Dynamic Structure Factor of an Electron Liquid*

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(Received 4 September 1974; revised manuscript received 17 March 1975)

It is shown that the recently observed interesting but somewhat unexpected features of the dynamic structure factor of an electron liquid can be understood on the basis of a simple modification of the theory of the dielectric response function of Vashishta and Singwi.

Recent inelastic x-ray and electron scattering experiments,[1-3] particularly those of Platzman and Eisenberger,[3] have revealed some very interesting features of the dynamical structure factor $S(\vec{q}, \omega)$ of the electron liquid in metals. Broadly speaking, these features are the following: (1) Contrary to what one might expect in the momentum-transfer region $q_F < q < 2q_F$, where q_F is the Fermi momentum, the excitation spectrum is comprised of two parts; one part is broad and corresponds to particle-hole excitations and the other is relatively sharper and has been interpreted as the continuation of the plasmon excitation in the particle-hole continuum. For $q < 2q_F$, the latter has larger strength than the former, and at $q \simeq 2q_F$, there occurs a switching over of the two strengths. For $q > 2q_F$, one observes only a single broad peak corresponding to free-particle excitations. (2) Surprisingly enough, the plasmon peak in the entire region $q_c < q < 2q_F$, where q_c is the critical wave vector at which the plasmon joins the particle-hole continuum, shows no dispersion.[1,2] Platzman and Eisenberger have even observed a small negative dispersion in the region $q_F < q < 2q_F$.

A very significant observation of Platzman and Eisenberger is that the above-mentioned features are common to such diverse systems as C, Be, and Al, thereby indicating that these features are not the result of simple one-electron properties of these metals, but are indeed the manifestations of the dynamical behavior of the electron gas. It is this aspect that renders the problem so interesting from a many-body theoretical point of view, and which shall mainly concern us here.

It has recently been pointed out by Kalia and Mukhopadhyay,[4] among others,[2,3] that the observed $S(\vec{q}, \omega)$ in the region $q_c < q < 2q_F$ cannot be understood in terms of the random-phase approximation (RPA). Nor can it be understood in terms of the dielectric response function of Vashishta and Singwi[5] (hereafter referred to as VS), which has otherwise been found to be very satisfactory in calculating various static properties.

The VS scheme goes beyond the RPA by introducing local-field effects which are incorporated in their function $G(q)$. This function is real and static. That the short-range correlations among electrons are properly taken into account in the original theory of Singwi *et al.*[6] has now been shown by several authors[7] using diagrammatic techniques. One important ingredient which is still missing in the VS theory is that the electrons and holes have a finite lifetime. This effect is not taken into account when one chooses a real local-field factor. We propose here to take this effect into account and work out its consequences. The modification of the VS theory, therefore, consists in adding to the free-particle energy $\epsilon(\vec{p})$, occurring in the energy denominators of the Lindhard function $\chi_0(\vec{q}, \omega)$, a term $i/\tau(\vec{p})$, where $\tau^{-1}(p)$ is given by the imaginary part of the self-energy $\Sigma(\vec{p}, \epsilon(\vec{p}))$. The latter, following Hedin,[8] has been calculated in the lowest-order approximation and evaluated at the free-particle energy $\epsilon(\vec{p})$. The real part of $\Sigma(\vec{p}, \epsilon(\vec{p}))$ is already contained in the local-field factor $G(q)$ in an average fashion. Through the above procedure, the f-sum rule is preserved. The response function $\chi(\vec{q}, \omega)$ in the VS theory is

$$\chi(\vec{q}, \omega) = \frac{\chi_0(\vec{q}, \omega)}{1 - (4\pi e^2/q^2)[1 - G(q)]\chi_0(\vec{q}, \omega)}. \quad (1)$$

$G(q)$ has been tabulated by VS for various values of r_s. $\chi_0(\vec{q}, \omega)$ in Eq. (1) should now contain the modification discussed above. The expression for the self-energy in the lowest-order approximation is

$$\Sigma(\vec{p}, \omega) = i \iint \frac{d^3q\, d\omega'}{(2\pi)^4} \frac{4\pi e^2}{q^2 \epsilon_{VS}(\vec{q}, \omega')} \times G_0(\vec{p} - \vec{q}, \omega - \omega') \exp(-i\delta_{\omega'}), \quad (2)$$

where G_0 is the free-particle Green's function and δ is a positive infinitesimal. $\epsilon_{VS}(\vec{q}, \omega)$ is the dielectric function of Vashishta and Singwi.[5] $S(\vec{q},$

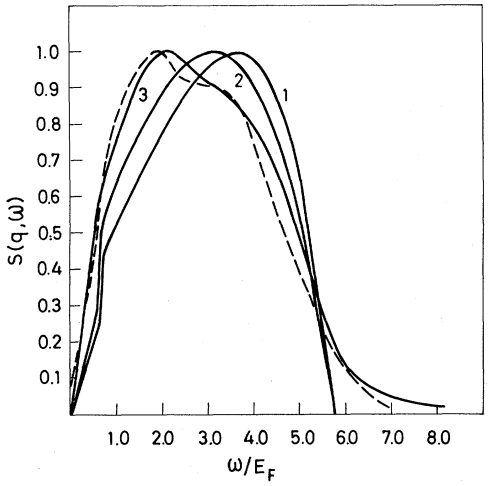

FIG. 1. $S(q,\omega)$ versus ω/E_F for $q/q_F = 1.6$ for Al. Peak heights of all curves have been normalized to unity. Curve 1, RPA; curve 2, VS theory; curve 3, modified VS theory. The dashed curve represents experimental data of Platzman and Eisenberger (Ref. 3).

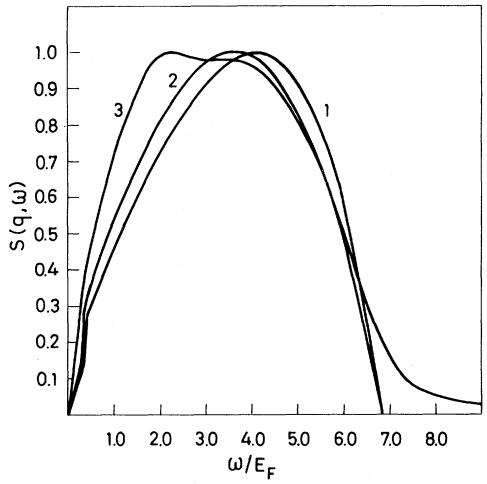

FIG. 2. $S(q,\omega)$ versus ω/E_F for $q/q_F = 1.8$ for Al. Peak heights of all curves have been normalized to unity. Curve 1, RPA; curve 2, VS theory; curve 3, modified VS theory.

ω) is related to the imaginary part $\chi''(\vec{q},\omega)$, through

$$S(\vec{q},\omega) = -(n\pi)^{-1}\chi''(\vec{q},\omega), \quad \omega > 0, \qquad = 0, \quad \omega < 0, \tag{3}$$

n being the electron density.

Numerical calculations, although tedious, are straightforward. Calculation of $S(\vec{q},\omega)$ was performed for Al ($r_s = 2.0$) for several different values of q, in the interval $q_c < q < 2.5q_F$. Calculated line shapes (curves 3) for three typical values of $q/q_F = 1.6$, 1.8, and 2.0 are shown, respectively, in Figs. 1, 2, and 3. For comparison, we have also shown the line shapes as calculated using the RPA (curves 1) and the unmodified VS scheme (curves 2). Peak heights of all curves have been normalized to unity. In these figures there are several points to note: (1) Curves 1 and 2 show no evidence of any structure—in fact they show no structure for any of the q's investigated. (2) The maximum of curve 2 is shifted to the lower-energy side relative to the maximum of curve 1. This shift is not small and for some q ($\approx 1.3q_F$) it is as large as 5 eV; it is entirely due to the local-field correction $G(q)$. (3) In curve 3, one can discern the presence of a well-developed shoulder, thereby indicating the presence of two peaks—one broad and the other relatively sharper. (4) For $q/q_F = 1.6$, the shoulder occurs at $\omega/E_F = 3.3$ and lies to the right of the peak at $\omega/E_F = 2.1$. The dashed curve in Fig. 1 is taken from the recent work of Platzman and Eisenberger[3] and is fairly close to the calculated curve. (5) For $q/q_F = 1.8$, although the peak still lies around $\omega/E_F = 2.2$, its strength has now diminished relative to its strength for $q/q_F = 1.6$, the ratio of their strengths being 0.86. In fact for $q/q_F = 1.8$, both the peak and the shoulder are

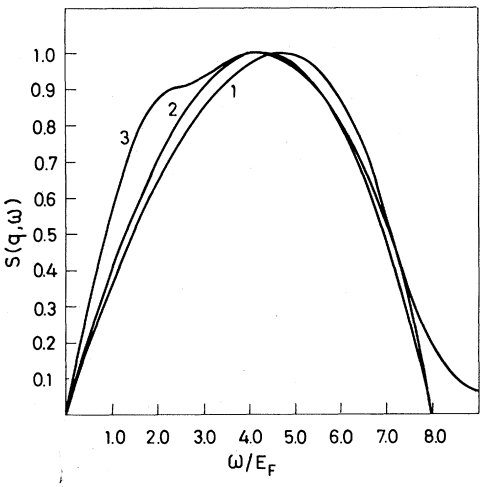

FIG. 3. $S(q,\omega)$ versus ω/E_F for $q/q_F = 2.0$ for Al. Peak heights of all curves have been normalized to unity. Curve 1, RPA; curve 2, VS theory; curve 3, modified theory.

almost of equal strength. (6) At $q/q_F = 2.0$, one notes a switching over of the two strengths. (7) For $q > 2q_F$ (not shown in figures), the plasmon peak diminishes in strength but continues to occur at nearly the same position, and finally at $q = 2.5q_F$ it is completely swallowed by the broad particle-hole excitation peak. The peak position now lies at the recoil energy $q^2/2m$ and the excitations are free-particle-like. The calculated area under the peak, i.e., $S(q)$, is nearly equal to unity.

Our calculations thus reveal the presence of a plasmon band in the region $q_c < q < 2q_F$, where it would not exist in the RPA. They also reveal the unexpected feature that the plasmon shows no dispersion in such a wide range of q values. This result is in accord with the observations of Miliotis[1] for Be ($r_s = 1.87$) and those of Zacharias[2] for Al ($r_s = 2.0$), and with the more recent result of Eisenberger *et al.*[9] on Li. It is somewhat at variance with the observations of Platzman and Eisenberger[3] on Be, Al, and C in the sense that these authors have observed a small negative dispersion in the range $q_F < q < 2q_F$. Also for Be (along the A axis) and for $q = 1.76q_F$, they observe a distinct separation of the two peaks, which we do not find in Al. This discrepancy could possibly be due to the periodicity of the lattice or to something lacking in the theory or to both.

We have thus shown that it is possible to understand the main but somewhat unexpected features of $S(\vec{q}, \omega)$ on the basis of a simple modification of the VS theory; and it is, therefore, not necessary to invoke[3] the presence of an incipient Wigner lattice at metallic densities. The theory has its defects too. In its present form it violates the continuity equation. Nevertheless, we believe that the essential new physics is taken care of by the theory.

We have just completed calculations of $S(\vec{q}, \omega)$ for sodium ($r_s = 4$), and we find results quite similar to those for Al ($r_s = 2$) except that the structure in $S(\vec{q}, \omega)$ in the former is somewhat more marked. This was expected because of stronger electron-electron correlations at low densities. Our calculations thus seem to support the conclusion[9] that the observed features of $S(q, \omega)$ have a universal character.

We are thankful to Alf Sjölander, Stig Lundqvist, and Lars Hedin for many stimulating discussions. One of us (K.S.S.) would like to thank P. Zacharias and H. Raether for discussion concerning the experimental aspects of the problem.

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*Work partly supported by the Advanced Research Projects Agency of the Department of Defense through the Northwestern University Materials Research Center and by the National Science Foundation under Grant No. GH-39127.

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