac{d^3 p'}{(2\pi)^3} \frac{g_{\vec{k}\omega}(p')}{(p'^2 + x^2)} \tag{9}$$

while $I_3(\beta)$ and $I_5(\beta_1)$ stand for $-\dfrac{d}{dx^2} I(x)$ with $x = \beta$ and β_1, respectively.

In performing integrals I_1 and $I(x)$, we consider the Fermi distribution function at $T = 0$, and use as a first approximation $p^2/2m$ for $\varepsilon_{\vec{p}}$ and write for $g_{\vec{k}\omega}(\vec{p})$:

$$g_{\vec{k}\omega}(\vec{p}) = \frac{(f_{\vec{p}+\vec{k}} - f_{\vec{p}})}{\left[\frac{p^2}{2m} - \frac{(\vec{p}+\vec{k})^2}{2m} + \omega + i\eta\right]}. \tag{10}$$

The values of these integrals have been given in our earlier paper[7]. We also note that the proper vertex function, $\tilde{\Lambda}_{\vec{k}\omega}(\vec{p})$, satisfies the Ward identity relation[8]:

$$\lim_{\omega\to 0}\left[\lim_{\vec{k}\to 0}\tilde{\Lambda}(\vec{p})\right] = Z_{\vec{p}}^{-1} \tag{11}$$

where Z_p is the wave function renormalization constant. In the static limit Z_p tends to unity for all $\vec{p}$. Thus in this limit the Ward identity relation Eq. (11) becomes:

$$\lim_{\omega\to 0}\left[\lim_{k\to 0}\tilde{\Lambda}_{\vec{k}\omega}(\vec{p})\right] = 1 \text{ for all } \vec{p}. \tag{12}$$

This condition is satisfied in our model.

By comparing with the expression for the dielectric function, in terms of $Q_0(\vec{k}, \omega)$ and local field correction factor, $G(\vec{k}, \omega)$

$$\varepsilon(\vec{k}, \omega) = 1 + \frac{Q_0(\vec{k}, \omega)}{[1 - G(\vec{k}, \omega)\, Q_0(\vec{k}, \omega)]} \tag{13}$$

the frequency dependent local field correction factor, $G(k, \omega)$, in the present model is given as

$$G(k, \omega) = \frac{f(\vec{k}, \omega)}{Q_0(\vec{k}, \omega)\,[Q_0(\vec{k}, \omega) + f(\vec{k}, \omega)]}. \tag{14}$$

We find that in the limit $\vec{k} \to \infty$, the frequency independent local field correction factor has the form:

$$\lim_{\vec{k}\to\infty} G(\vec{k}, 0) = \frac{(\lambda_1^2 + \lambda_2^2)}{\beta^2} \quad \frac{2}{9}. \tag{15}$$

Niklasson[9] and Kimball[10] have shown that the pair distribution function at small interparticle distances is related to the static structure factor $S(\vec{k})$ at large $\vec{k}$ limit by

$$g(0) = -\frac{a_0}{8\pi n}\lim_{\vec{k}\to\infty} k^4\,[S(\vec{k}) - 1] \tag{16}$$

where a_0 is the Bohr radius and n is the electron density. The static structure factor is given as a frequency integral of the inverse dielectric function[11]. Assuming $G(\vec{k}, \omega)$ to be frequency independent ($\omega = 0$ in Eq. (14)) in the expression for $[\varepsilon(\vec{k}, \omega)]^{-1}$ we can solve for the structure factor $S(\vec{k})$ and in the limit $\vec{k} \to \infty$, obtain:

$$g(0) = -\frac{a_0}{8\pi n} \lim_{\vec{k}\to\infty} k^4 [S(\vec{k}) - 1] = 1 - \frac{(\lambda_1^2 + \lambda_2^2)}{\beta^2} \cdot \frac{2}{9} = 1 - \lim_{\vec{k}\to\infty} G(\vec{k}, 0) \quad (17)$$

a relationship in agreement with Kimball.

The collective plasma mode in the electron gas can be found from the vanishing of the real part of the dielectric function. The required plasma dispersion in the long wavelength limit $\vec{k} \to 0$, becomes:

$$\omega_p(\vec{k}) = \omega_p(0) \left\{1 + \frac{k^2}{k_{TF}^2}\left[\frac{9}{10} - \frac{(\lambda_1^2 + \lambda_2^2)}{4\beta^2\delta^2} k_{TF}^2\right] + \ldots\right\} \quad (18)$$

$\omega_p(0)$ being the plasma frequency, $\omega_p(0) = \sqrt{\frac{4\pi n e^2}{m}}$ and $k_{TF}^2 = \frac{3\omega_p^2(0)}{v_F^2}$.

If the plasma frequency is written as

$$\omega_p(\vec{k}) = \omega_p(0) + \tilde{\beta} k^2 \quad (19)$$

then the ratio $\beta/\tilde{\beta}_{RPA}$ of the dispersion parameter becomes:

$$\tilde{\beta}/\tilde{\beta}_{RPA} = 1 - \frac{5}{9} \cdot \frac{(\lambda_1^2 + \lambda_2^2)}{\beta^2\delta^2} \cdot \frac{k_{TF}^2}{2} \quad (20)$$

where δ^2 is the value of β_1^2 at $k^2 = 0$ and $\tilde{\beta}_{RPA}$ is obtained from Eqs. (18) and (19) by dropping the $(\lambda_1^2 + \lambda_2^2)$ — dependent terms.

An easily calculable expression for the dynamic structure factor, $S(\vec{k}, \omega)$, can be obtained in our model using the complex nature of $Q_0(\vec{k}, \omega)$ and $G(\vec{k}, \omega)$ and the expression relating $S(\vec{k}, \omega)$ to the inverse of dielectric function (11), such that

$$S(\vec{k}, \omega) = \frac{\hbar k^2}{4\pi^2 e^2 n} \left\{\frac{\operatorname{Im} Q_0(\vec{k}, \omega) + [(\operatorname{Re} Q_0(\vec{k}, \omega))^2 + (\operatorname{Im} Q_0(\vec{k}, \omega))^2] \operatorname{Im} G(\vec{k}, \omega)}{(J(\vec{k}, \omega))^2 + (M(\vec{k}, \omega))^2}\right\} \quad (21)$$

where

$$J(\vec{k}, \omega) = 1 + \operatorname{Re} Q_0(\vec{k}, \omega) +$$

$$+ \operatorname{Im} Q_0(\vec{k}, \omega) \operatorname{Im} G(\vec{k}, \omega) - \operatorname{Re} Q_0(\vec{k}, \omega) \operatorname{Re} G(\vec{k}, \omega)$$

and

$$M(\vec{k}, \omega) = \text{Im}\, Q_0(\vec{k}, \omega) - \text{Re}\, Q_0(\vec{k}, \omega)\, \text{Im}\, G(\vec{k}, \omega) -$$

$$- \text{Im}\, Q_0(\vec{k}, \omega)\, \text{Re}\, G(\vec{k}, \omega).$$

In the next section we discuss and give the numerical results of the above quantities.

3. *Discussion*

In order to calculate the various quantities of interest, related to $\varepsilon(\vec{k}, \omega)$, we must know the values of the screening parameters λ_1^2, λ_2^2, β^2 and β_1^2. We choose the parameters λ_1^2, λ_2^2 and β^2 by making use of relation given by Eq. (17). For this we use $r_s \left[r_s = \left(\frac{4\pi n a_0^3}{3} \right)^{-1/3} \right]$ dependent values of $g(0)$ as given by Zabolitz-

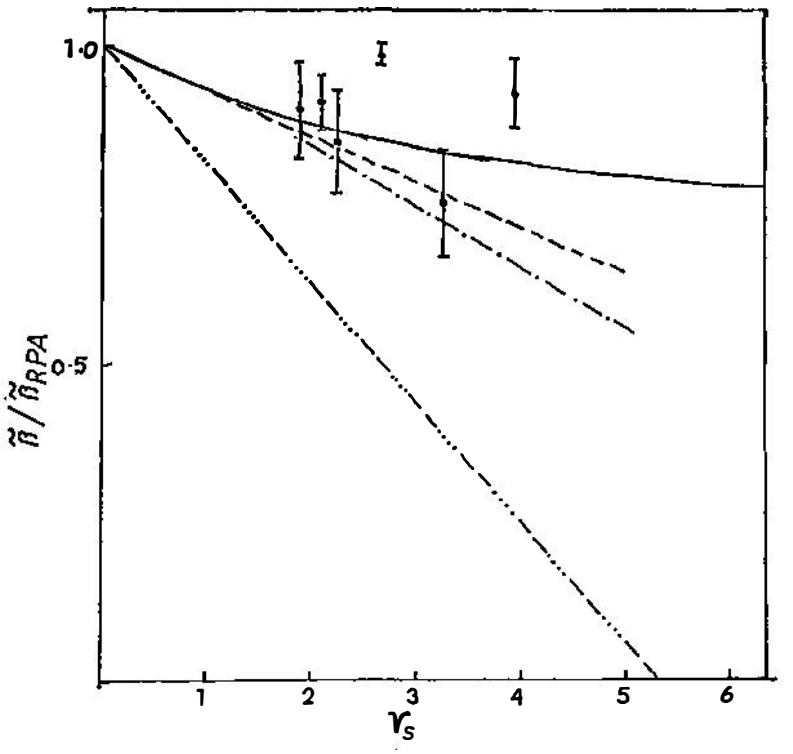

Fig. 1. Variation of dispersion parameter ratio, $\tilde{\beta}/\tilde{\beta}_{RPA}$, with metallic electron densities represented by r_s, as given by experimental results of Raether and various theories. --- Vashishta and Singwi; -·- Rajagopal, Rath and Kimball; --·····-- Hubbard; ——— Present model calculations.

ky[12]. It may be pointed out that the value of the pair distribution function $g(r)$ due to Zabolitzky are in good agreement with Monte Carlo data on $g(r)$ obtained by Ceperley[13] for $r_s = 1, 3, 5$. A choice of $\lambda_1^2 = a(k_F^2 + k_{TF}^2)$, $\lambda_2^2 = 2.5\, k_{TF}^2$ and $\beta^2 = b(k_F^2 + k_{TF}^2)$ with the values $a = 1.61$ and $b = 0.82$, gives a good fit to Zabolitzky results of $g(0)$ at various metallic densities. k_F^2 and k_{TF}^2 are r_s dependent, $k_F = 1/\alpha r_s a_0$, $a = 0.52$. Making use of the above mentioned values of λ_1^2, λ_2^2, β^2 and $\beta_1^2 = k^2 + 4(k_F^2 + k_{TF}^2)$, the calculated values of $\tilde{\beta}/\tilde{\beta}_{RPA}$, given by Eq. (20) yield result which are in good agreement with experimental data[14], at various metallic densities. In Fig. 1 we have presented our calculated values of the plasma dispersion ratio $\tilde{\beta}/\tilde{\beta}_{RPA}$, and compared them with the experimental data and other theoretical calculations[15-17]. In Fig. 2, we have plotted the variation of $G(\vec{k}, \omega = 0)$ with k (k expressed in units of k_F) and compared with other theoretical studies[15-19]. We observe a peak in the evaluated values of $G(\vec{k}, \omega = 0)$ at $k = 2k_F$, similar to the ones predicted by the theories of Toigo and Woodruff[18] and Brosens et al.[19], who obtain a frequency dependent local field correction factor.

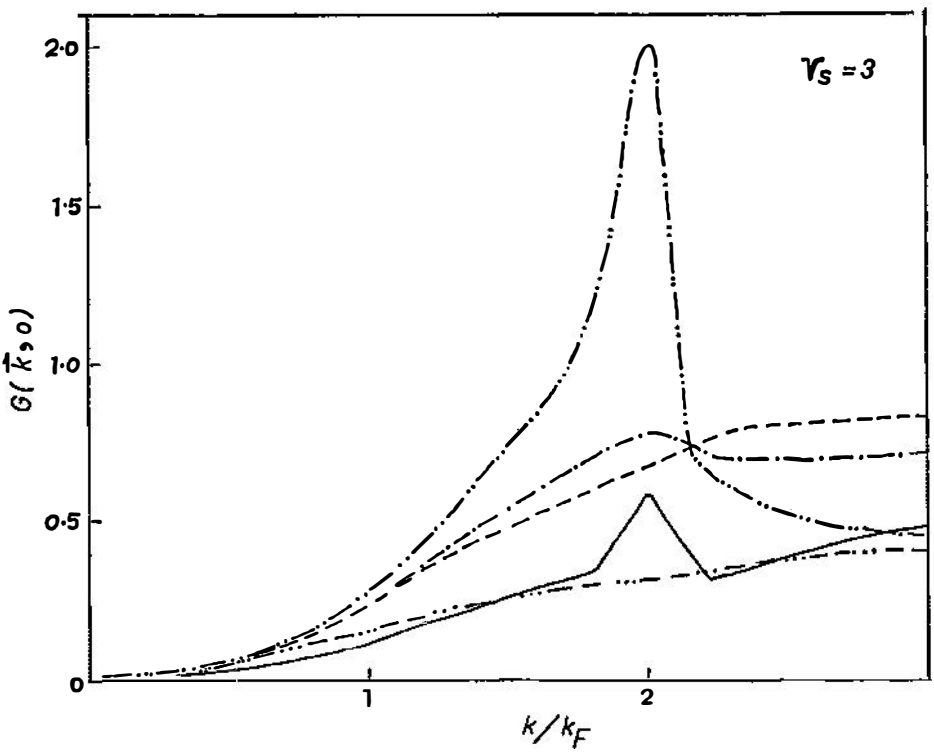

Fig. 2. Local field correction factor $G(\vec{k}, 0)$, for $r_s = 3$, as given by various theories. --- Vashishta and Singwi; -·- Toigo and Woodruff; -·-·- Brosens et al.; --·····-- Hubbard; —— Present model calculations.

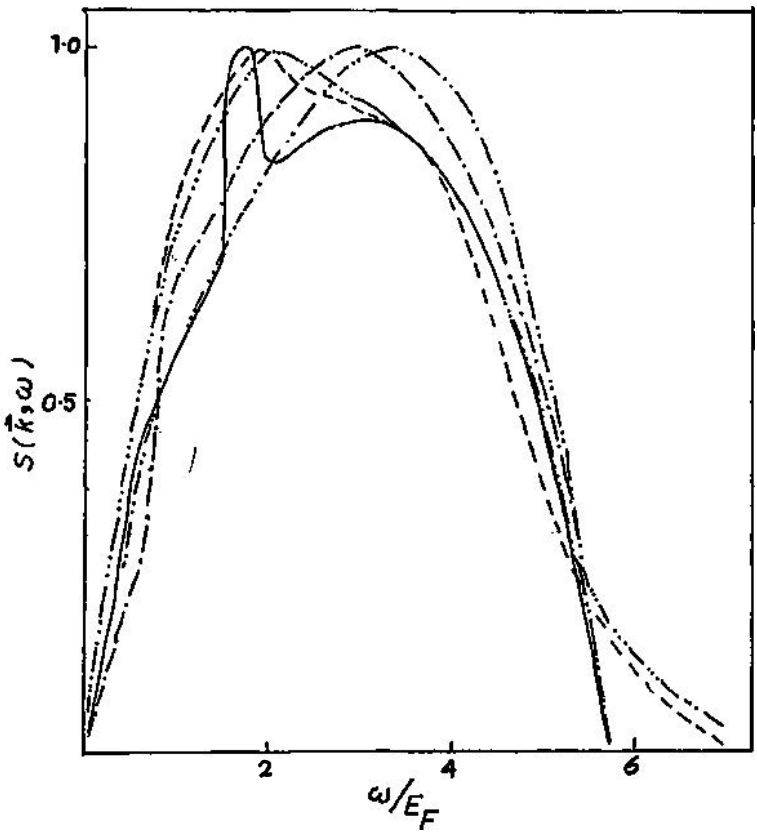

Fig. 3. $S(k, \omega)$ for $r_s = 2$ and $k = 1.6\ k_F$. --- experimental data for Platzman and Eisenberger; - · · · - Mukhopadhyay et al.; - · - RPA; —— Present model calculations; - · - Vashishta and Singwi.

In Fig. 3, we have shown the variation of $S(\vec{k}, \omega)$ with ω, for value of the wave-vector $k = 1.6\ k_F$ for $r_s = 2$ and compared with the experimental graph obtained by Platzman and Eisenberger[2] and other theories[3,15]. The $S(\vec{k}, \omega)$ obtained from $\varepsilon_{RPA}(\vec{k}, \omega)$ does not show any double peak structure. On the other hand the $S(\vec{k}, \omega)$ that we obtain shows a double peak structure which appears to be a consequence of the dynamical nature of the local field correction factor. One part of the excitation spectrum is broad and it corresponds to the particle--hole continuation of the plasmon spectrum in the particle-hole continuum. In Fig. 4 we notice that for large values of wave vector, for eg. $k = 2.6\ k_F$ there no longer is a double peak and the particle-hole excitations dominate. We have also compared the dynamic structure factor for Al ($r_s = 2$) at wave vector $k = 1.8\ k_F$ with the theoretical curve obtained by Awa et al.[10] and observe the qualitative agreement of both curves.

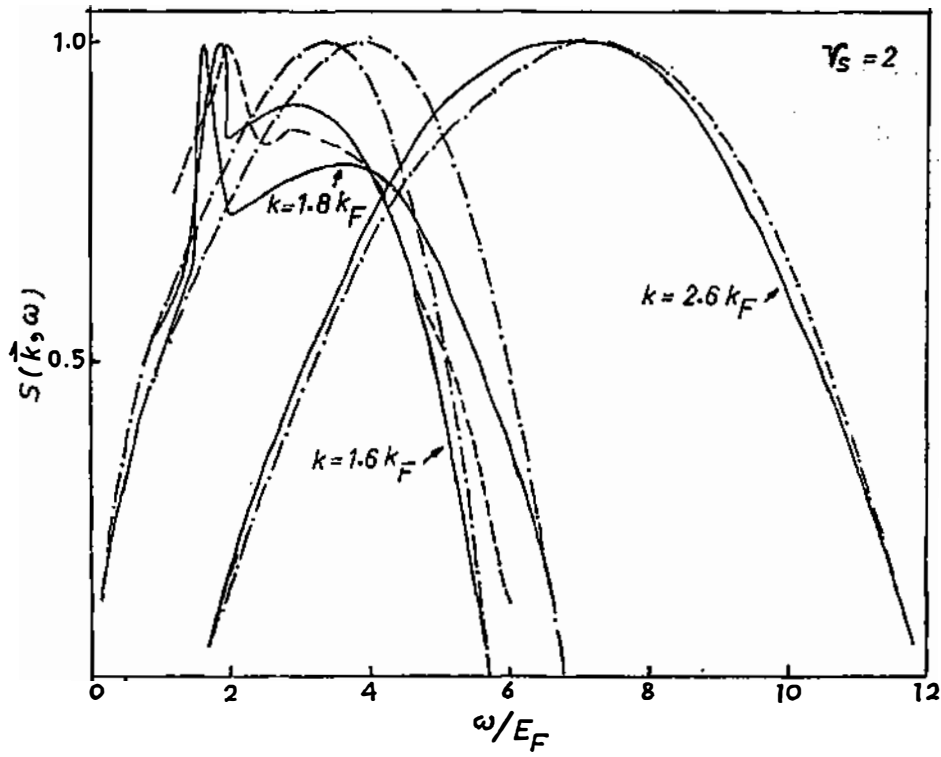

Fig. 4. $S(\vec{k}, \omega)$ for $r_s = 2$ and $k = 1.6\,k_F$, $1.8\,k_F$, $2.0\,k_F$. —— Present model calculations; -·- RPA; --- Awa et al.

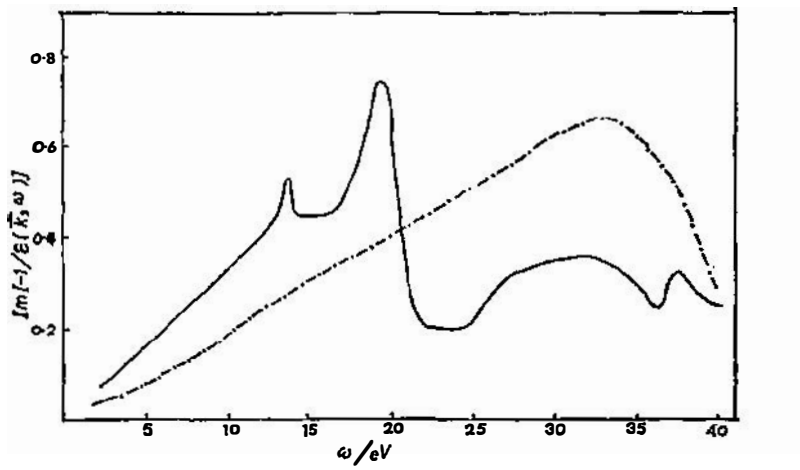

Fig. 5. Variation of Im $(-1/\varepsilon(\vec{k}, \omega))$ with ω, at $k = 1.14\,k_F$. —— Present model calculation; ---RPA.

Another interesting problem which has been of interest, is the study of energy loss spectra as a function of frequency, ω [20], which gives a measure of the influence of correlations between electrons. In Fig. 5 we have plotted the energy loss function $\mathrm{Im}\,(-1/\varepsilon\,(\vec{k}, \omega))$ for Al ($r_s = 2$) as a function of ω at a constant $k = 1.14\,k_F$. We note the presence of energy loss peaks at 13.6, 19.6, 31. 4 and 37.8 eV which cover the plasmon resonance range. Of the sum rules [21] which provide a check on the consistency of a given theory in the electron gas, two of them, the f-sum rule, that is

$$\int_0^\infty \omega\, S\,(\vec{k}, \omega)\, \mathrm{d}\omega = \frac{nk^2}{2m}$$

and the conductivity sum rule

$$\int_0^\infty \omega\, S\,(\vec{k}, \omega)\, |\varepsilon\,(\vec{k}, \omega)|^2\, \mathrm{d}\omega = \frac{nk^2}{2m}$$

are well satisfied in our model. The perfect screening sum rule, that is

$$\lim_{\vec{k}\to 0} \int_0^\infty \frac{S\,(\vec{k}, \omega)}{\omega}\, \mathrm{d}\omega = k^2/8\pi e^2$$

and the compressibility sum rule

$$\lim_{\vec{k}\to 0} \int_0^\infty \frac{S\,(\vec{k}, \omega)}{\omega}\, |\varepsilon\,(\vec{k}, \omega)|^2\, \mathrm{d}\omega = \frac{n}{2ms^2}$$

where s is the isothermal sound velocity in the electron gas, are not satisfied in our model. Our model therefore suffers from these difficulties.

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DINAMIČKI EFEKTI U ELEKTRONSKOM FLUIDU S NELOKALNOM INTERAKCIJOM ELEKTRON-ŠUPLJINA

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Pretpostavljajući da je interakcija elektron-šupljina nelokalna i separabilnog oblika, proračunat je dinamički strukturni faktor rješavanjem integralne jednadžbe. Dobiveni rezultati konzistentni su s ranijim teorijama i s eksperimentima. Izračunata disperziona relacija plazme pokazuje zadovoljavajuće slaganje s eksperimentalno utvrđenim vrijednostima.