Calculation of the Dielectric Function for a Degenerate Electron Gas with Interaction. II. Frequency Dependence*

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Starting from an expression for the dielectric function earlier derived, we calculate explicitly the ω dependence of the $G(k, \omega)$ function which describes correlation and exchange effects. The full frequency dependence of this function is found to be rather significant; in particular it improves the accuracy with which the f sum rule is satisfied, which confirms the goodness of the approximations involved in the calculation of the dielectric function.

I. INTRODUCTION

In a previous paper,[1] hereafter referred to as I, a formula for the wave-vector- and frequency-dependent dielectric function was obtained by a moment-conserving decoupling procedure which had the effect of enforcing the f sum rule on $\epsilon(k, \omega)$. The $\epsilon(k, \omega)$ obtained was of the Hubbard[2] form

$$\epsilon(k, \omega) = 1 + \frac{Q_0(k, \omega)}{1 - G(k, \omega) Q_0(k, \omega)} , \tag{1.1}$$

where $Q_0(k, \omega)$ is the usual Lindhard function and $G(k, \omega)$ is a function which includes electron self-energy and exchange effects. It is apparent that a complete knowledge of $G(k, \omega)$ is required for a complete knowledge of the properties of the system. In this note we extend I by calculating the ω dependence of $G(k, \omega)$, which was previously neglected ("static limit"), and we show, in fact, that the ω dependence is rather strong and has important effects.

II. CALCULATIONS

We start from Eq. (3.5) of I, noticing that the function $P_0(k, \omega)$ defined there can be written as

$$P_0(k, \omega) = 3(\alpha r_s/\pi k^2)(2\pi)^4 T(k, \omega) , \tag{2.1}$$

where $\alpha = (4/9\pi)^{1/3}$, r_s is the usual parameter related to the density of the electron gas, k is in units of the Fermi wave vector (k_F), the frequencies are in units of the Fermi frequency, and

$$T(k, \omega) = \sum_{\vec{q}_1, \vec{q}_2} v_{\vec{q}_1 - \vec{q}_2} \frac{\omega(\vec{q}_1, \vec{k}) - \omega(\vec{q}_2, \vec{k})}{\omega - \omega(\vec{q}_1, \vec{k}) + i\delta} \times (n_{\vec{q}_1 + \vec{k}} - n_{\vec{q}_1})(n_{\vec{q}_2} - n_{\vec{q}_2 + \vec{k}}) , \tag{2.2}$$

with $\omega(\vec{q}, \vec{k}) = (\vec{q} + \vec{k})^2 - q^2$ and $v_{\vec{q}_1 - \vec{q}_2} = 1/|\vec{q}_1 - \vec{q}_2|^2$. Also, $n_{\vec{q}}$ is the Fermi distribution function, which, for the case of the completely degenerate electron gas under consideration is the unit-step function.

The summation over $\vec{q}_2$ is easily performed analytically to give

$$T(k, \omega) = \frac{1}{(2\pi)^2} \sum_{\vec{q}} (n_{\vec{q} + \vec{k}} - n_{\vec{q}}) \frac{F(\vec{q} + \vec{k}, \vec{k}) - F(\vec{q}, \vec{k})}{\omega - \omega(\vec{q}, \vec{k}) + i\delta} , \tag{2.3}$$

with

$$F(\vec{p}, \vec{k}) = \frac{\vec{p} \cdot \vec{k}}{p^2} \left(\frac{1 + p^2}{4} + \frac{(1 - p^2)^2}{8p} \ln \left| \frac{1 - p}{1 + p} \right| \right) . \tag{2.4}$$

Exploiting the symmetry properties of $F(\vec{p}, \vec{k})$ and $\omega(\vec{p}, \vec{k})$,

$$\begin{aligned} F(\vec{p}, \vec{k}) &= -F(-\vec{p}, \vec{k}) , \\ \omega(\vec{p}, \vec{k}) &= -\omega(-\vec{p} - \vec{k}, \vec{k}) , \end{aligned} \tag{2.5}$$

we easily see that Eq. (2.3) may be rewritten as

$$T(k, \omega) = \frac{1}{(2\pi)^2} \sum_{\vec{q}} n_{\vec{q}} [F(\vec{q} + \vec{k}, \vec{k}) - F(\vec{q}, \vec{k})] \times \left(\frac{1}{\omega + \omega(\vec{q}, \vec{k}) + i\delta} - \frac{1}{\omega - \omega(\vec{q}, \vec{k}) + i\delta} \right) . \tag{2.6}$$

At this point we change the sum into an integral and make use of the relation

$$\frac{1}{x + i\delta} = P\left(\frac{1}{x}\right) - i\pi\delta(x) \tag{2.7}$$

to separate $T(k, \omega)$ into its real and imaginary parts $T_1(k, \omega)$ and $T_2(k, \omega)$. The symbol P implies a principal-value integration of the Cauchy type.

We first consider the real part

$$T_1(k, \omega) = \frac{1}{(2\pi)^4} \int_0^1 q^2 \, dq \int_{-1}^1 dx \, F(\vec{q} + \vec{k}, \vec{k}) \left(\frac{1}{\omega + \omega(\vec{q}, \vec{k})} - \frac{1}{\omega - \omega(\vec{q}, \vec{k})} \right)$$

$$-\frac{1}{(2\pi)^4}\int_0^1 q^2\,dq\int_{-1}^1 dx\,F(\vec{q},\vec{k})\left(\frac{1}{\omega+\omega(q,k)}-\frac{1}{\omega-\omega(q,k)}\right), \qquad (2.8)$$

where

$$x=(\vec{q}+\vec{k})\cdot\vec{k}/|\vec{q}+\vec{k}|k \text{ or } x=\vec{q}\cdot\vec{k}/qk\ .$$

Changing the variables of integration in the first term on the right-hand side of Eq. (2.8) to

$$p=(q^2+k^2+2qkx)^{1/2}\ ,\quad z=-(k+qx)/(q^2+k^2+2qkx)^{1/2}\ , \qquad (2.9)$$

and noticing that this corresponds to $\vec{q}+\vec{k}=-\vec{p}$ we can write

$$T_1(k,\omega)=\frac{1}{(2\pi)^4}\left[\int_0^1\int_{-1}^1 q^2\,dq\,dx\,F(\vec{q},\vec{k})\left(\frac{1}{\omega-\omega(\vec{q},\vec{k})}-\frac{1}{\omega+\omega(\vec{q},\vec{k})}\right)\right.$$
$$\left.-\iint_D p^2\,dp\,dz\,F(\vec{p},\vec{k})\left(\frac{1}{\omega-\omega(\vec{p},\vec{k})}-\frac{1}{\omega+\omega(\vec{p},\vec{k})}\right)\right], \qquad (2.10)$$

where the domain of integration D is defined by the following conditions:

$$\begin{aligned} &k<1\ , && 0<p<1-k, && -1<z<1\ ,\\ &&& 1-k<p<1+k, && -1<z<(1-p^2-k^2)/2pk\ ;\\ &k>1, && k-1<p<k+1, && -1<z<(1-p^2-k^2)/2pk\ . \end{aligned} \qquad (2.11)$$

The x and z integrations can now be performed analytically to give finally

$$T_1(k,\omega)=\frac{1}{(2\pi)^4}\left[\int_{1-k}^{1+k} dq\,f(q)\left(\frac{1-(q-k)^2}{qk}+\frac{\omega-k^2}{2qk}\ln\left|\frac{1-q^2-\omega}{2qk+\omega-k^2}\right|+\frac{\omega+k^2}{2qk}\ln\left|\frac{2qk-\omega-k^2}{1-q^2+\omega}\right|\right)\right.$$
$$\left.-\int_{1-k\theta(1-k)}^1 dq\,f(q)\left(4+\frac{\omega-k^2}{2qk}\ln\left|\frac{2qk-\omega+k^2}{2qk+\omega-k^2}\right|+\frac{\omega+k^2}{2qk}\ln\left|\frac{2qk-\omega-k^2}{2qk+\omega+k^2}\right|\right)\right], \qquad (2.12)$$

with

$$f(q)=\frac{1}{2}\left[\frac{1+q^2}{4}+\frac{(q^2-1)^2}{8q}\ln\left|\frac{1-q}{1+q}\right|\right] \qquad (2.13)$$

and where $\theta(1-k)$ is the step function.

Let us now consider the imaginary part of $T(k,\omega)$. From Eq. (2.6), we obtain

$$T_2(k,\omega)=\frac{\pi}{(2\pi)^4}\int_{-1}^1 dx\int_0^1 q^2\,dq\,\frac{\phi(q,k,x)}{|2kx|}$$
$$\times\left[\delta\left(q-\frac{\omega-k^2}{2kx}\right)-\delta\left(q+\frac{\omega+k^2}{2kx}\right)\right], \qquad (2.14)$$

where

$$\phi(q,k,x)=F(\vec{q}+\vec{k},\vec{k})-F(\vec{q},\vec{k})\ , \qquad (2.15)$$

with $x=\vec{q}\cdot\vec{k}/qk$. The integration over q is easily performed if one notes that, due to the finite domain of integration, each δ function will contribute only under particular conditions. More exactly, the first δ function contributes for the following ranges of the integration variable x:

$$\begin{aligned} &\frac{\omega-k^2}{2k}<x<1, && k^2<\omega<k^2+2k, && \text{any } k\ ;\\ &-1<x<\frac{\omega-k^2}{2k} && \begin{cases}0<\omega<k^2, & k<2\ ,\\ k^2-2k<\omega<k^2, & k>2\ ;\end{cases} \end{aligned} \qquad (2.16)$$

while the second δ function contributes only when

$$-1<x<-\frac{\omega+k^2}{2k},\quad 0<\omega<2k-k^2,\quad k<2\ . \qquad (2.17)$$

III. RESULTS AND CONCLUSIONS

The integrals (2.12) and (2.14) were carried out numerically and the function $G(k,\omega)$ was obtained[3] using the relation

$$G(k,\omega)=P_0(k,\omega)/Q_0(k,\omega)\ . \qquad (3.1)$$

A useful check on the calculations was based on comparing values of $G(k,0)$ calculated in two independent ways. $G(k,0)$ as calculated here agrees to within 1% with the values previously obtained and

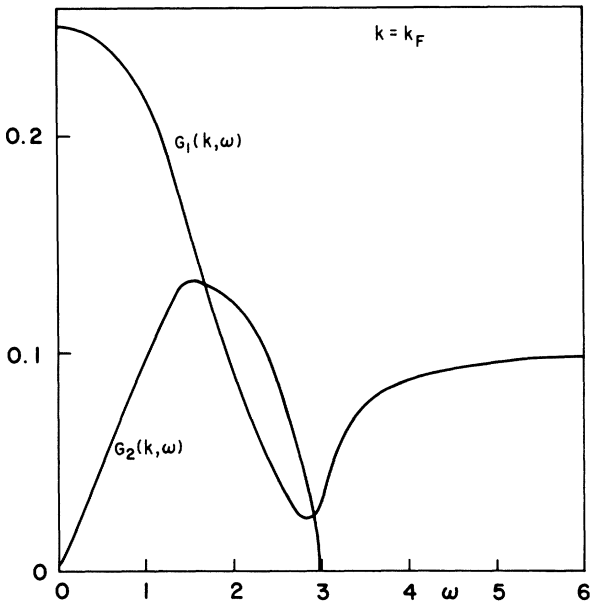

FIG. 1. $G_1(k, \omega)$ and $G_2(k, \omega)$ vs ω for $k = k_F$. $G_1(k, \omega)$ remains flat for values of ω larger than 6.

published in I for $k \gtrsim 2$, while for large k, $G(k, 0)$ approaches the asymptotic value $\frac{2}{3}$. The discrepancies are attributable, of course, to the fact that in I the values of $G(k, 0)$ were obtained by numerical evaluation of a fourfold integral, while in the present paper only one-dimensional integrals are calculated numerically. In Fig. 1 the real and imaginary parts of $G(k, \omega)$ are shown as functions of ω for $k = k_F$. As may be seen, the ω dependence is rather large, particularly at small ω values. The decrease in $G_1(k, \omega)$ from its static value, together with a nonzero $G_2(k, \omega)$, has the effect of decreasing the values of $\epsilon_1(k, \omega)$ and $\epsilon_2(k, \omega)$ from the values obtained by approximating $G(k, \omega)$ by $G(k, 0)$ in Eq. (1.1). In Figs. 2 and 3, $\epsilon_1(k, \omega)$ and $\epsilon_2(k, \omega)$ including the full ω dependence are compared with the functions obtained using $G(k, 0)$ $[\epsilon^{I}(k, \omega)]$ and with the random-phase-approximation results $[\epsilon^{RPA}(k, \omega)]$, again at $k = k_F$. It will be noted that the maximum in $\epsilon_2(k, \omega)$ is shifted to a lower ω value than it has in the RPA. This effect, however, is not peculiar to the presently assumed ω dependence; it can be easily seen, in fact, that any dielectric function in which self-energy and correlation effects are included using the Hubbard form (1.1) exhibits that effect.

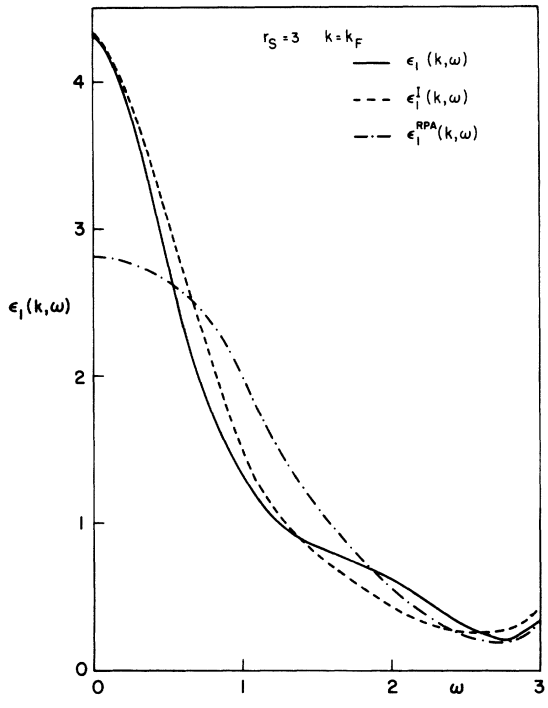

FIG. 2. Real part of the dielectric function for $r_s = 3$, $k = k_F$.

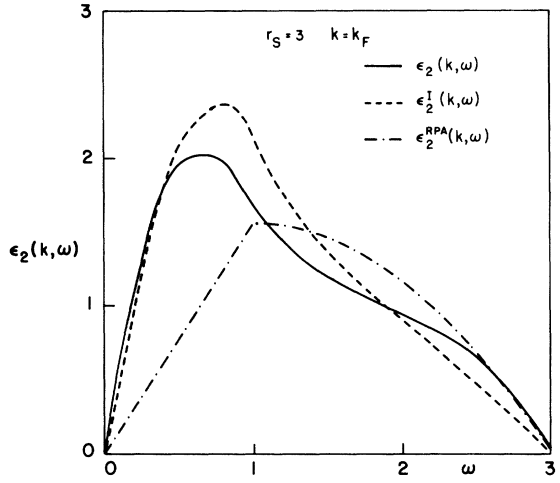

FIG. 3. Imaginary part of the dielectric function for $r_s = 3$, $k = k_F$.

Finally, as Eq. (3.5) of I was obtained by imposing the f sum rule, in our notation

$$\int_0^\infty S(k, \omega)\, \omega\, d\omega = Nk^2 , \tag{3.2}$$

we have checked our calculations and approximations by calculating the integral in Eq. (3.2). We find that, neglecting the ω dependence, the sum rule is satisfied with an accuracy of 10^{-3}, while with the full ω dependence the accuracy is improved to a value varying between 10^{-4} and 10^{-5}, thus confirming the goodness of the approximations used in deriving Eq. (3.5) of I, particularly the decoupling of the expectation value of a product of four Fermi operators according to

$$\langle a^\dagger_{q_1} a^\dagger_{q_2} a_{q_3} a_{q_4}\rangle \cong \langle a^\dagger_{q_1} a_{q_4}\rangle \langle a^\dagger_{q_2} a_{q_3}\rangle - \langle a^\dagger_{q_1} a_{q_3}\rangle \langle a^\dagger_{q_2} a_{q_4}\rangle , \quad (3.3)$$

and the neglecting of term (A5) of I. We can, in fact, claim that the effects neglected will give a contribution to the integral in Eq. (3.2) not larger than one part in 10^4. It must, however, be mentioned that if one wants to calculate the Pauli or spin paramagnetic susceptibility using the same Green's-function decoupling method used in I, not only must one take into account term (A5) of I, but one also has to improve upon the Hartree-Fock decoupling (3.3); in the contrary case one finds for the spin susceptibility the Hartree-Fock result, which implies[4] a ferromagnetic instability in the electron gas at $r_s \simeq 6$ which has never been observed.

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X-Ray Edge Problem with Finite Hole Mass*

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The methods used by Schotte and Schotte to study Mahan's x-ray edge problem are extended to the case of finite hole mass. The singular behavior is expected to continue down to a distance $\Delta\omega \propto 1/M\delta$ above the absoprtion edge for attractive electron-hole interactions.

I. INTRODUCTION

When an infinitely heavy hole interacts with an electron gas, the absorption and emission spectra due, respectively, to the creation and annihilation of the hole change their shape. In the absence of electron-hole interactions, the spectra have the usual threshold edge $\theta(\omega - \omega_0)$, but in the presence of this interaction, the threshold acquires a $(\omega - \omega_0)^{-\epsilon}$ singularity (see Fig. 1).

This behavior was first surmised by Mahan,[1] and can be calculated exactly using the path-integral approach due to Nozières and De Dominicis,[2] or that due to Schotte and Schotte.[3]

If the hole mass is now allowed to be finite, the problem becomes more complicated, and it no longer seems possible to use the methods of Ref. 2. See Refs. 4–6 for some approaches to the problem.

In this article we shall extend the method of Ref. 3 to the case of finite hole mass. In this method, the electron Fermi gas is replaced by the Bose gas of its density oscillations; this allows us to use the path-integral theory of a system interacting with an ensemble of independent harmonic oscillators. In the one-dimensional gas of S electrons (the only ones that can interact with a stationary hole via a Dirac's δ function interaction), Schotte and Schotte, following Tomonaga,[7] define density-wave operators

$$\rho_k = \sum_{\vec{k}_1 - \vec{k}_2 = \vec{k}} \frac{1}{\sqrt{N}}\, a^\dagger_{k_1} a_{k_2} ,$$

$$E(k_1) - E(k_2) = k v_F ,$$

where N is the number of electrons and k_0 is the momentum at the top of the conduction band. To within a good approximation (see Tomonaga), the ρ_k obey boson commutation relations, and have the dispersion law

$$E_k = k v_F ,$$

where v_F is the Fermi velocity.

Schotte and Schotte also transform the electron creation and annihilation operators appearing in the problem into boson operators. If an electron is created at the origin at time $t = 0$, and annihilated there at time t_0, these two fermion operators can