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Dielectric function of the electron gas with dynamical-exchange decoupling. I. Analytical treatment*

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Dynamical-exchange effects in the dielectric function of the electron gas can be described by a frequency-dependent local-field correction $G(q,\omega)$. In an earlier derivation, we deduced an explicit expression for $G(q,\omega)$ as a sixfold integral, which was obtained from the dynamical-exchange decoupling in the equation of motion for the Wigner distribution function, and a variational treatment of the resulting integro-differential equation. Explicit dynamical calculations were presented. In this paper the formal expression for $G(q,\omega)$ is reduced to a double integral in a convenient form for numerical purposes, using various Fourier representations in the integrand. Several limiting cases are evaluated analytically, from which it follows that dynamical-exchange effects drastically influence the structure of the dielectric function. Some numerical results on the frequency-dependent dielectric function with dynamical-exchange decoupling are presented.

I. INTRODUCTION

Many properties of simple metals can be described and calculated from the dielectric function. In studying the effects that are essentially due to the electron-electron interactions, the jellium model is widely used. In this model, the discrete-ion lattice is supposed not to have essential influence on the dielectric function $\epsilon(q,\omega)$ and is replaced by a uniform positive background.

In the well-known randon-phase approximation (RPA),[1] $\epsilon(q,\omega)$ was first calculated by Lindhard,[2] who studied the motion of the electrons in the presence of an electromagnetic field, under the assumption that this motion is governed by classical laws.

Because the RPA only takes into account the long-range interaction of the classical Hartree potential, a satisfactory description of the long-wavelength collective excitations is obtained. However, due to the neglect of the exchange and correlation interactions, the RPA insufficiently describes short-range effects, which, for instance, is reflected in a negative pair correlation function for small interparticle distances from RPA.[3]

By summing up several exchange diagrams, Hubbard[4] introduced a first correction to the RPA, in the form of a frequency-independent function $G(q)$, and various improvements on this local-field correction, going beyond Hubbard's expansion, have been proposed.[5-19]

Several approximations have also been made by other workers,[20-26] leading to a frequency-dependent local-field correction $G(q,\omega)$, and it has been shown[29] that an internally consistent theory of the electron gas cannot be obtained if this frequency dependence is neglected. However, the explicit calculations of $G(q,\omega)$ were restricted to the static limit $\omega=0$ and to a few limiting cases. But even this partial information from approximate treatments, as well as some interesting general properties of $G(q,\omega)$,[26] already indicate appreciable effects of the exchange interaction on the dielectric response of the electron gas.

Therefore, the present authors[27] tried to evaluate the dynamical-exchange influence on the dielectric function explicitly, including the full wave vector and frequency dependence, and derived general expressions for the transverse and longitudinal dielectric function of jellium, including exchange. $G(q,\omega)$ was obtained as a sixfold integral that could only be solved analytically in a few limiting cases. This solution was obtained by considering the equation of motion for the Wigner distribution function, and where dynamical-exchange effects were included by making the exchange decoupling in the equation of motion. By a variational procedure, an approximate solution of the resulting integrodifferential equation was obtained that *rigorously* satisfies the equation of motion for the charge and current density. Various limits were also studied.

The same general form for $G(q,\omega)$ as a sixfold integral is also obtained if one variationally solves the integral equation for the irreducible vertex function with linear exchange processes as derived in Ref. 23, but with a screened Coulomb interaction, and without explicit evaluation.

The same formal expression for $G(q,\omega)$ which we derived was afterwards also obtained in Ref. 28 from the equation of motion for the double-time-retarded commutator of the charge-density-fluctuation operators.

The static limit $G(q,0)$ has been evaluated[30] and shows a sharp peak near $q=2k_F$, in contrast to earlier theories.

The limiting cases in which the sixfold integral for $G(q,\omega)$ can be calculated analytically suggest that dynamical-exchange effects might appreciably influence the dielectric function. These indications are confirmed by our explicit evaluation of $G(q,\omega)$ with dynamical-exchange decoupling.[31] In Ref. 31, we presented numerical results for $\epsilon(q,\omega)$ and for $\text{Im}\,\epsilon^{-1}(q,\omega)$, obtained by reducing the sixfold integral for $G(q,\omega)$ into a double integral with elementary analytical methods, and by evaluating the remaining double integral numerically. As far as we know, this is the first calculation of $G(q,\omega)$ with dynamical-exchange decoupling at arbitrary wave vector and frequency. However, no detailed information was given about the analytical and numerical methods used.

In Ref. 31 we also deduced an important scaling property of $G(q,\omega)$ with respect to density. Expressing the wave vector in units of the Fermi wave vector k_F, and the frequency in units of twice the Fermi energy E_F:

$$k=q/k_F,\quad \nu=\hbar\omega/2E_F\,, \tag{1}$$

we proved the theorem that $G(kk_F,2\nu E_F/\hbar)$ is a universal function of k and ν for all densities. In these units, we obtained the explicit expression

$$G(kk_F,2\nu E_F/\hbar)=f(k,\nu)\int d^3r\int d^3r'\,\frac{1}{|\vec{r}-\vec{r}'|^2}\,[\mathfrak{N}(\vec{r}+\tfrac{1}{2}\vec{k})-\mathfrak{N}(\vec{r}-\tfrac{1}{2}\vec{k})][\mathfrak{N}(\vec{r}'+\tfrac{1}{2}\vec{k})-\mathfrak{N}(\vec{r}'-\tfrac{1}{2}\vec{k})]$$
$$\times\frac{1}{\nu+i\epsilon-\vec{r}\cdot\vec{k}}\left(\frac{1}{\nu+i\epsilon-\vec{r}'\cdot\vec{k}}-\frac{1}{\nu+i\epsilon-\vec{r}\cdot\vec{k}}\right), \tag{2}$$

with

$$\mathfrak{N}(\vec{r})=\begin{cases}1, & |\vec{r}|\le 1\\ 0, & |\vec{r}|>1\end{cases} \tag{3}$$

$$f(k,\nu)=\frac{1}{2}\,\frac{m^2e^4}{\pi^4\hbar^4k^2k_F^2Q_0^2(k\,k_F,2\nu E_F/\hbar)}\,, \tag{4}$$

and where Q_0 is the Lindhard polarizability, given by

$$Q_0(k\,k_F,2\nu E_F/\hbar)=\frac{me^2}{\pi^2\hbar^2k_F}\frac{1}{k^2}\times\int d^3r\,\frac{\mathfrak{N}(\vec{r}+\tfrac{1}{2}\vec{k})-\mathfrak{N}(\vec{r}-\tfrac{1}{2}\vec{k})}{\nu+i\delta-\vec{r}\cdot\vec{k}}\,. \tag{5}$$

With these definitions, the dielectric function takes the form

$$\epsilon(q,\omega)=1+Q_0(q,\omega)/[1-G(q,\omega)Q_0(q,\omega)]\,. \tag{6}$$

Furthermore, we have shown in Ref. 32 that the high-frequency limit and the static limit of our expression (2) for $G(q,\omega)$ are internally consistent, in the sense that these limits both lead to the same value of the pair correlation function at the origin.

The sixfold integral (2) forms a key problem in studying dynamical-exchange effects. Therefore, much effort has been put into the evaluation of this integral. The final form we succeeded in obtaining is quite appropriate for practical applications, and because of its general interest, the derivation of this final result is given in full detail in the present paper.

In this paper (hereafter I), we do not develop the method we proposed in Ref. 31, but present an alternative procedure, based on Fourier representations of the integrand, which allow one to reduce the sixfold integral (2) to a double integral, transformed into a convenient form for numerical purposes. The method applies to arbitrary frequency and is not restricted to the static limit. The general dependence of $G(q,\omega)$ on wave vector and frequency is discussed, and in Appendix A the high-frequency limit of $G(q,\omega)$ is calculated analytically.

In paper II, a summary will be given of the various internal-consistency requirements and sum rules that could be tested and are satisfied within this theory, and numerical results for the dielectric function with dynamical-exchange decoupling will be presented at arbitrary wave vector and frequency. The implications for various electronic densities will also be discussed.

II. ANALYTICAL TREATMENT OF $G(q,\omega)$

From our earlier derivation,[27,31] the influence of exchange effects on the dielectric function is described by the function $G(q,\omega)$, given in (2) as a sixfold integral, which is obviously not appropriate for numerical evaluation. In order to achieve the twofold goal of reducing computation time and simultaneously solving the accuracy problem, two independent methods were worked out.

An outline of our first method, based on the straightforward evaluation of (2) towards a double integral, was presented previously.[31] This procedure, however, requires more computation time and turns out to be slightly less accurate than a second method, which is based on Fourier transforms, and which is presented in this section.

A. Fourier transformation

The possible sources of inaccuracies in evaluating (2) from the subtraction of integrals over two displaced Fermi spheres can be eliminated by introducing the Fourier transform of the reduced Fermi function (3), expressed in cylindrical coordinates. The singular behavior of the factor $|\vec{r}-\vec{r}'|^{-2}$ also becomes easier to treat if one makes use of its Fourier transform. Furthermore taking the Fourier transforms of the frequency-dependent factors, one obtains a 17-fold integral, where one recognizes the representations of two three-dimensional δ functions.

Performing some of the resulting integrations, Eq. (2) eventually transforms into

$$G(k\,k_F, 2\nu E_F/\hbar) = 4f(k,\nu)\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \frac{k(z-z')}{(\nu+i\epsilon-kz)^2(\nu+i\epsilon-kz')}\psi_k(z,z')\,, \tag{7}$$

where $\psi_k(z,z')$ is defined as the fivefold integral

$$\psi_k(z,z') = \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \int_0^{\infty} \frac{d\xi_\perp}{\xi_\perp} \int_{-1}^{1} dx \int_{-1}^{1} dx'\, K_0(\xi_\perp|z-z'|)e^{ip(z+x)}e^{ip'(z'+x')}\sin\frac{pk}{2}\sin\frac{p'k}{2} \times (1-x^2)^{1/2}J_1[\xi_\perp(1-x^2)^{1/2}](1-x'^2)^{1/2}J_1[\xi_\perp(1-x'^2)^{1/2}]\,. \tag{8}$$

We note that in (8), the integration over p would yield a difference of two δ functions, only allowing for z to take the values $z=-x\pm\frac{1}{2}k$, while $|x|\leq 1$ because of the integration limits of x. Therefore $\psi_k(z,z')$ only differs from zero in the region $-1-\frac{1}{2}k\leq z\leq 1+\frac{1}{2}k$. We thus obtain the important property that $\psi_k(\pm\infty,z')=0$. This makes it possible to reduce the second-order pole in (7) to a pole of first order by an integration by parts, using

$$\frac{1}{(\nu+i\epsilon-kz)^2} = \frac{1}{k}\frac{d}{dz}\frac{1}{\nu+i\epsilon-kz}\,. \tag{9}$$

One then obtains

$$G(k\,k_F, 2\nu E_F/\hbar) = -4f(k,\nu)\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \frac{1}{\nu+i\epsilon-kz}\frac{1}{\nu+i\epsilon-kz'}\frac{d}{dz}[(z-z')\psi_k(z,z')]\,. \tag{10}$$

Performing next the differentiation with respect to z, and decoupling the products of the denominators in (10) as

$$[1/(\nu+i\epsilon-kz)][1/(\nu+i\epsilon-kz')] = [1/k(z-z')][1/(\nu+i\epsilon-kz)-1/(\nu+i\epsilon-kz')]\,, \tag{11}$$

the integrand then consists of four terms

$$G(k\,k_F, 2\nu E_F/\hbar) = -\frac{4f(k,\nu)}{k}\int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \left(\frac{1}{\nu+i\epsilon-kz}\frac{\psi_k(z,z')}{z-z'} + \frac{1}{\nu+i\epsilon-kz}\frac{d}{dz}\psi_k(z,z') - \frac{1}{\nu+i\epsilon-kz'}\frac{\psi_k(z,z')}{z-z'} - \frac{1}{\nu+i\epsilon-kz'}\frac{d}{dz}\psi_k(z,z')\right). \tag{12}$$

The last term on the right-hand side of (12) can easily be integrated with respect to z, which gives zero because $\psi_k(\pm\infty,z')=0$. The first and third terms on the right-hand side give an equal contribution for symmetry reasons, because it follows from (8) that $\psi_k(z,z')=\psi_k(z',z)$. Therefore, (12) separates into two terms

$$G(k\,k_F, 2\nu E_F/\hbar) = f(k,\nu)[G_1(k,\nu)+G_2(k,\nu)]\,, \tag{13}$$

where

$$G_1(k,\nu) = -\frac{4}{k}\int_{-\infty}^{\infty} dz \frac{1}{\nu+i\epsilon-kz}\frac{d}{dz}\int_{-\infty}^{\infty} dz'\,\psi_k(z,z')\,, \tag{14}$$

$$G_2(k,\nu) = -\frac{8}{k}\int_{-\infty}^{\infty} dz \frac{1}{\nu+i\epsilon-kz}\int_{-\infty}^{\infty} dz' \frac{\psi_k(z,z')}{z-z'}\,, \tag{15}$$

and where $\psi_k(z,z')$ is defined in (8).

The term $G_1(k,\nu)$ essentially results from the pole of second order in the original sixfold integral and can be written as a single integral. The term $G_2(k,\nu)$ can be reduced to a double but numerically tractable integral.

B. $G_2(k,\nu)$ as a double integral

Writing the modified Bessel function K_0 of the second kind in its integral representation

$$\int_{-\infty}^{\infty} d\xi_z \frac{e^{i\xi_z(z-z')}}{(\xi_\perp^2+\xi_z^2)^{1/2}} = 2K_0(\xi_\perp |z-z'|)\,, \tag{16}$$

and performing the integrals over z and z' in (15), using (8), one obtains

$$\begin{aligned} G_2(k,\nu) = -8\frac{\pi^2}{k^2}\int_0^\infty \frac{d\xi_\perp}{\xi_\perp}\int_{-\infty}^{\infty} d\xi_z \int_{-1}^{1} dx \int_{-1}^{1} dx' \int_{-\infty}^{\infty} dp'[\Theta(p'-\xi_z)-\Theta(\xi_z-p')] \\ \times \int_{-p'}^{\infty} dp \frac{1}{(\xi_\perp^2+\xi_z^2)^{1/2}} \exp\left(i\frac{p+p'}{k}(\nu+i\epsilon)\right) e^{ipx} e^{ip'x'} \sin\frac{pk}{2}\sin\frac{p'k}{2} \\ \times (1-x^2)^{1/2} J_1[\xi_\perp(1-x^2)^{1/2}](1-x'^2)^{1/2} J_1[\xi_\perp(1-x'^2)^{1/2}]\,, \end{aligned} \tag{17}$$

where

$$\Theta(x) = \begin{cases} 1, & x \leq 0 \\ 0, & x > 0\,. \end{cases} \tag{18}$$

The integration over x' then gives (Ref. 33, p. 376)

$$\int_{-1}^{1} dx' e^{ip'x'}(1-x'^2)^{1/2} J_1[\xi_\perp(1-x'^2)^{1/2}] = \sqrt{2\pi}\,\xi_\perp J_{3/2}[(\xi_\perp^2+p'^2)^{1/2}]/(\xi_\perp^2+p'^2)^{3/4}\,.$$

If one subsequently interchanges the integration over p' and ξ_z, evaluates the integral over ξ_z, substitutes p' by ξ_z and p by $\tau-\xi_z$, introduces the polar coordinates (ξ,θ) instead of ξ_z and $\xi_\perp$, and performs a partial integration with respect to ξ, using

$$\frac{J_{3/2}(\xi)}{\xi^{3/2}} = -\left(\frac{2}{\pi}\right)^{1/2}\frac{d}{d\xi}\frac{\sin\xi}{\xi}\,, \tag{19}$$

then (17) transforms into

$$\begin{aligned} G_2(k,\nu) = \frac{32\pi^2}{k^2}\int_0^\pi d\theta \int_{-1}^{1} dx \int_0^\infty d\tau\, sh^{-1}(\cot\theta)\exp\left[i\tau\left(\frac{\nu+i\epsilon}{k}+x\right)\right](1-x^2)^{1/2} \\ \times \int_0^\infty d\xi \frac{\sin\xi}{\xi}\frac{d}{d\xi}\left[\sin\left(\frac{\tau-\xi\cos\theta}{2}k\right)\sin\left(\frac{\xi\cos\theta}{2}k\right) e^{-i\xi x\cos\theta} J_1[\xi\sin\theta(1-x^2)^{1/2}]\right]. \end{aligned} \tag{20}$$

From the elementary relation

$$\int_0^\pi d\theta f(\sin\theta,\cos\theta) = \int_0^{\pi/2} d\theta[f(\sin\theta,\cos\theta)+f(\sin\theta,-\cos\theta)]\,, \tag{21}$$

the range of the angular integration is restricted to $(0,\frac{1}{2}\pi)$. The integration over τ is straightforward. By recombining terms, one then finds

$$G_2(k,\nu) = \frac{2\pi^2}{k}\int_{-1}^{1} dz \left(\frac{\mathcal{H}(z,0)-\mathcal{H}(z,k)}{\nu+i\epsilon-kz-k^2/2}+\frac{\mathcal{H}(z,0)-\mathcal{H}(z,-k)}{\nu+i\epsilon-kz+k^2/2}\right)\,, \tag{22}$$

with

$$\mathcal{H}(z,k) = -8(1-z^2)^{1/2}\int_0^{\pi/2} d\theta\, sh^{-1}(\cot\theta) F((z+k)\cos\theta,(1-z^2)^{1/2}\sin\theta)\,, \tag{23}$$

and where the function $F(b,a)$ is defined as

$$F(b,a) = \int_0^\infty d\xi \frac{\sin\xi}{\xi}\frac{d}{d\xi}[J_1(a\xi)\sin b\xi]\,. \tag{24}$$

The integral (24) is explicitly evaluated in Appendix C in terms of elementary functions, giving

$$F(b,a)=\frac{1-b^2}{4a}\left\{\Theta(a-|1+b|)\left[1-\left(\frac{a}{1+b}\right)^2\right]^{1/2}-\Theta(a-|1-b|)\left[1-\left(\frac{a}{1-b}\right)^2\right]^{1/2}\right\}$$
$$+\frac{a}{4}\left\{\Theta(a-|1-b|)\ln\left|\frac{|1+b|+[(1+b)^2-a^2]^{1/2}}{|1-b|+[(1-b)^2-a^2]^{1/2}}\right|\right.$$
$$\left.+\Theta(a-|1+b|)\Theta(|1-b|-a)\ln\left|\frac{|1+b|+[(1+b)^2-a^2]^{1/2}}{a}\right|\right\}. \quad (25)$$

One readily shows that the singularity of $sh^{-1}(\cot\theta)$ for $\theta\to 0$ in (23) is cancelled by the behavior of the function F, given in (25).

In summary, the formula (22), combined with (23) and (25) expresses $G_2(k,\nu)$ as a double integral. The integral (23) is easy to treat numerically, and the remaining integral (22) involves a principal-value problem. However, before considering this difficulty, we first discuss the evaluation of $G_1(k,\nu)$ from (14) as a single integral that takes the same form of (22).

C. $G_1(k,\nu)$ as a single integral

In order to evaluate $G_1(k,\nu)$ given in (14), with $\psi_k(z,z')$ given in (8), a useful identity is derived in Appendix D:

$$\int_0^\infty d\xi_\perp \frac{1}{\xi_\perp}K_0(\xi_\perp|z-z'|)J_1[\xi_\perp(1-x^2)^{1/2}]J_1[\xi_\perp(1-x'^2)^{1/2}]$$
$$=\frac{1}{2\pi(1-x^2)^{1/2}(1-x'^2)^{1/2}}\int_0^{(1-x^2)^{1/2}}\rho\,d\rho\int_0^{(1-x'^2)^{1/2}}\rho'\,d\rho'\int_0^{2\pi}d\varphi'\frac{1}{\rho^2+\rho'^2-2\rho\rho'\cos\varphi'+(z-z')^2}. \quad (26)$$

Noting that in (14) the integral $\int_{-\infty}^{\infty}dz'\psi_k(z,z')$ is needed, the expression (8) for $\psi_k(z,z')$ is rewritten with the help of (26), and the integration over p' is performed, resulting in a difference of δ functions

$$\int_{-\infty}^{\infty}dz'\psi_k(z,z')=\frac{1}{2i}\int_{-\infty}^{\infty}dz'\int_{-\infty}^{\infty}dp\sin\frac{pk}{2}\int_{-1}^{1}dx\,e^{ip(z+x)}\int_0^{(1-x^2)^{1/2}}\rho\,d\rho$$
$$\times\int_{-1}^{1}dx'\int_0^{(1-x'^2)^{1/2}}\rho'\,d\rho'\int_0^{2\pi}d\varphi'\frac{\delta(z'+x'+\frac{1}{2}k)-\delta(z'+x'-\frac{1}{2}k)}{\rho^2+\rho'^2-2\rho\rho'\cos\varphi'+(z-z')^2}. \quad (27)$$

One then performs the integral over z' with the help of the δ functions, and defines a vector $\vec{t}_\pm$ with components $-(z\pm k/2)$ in some arbitrary direction and $\vec{\rho}$ perpendicular to this direction. The integrations over z', ρ', and φ' can then be considered as a volume integral over a unit sphere,

$$\int_{-\infty}^{\infty}dz'\psi_k(z,z')=\frac{1}{2i}\int_{-\infty}^{\infty}dp\int_{-1}^{1}dx\int_0^{(1-x^2)^{1/2}}\rho\,d\rho\,e^{ip(z+x)}\sin\frac{pk}{2}\int d^3r'\,\mathfrak{N}(\vec{r}')\left(\frac{1}{|\vec{r}'-\vec{t}_+|^2}-\frac{1}{|\vec{r}'-\vec{t}_-|^2}\right), \quad (28)$$

where $\mathfrak{N}(\vec{r})$ is the Fermi function on a unit sphere defined above (3), and where $\vec{t}_\pm$ is a vector of length,

$$t_\pm\equiv|\vec{t}_\pm|=[\rho^2+(z\pm\tfrac{1}{2}k)^2]^{1/2}. \quad (29)$$

The volume integral over $\vec{r}'$ is easily performed:

$$\int d^3r'\,\mathfrak{N}(r')\frac{1}{|\vec{r}'-\vec{t}_\pm|^2}=2\pi\left(1+\frac{1-t_\pm^2}{2t_\pm}\ln\left|\frac{1+t_\pm}{1-t_\pm}\right|\right). \quad (30)$$

Combining then (14), (28), and (30) and integrating over p, one finds

$$G_1(k,\nu)=\frac{8}{k}\left(\frac{2\pi}{i}\right)^2\int_{-\infty}^{\infty}\frac{dz}{\nu+i\epsilon-kz}\frac{d}{dz}\left[\int_{-1}^{1}dx(\delta(z+x+\tfrac{1}{2}k)-\delta(z+x-\tfrac{1}{2}k))\right.$$
$$\left.\times\int_0^{(1-x^2)^{1/2}}\rho\,d\rho\left(\frac{1-t_-^2}{2t_-}\ln\left|\frac{1-t_-}{1+t_-}\right|-\frac{1-t_+^2}{2t_+}\ln\left|\frac{1-t_+}{1+t_+}\right|\right)\right]. \quad (31)$$

Integrating twice by parts one obtains

$$\int_{-\infty}^{\infty}\frac{dz}{\nu+i\epsilon-kz}\,\frac{d}{dz}\int_{-1}^{1}dx\,\delta(z+x\pm\tfrac{1}{2}k)g(x,z)$$
$$=\frac{1}{\nu+i\epsilon-kz}\int_{-1}^{1}dx\,\delta(z+x\pm\tfrac{1}{2}k)g(x,z)\Big|_{z=-\infty}^{z=\infty}$$
$$-\frac{1}{\nu+i\epsilon-kz}\,g(-z\mp\tfrac{1}{2}k,z)\Big|_{z=-(1\mp k/2)}^{z=1\mp k/2}$$
$$+\int_{-1\mp k/2}^{1\mp k/2}dz\,\frac{1}{\nu+i\epsilon-kz}\,\frac{d}{dz}\,g(-(z\pm\tfrac{1}{2}k),z)\,. \qquad (32)$$

Applying this more-general result (32) to the specific case (31), one easily checks that only the last term of (32) contributes. Furthermore, substituting the integration variable ρ by $u=\rho^2+(z\pm\frac{1}{2}k)^2$ in order to include all the z dependence in the integration limits of u, the differentiation with respect to z eliminates the integration over u. Recombining terms, one then finally obtains

$$G_1(k,\nu)=\frac{2\pi^2}{k}\int_{-1}^{1}dz\left(\frac{\mathcal{F}(z,-k)-\mathcal{F}(z,0)}{\nu+i\epsilon+\frac{1}{2}k^2-kz}+\frac{\mathcal{F}(z,k)-\mathcal{F}(z,0)}{\nu+i\epsilon-\frac{1}{2}k^2-kz}\right), \qquad (33)$$

where $\mathcal{F}(z,k)$ is given by

$$\mathcal{F}(z,k)=-k\frac{1-(1+k^2+2kz)}{[1+k^2+2kz]^{1/2}}\ln\left|\frac{1+[1+k^2+2kz]^{1/2}}{1-[1+k^2+2kz]^{1/2}}\right|$$
$$+(z+k)\frac{1-(z+k)^2}{[(z+k)^2]^{1/2}}\ln\left|\frac{1+[(z+k)^2]^{1/2}}{1-[(z+k)^2]^{1/2}}\right|\,. \qquad (34)$$

D. Final form of $G(kk_F, 2\nu E_F/\hbar)$

By recombining (13), (22), and (33), the full expression for $G(k\,k_F,2\nu E_F/\hbar)$ is thus given by

$$G(k\,k_F,2\nu E_F/\hbar)=\frac{2\pi^2}{k}f(k,\nu)\times\int_{-1}^{1}dz\left(\frac{\mathcal{T}(z,k)}{\nu+i\epsilon-k^2/2-kz}+\frac{\mathcal{T}(z,-k)}{\nu+i\epsilon+k^2/2-kz}\right), \qquad (35)$$

with

$$\mathcal{T}(z,k)=[\mathcal{H}(z,0)-\mathcal{H}(z,k)]-[\mathcal{F}(z,0)-\mathcal{F}(z,k)]\,. \qquad (36)$$

The function $\mathcal{F}(z,k)$ is given in (34) as an elementary function, and $\mathcal{H}(z,k)$ is a single integral, given in (23) and (25).

One then easily checks the symmetry property

$$\mathcal{T}(z,k)=-\mathcal{T}(-z,-k)\,, \qquad (37)$$

and thus (35) can be rewritten in the form

$$G(k\,k_F,2\nu E_F/\hbar)=\frac{2\pi^2}{k}f(k,\nu)\times\int_{-1}^{1}dz\,\mathcal{T}(z,k)\left(\frac{1}{\nu+i\epsilon-k^2/2-kz}-\frac{1}{\nu+i\epsilon+k^2/2+kz}\right). \qquad (38)$$

As discussed above, the evaluation of $\mathcal{H}(z,k)$ presents no numerical difficulties, and the function is shown in Fig. 1 for several values of k. The function $\mathcal{T}(z,k)$, given in (36), can then easily be obtained, because $\mathcal{F}(z,k)$ is an elementary function (34). The result is shown in Fig. 2 for various values of k. The function $\mathcal{T}(z,k)$ shows no singular behavior, and thus the numerical evaluation of (38) can be performed by standard techniques, except when the denominators in (38) tend to cancel each other, or when one of the poles approaches the integration limit. But these two remaining problems can be treated analytically.

Under the condition $|\nu|\gg|\frac{1}{2}k^2\pm k|$, the denominators in (38) are almost equal, which might introduce numerical inaccuracy. We considered this problem previously in the limit $k\to 0$ (Ref. 27), and now discuss it in general in Appendix A, where $G(kk_F,2\nu E_F/\hbar)$ is calculated analytically for $|\nu|\gg|\frac{1}{2}k^2\pm k|$.

A second problem in evaluating (38) arises from the possibility that one of the poles approaches an integration limit. Because

$$\int_a^b\frac{f(x)}{p+i\epsilon-x}\,dx=\int_a^b dx\,\frac{f(x)-f(p)}{p+i\epsilon-x}-f(p)\ln\frac{b-p-i\epsilon}{a-p-i\epsilon}\,, \qquad (39)$$

a logarithmic singularity might occur for $|\nu|=|\frac{1}{2}k^2\pm k|$ if $\mathcal{T}(\pm1,k)$ differs from zero. From (23) and (24) it is obvious that $\mathcal{H}(\pm1,k)=0$, as is clear from Fig. 1. Furthermore it follows from (34) that $\mathcal{F}(\pm1,0)=0$. Therefore (36) yields that $\mathcal{T}(\pm1,k)=\mathcal{F}(\pm1,k)$, which results in

$$\mathcal{T}(\pm1,k)=k^2\,\frac{k\pm2}{|k\pm1|}\ln\left|\frac{1+|k\pm1|}{1-|k\pm1|}\right|+(k\pm1)\,\frac{1-(k\pm1)^2}{|k\pm1|}\ln\left|\frac{1+|k\pm1|}{1+|k\pm1|}\right|. \qquad (40)$$

Consequently, $G(k\,k_F,2\nu E_F/\hbar)$ shows a logarithmic singularity in the region $|\nu|\simeq|\frac{1}{2}k^2\pm k|$, because $\mathcal{T}(\pm1,k)\neq0$, provided that $f(k,\nu)$ differs from zero:

$$G(k\,k_F,2\nu E_F/\hbar)\big|_{|\nu|\simeq|k^2/2\pm k|}\simeq\pm f(k,\nu)\frac{2\pi^2}{k^2}k\,\frac{2\pm k}{1\pm k}\ln\left|\frac{2\pm k}{k}\right|\ln\left|\nu-\left|\frac{k^2}{2}\pm k\right|\right|\,. \qquad (41)$$

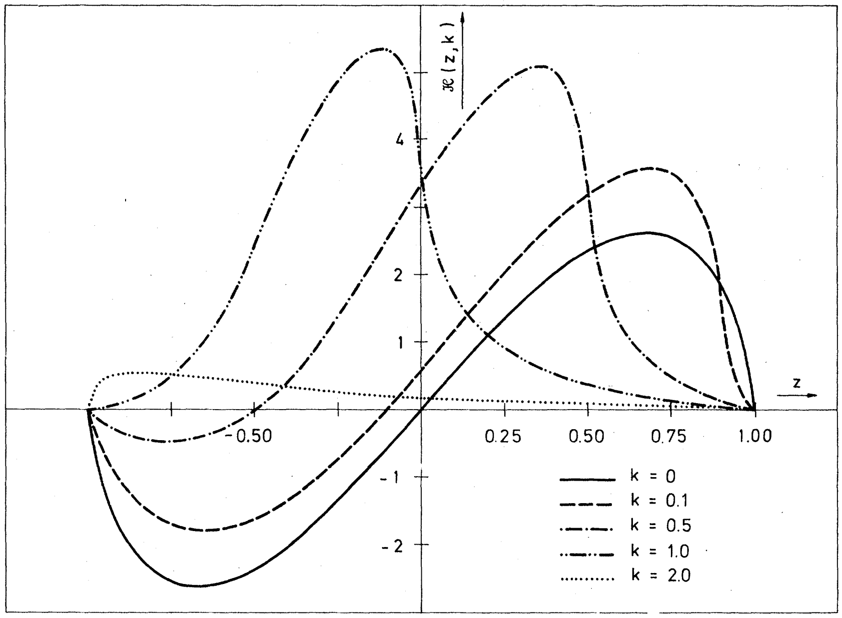

FIG. 1. Function $\mathcal{K}(z,k)$ defined in (23) and (25) as a function of z for various values of k.

From the expression (4) for $f(k,\nu)$ in terms of the Lindhard polarizability Q_0, it follows that $f(k,\nu) \sim k^2$ for $k \to 0$ in the static limit $\nu = 0$. The logarithmic singularity (41) therefore smooths out near the origin. Also in the static limit at $k=2$, the singularity is cancelled by the factor $(2-k)$ multiplying the logarithmic functions.

It should, however, be emphasized that this singularity (41) might be a mathematical artifact. Because it is a logarithmic singularity, its influence extends over a very narrow region in frequency. Furthermore, it would be smoothed out by any physical effect which removes the cutoff in the Fermi function.

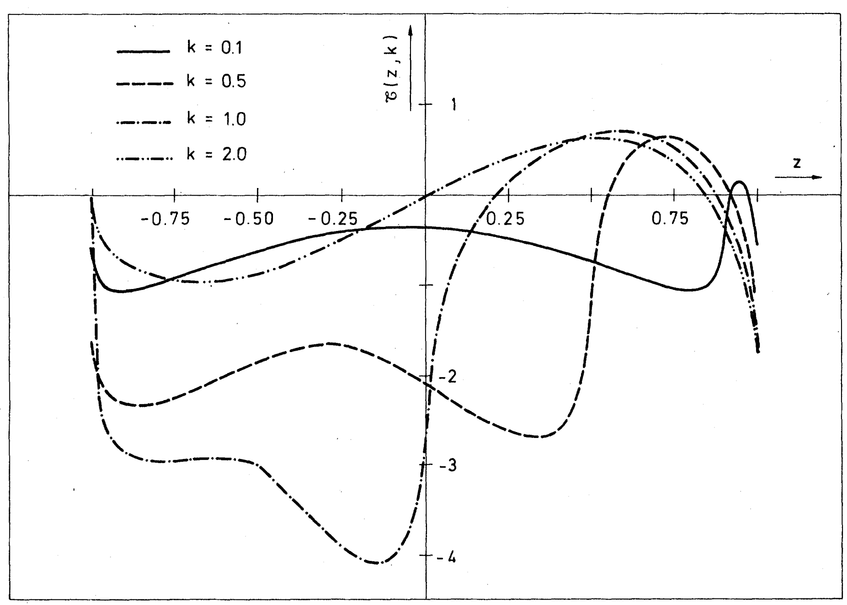

FIG. 2. Function $\mathcal{T}(z,k)$ defined in (36) and forming one of the basic ingredients in the evaluation of $G(q,\omega)$ [see (38)], as a function of z for various values of k.

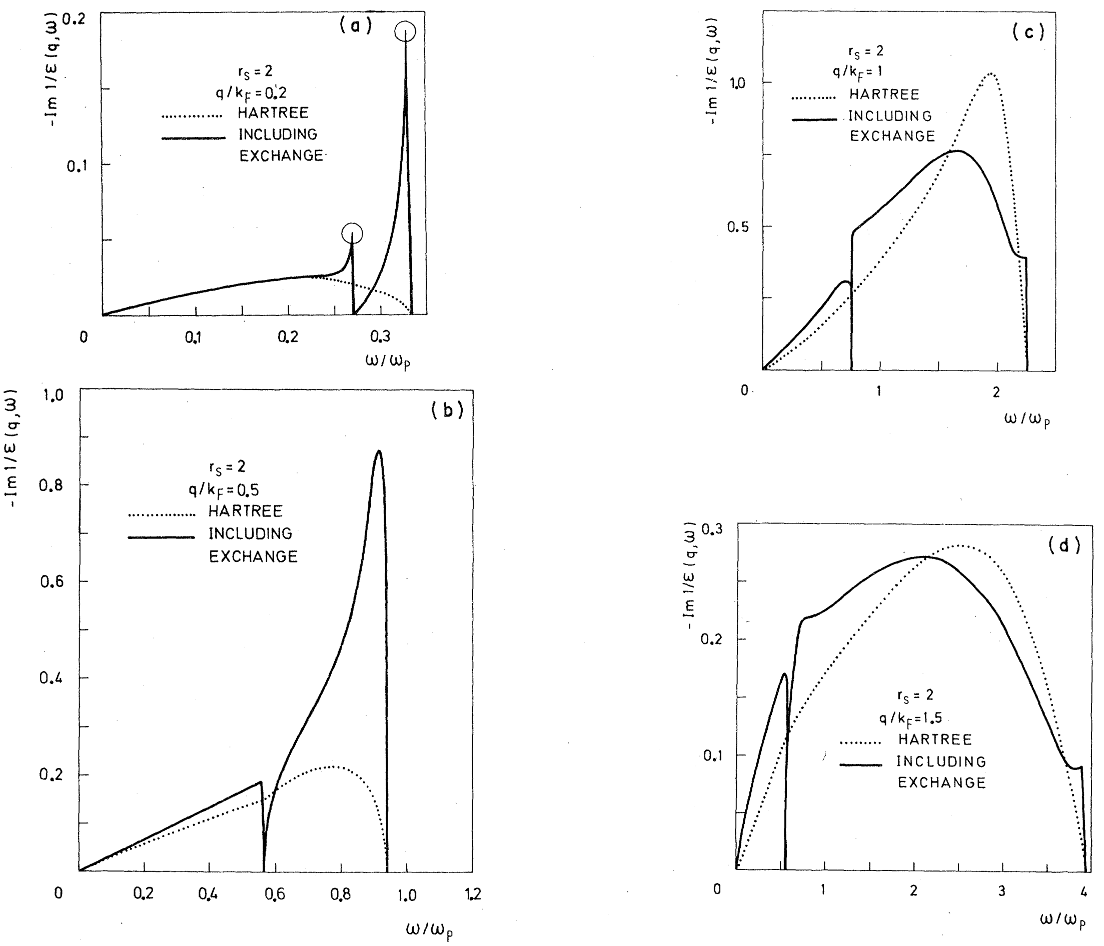

FIG. 3. $-\mathrm{Im}\ \epsilon^{-1}(q,\omega)$ as a function of ω at $r_s=2$, for (a) $q/k_F=0.2$, (b) 0.5, (c) 1.0, and (d) 1.5. The dotted line indicates the RPA, and the full line represents the results from dynamical-exchange decoupling. The circles in Fig. 2(a) indicate that the magnitude of the peaks is not precisely known, due to numerical inaccuracy.

Two immediate mathematical consequences result from the singularity (41). At the parabolas $|\nu| = |\frac{1}{2}k^2 \pm k|$, the real part of the dielectric function equals 1, whereas the imaginary part of the inverse dielectric function becomes 0. This is readily seen from (6). Thus the dynamical structure factor, including exchange, has a zero as a function of frequency at the parabola $\nu = |k - \frac{1}{2}k^2|$, whereas in the RPA approximation only a discontinuity in the derivative occurs. This phenomenon is illustrated in a few plots of $-\mathrm{Im}\,\epsilon^{-1}(q,\omega)$ in Fig. 3.

As a second consequence of this logarithmic singularity, the zeros of $\epsilon(q,\omega)$ do not penetrate into the particle-hole continuum, but only approach it asymptotically. Near the continuum, their oscillator strength strongly decreases and is taken over by the maxima of $\mathrm{Im}\,\epsilon^{-1}(q,\omega)$ in the continuum. Because at very high frequencies $Q_0(q,\omega)$ is negative and $G(q,\omega)$ is positive, as shown in Appendix A, far above the continuum $1 - G(q,\omega)Q_0(q,\omega)$ is positive. At the upper boundary of the continuum, $G(q,\omega) = -\infty$ from (41), and because $Q_0(q,\omega)$ is negative, it follows that $1 - G(q,\omega)Q_0(q,\omega) = -\infty$ at this upper boundary. Thus, with decreasing frequency, $1 - G(q,\omega)Q_0(q,\omega)$ decreases from some positive value at very high frequency to $-\infty$ at $\omega = \hbar(qk_F + \frac{1}{2}q^2)/m$, passing through zero at some critical value ω_c. From (6) it thus follows that $\epsilon(q,\omega)$ diverges at $\omega = \omega_c$, and because $Q_0(q,\omega)$ is negative, $\epsilon(q,\omega)$ tends to $-\infty$ for ω decreasing towards ω_c. However, because $\epsilon(q,\omega$ is positive at very high frequency, a zero in $\epsilon(q,\omega)$ has to be found above ω_c. It should be noted that a similar singular behavior of $\mathrm{Re}\,\epsilon(q,\omega)$ also appears above $\omega = \hbar(qk_F - \frac{1}{2}q^2)/m$, but because $G(q,\omega)$ and $Q_0(q,\omega)$ have an imaginary part, the pole in $\mathrm{Re}\,\epsilon(q,\omega)$ is replaced there by a strongly peaked structure.
In Fig. 4, $\mathrm{Re}\,\epsilon(q,\omega)$ is shown as a function of frequency for several values of the wave vector.

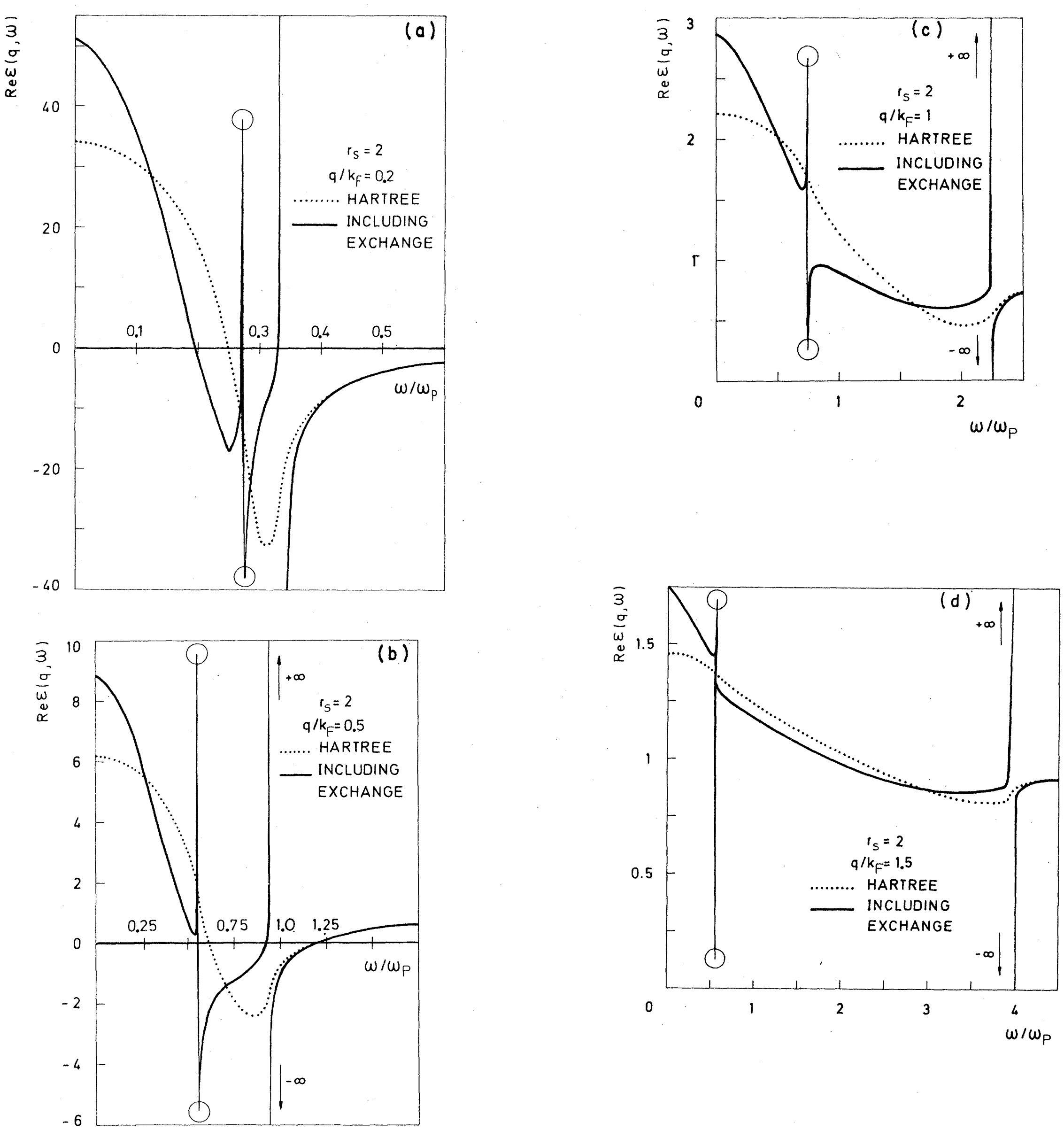

FIG. 4. Re $\epsilon(q,\omega)$ as a function of ω at $r_s=2$, for $q/k_F=$ (a) 0.2, (b) 0.5, (c) 1.0, and (d) 1.5. The dotted line indicates the RPA, and the full line represents the results from dynamical-exchange decoupling. The circles indicate that the magnitude of the peaks is not precisely known, due to numerical inaccuracy.

We emphasize again that the maximum in the structure factor penetrates in the continuum, although the zeros of $\epsilon(q,\omega)$ do not. In approaching the continuum, the oscillator strength of these zeros decreases and goes over into the maxima of Im$\epsilon^{-1}(q,\omega)$.

III. CONCLUSION

The equation of motion for the Wigner distribution, including exchange effects via the dynamical-exchange decoupling, as presented in Ref. 27, was already deduced in Ref. 20, where an iteration to first order was proposed in order to solve the resulting integrodifferential equation approximately. In the static limit, this iterative result was also obtained from a diagrammatic expansion.[12] In a previous paper, we have shown that this iteration to first order provides the terms to order e^4 in the geometric progression of our variational dielectric function in powers of e^2.

The variational procedure was also proposed previously to treat integral equations of the same type,[10,22,23] where a similar trial solution, as in Ref. 27, neglecting the momentum dependence, was used.

But the application we proposed in the equation of motion for the Wigner distribution function clearly indicates that the bare exchange effects are treated dynamically and to the full extent, and that all other correlations are neglected.

It should also be emphasized that the derivation of the dielectric function by Toigo and Woodruff[21] is a first attempt to include dynamical-exchange effects. We discussed the relation between this first-frequency-moment conserving method and the variational procedure in Ref. 32. Along the same lines as in Ref. 21, a dielectric function can be derived by conserving frequency moments to infinite order in the Hartree-Fock (HF) approximation.[28] The resulting expression for $G(q,\omega)$ happens to be identical to the one we derived earlier in Ref. 27, but in Ref. 28 no explicit evaluation was performed. The conservation of the frequency moments in the equation of motion for the double-time-retarded commutator of the charge-density-fluctuation operators thus seems to be equivalent to satisfying the integrated equation of motion which we obtained by a variational technique.

The sixfold integral (2) for $G(q,\omega)$, including dynamical-exchange effects, can thus formally be obtained by several methods. But as far as we know, the reduction to a twofold integral and its explicit evaluation at arbitrary frequency and wave vector are for the first time presented in Ref. 31.

The sixfold integral (2) is the key problem for the study of dynamical-exchange effects. In this paper we derive in detail how, by using Fourier representations, it is transformed analytically into a double integral and is written in a simple form, adapted for numerical purposes. This evaluation reveals appreciable exchange effects in the dielectric function, having implications on the plasmon dispersion and on the frequencies of the maxima in the structure factor.[34,35]

Near the boundaries of the particle-hole continuum, the logarithmic singularity in $G(q,\omega)$ induces drastic exchange effects. But the physical significance of this singular behavior is restricted, because it results from the cutoff in the Fermi function. Finite-temperature and higher-order correlation effects would remove the discontinuity in the equilibrium distribution, and therefore smooth out the logarithmic singularity in $G(q,\omega)$. The overall exchange effects at arbitrary wave vector and frequency are thus more important physically than the singular behavior found in a limited (q,ω) domain.

In paper II, the dynamical-exchange-decoupling method will be tested for its internal consistency from several sum rules and consistency requirements, and an extensive survey of numerical results will be presented.

ACKNOWLEDGMENTS

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APPENDIX A: EVALUATION OF $G(kk_F, 2\nu E_F/\hbar)$ IF $|\nu| \gg |k^2/2 \pm k|$

As discussed in Sec. II, the final expression (38) for $G(k k_F, 2\nu E_F/\hbar)$ presents numerical difficulties for frequencies far above the continuum, because both denominators then tend to cancel each other. However, this limit can be evaluated analytically for arbitrary wave vectors.

From symmetry, the sixfold integral (2) for $G(k k_F, 2\nu E_F/\hbar)$ can be rewritten

$$G(k k_F, 2\nu E_F/\hbar) = -\tfrac{1}{2} f(k,\nu) \int d^3r \int d^3r' \frac{[(\vec{r}-\vec{r}')\cdot\vec{k}]^2}{|\vec{r}-\vec{r}'|^2} \frac{1}{(\nu + i\epsilon - \vec{r}\cdot\vec{k})^2} \frac{1}{(\nu + i\epsilon - \vec{r}'\cdot\vec{k})^2} \times [\mathfrak{N}(\vec{r}+\tfrac{1}{2}\vec{k}) - \mathfrak{N}(\vec{r}-\tfrac{1}{2}\vec{k})][\mathfrak{N}(\vec{r}'+\tfrac{1}{2}\vec{k}) - \mathfrak{N}(\vec{r}'-\tfrac{1}{2}\vec{k})], \quad (A1)$$

where $f(k,\nu)$ is defined in (4), and $\mathfrak{N}(\vec{r})$ is the reduced Fermi function in a unit sphere, as given in (3).

In the limit $\nu \gg |k^2/2 \pm k|$, the $\vec{k}$ dependence in the denominators of (A1) can be neglected. Then (A1) becomes

$$G(k k_F, 2\nu E_F/\hbar) \simeq -\frac{1}{2} \frac{f(k,\nu)}{\nu^4} [I(\tfrac{1}{2},\tfrac{1}{2},k) - I(\tfrac{1}{2},-\tfrac{1}{2},k) - I(-\tfrac{1}{2},\tfrac{1}{2},k) + I(-\tfrac{1}{2},-\tfrac{1}{2},k)], \quad (A2)$$

with

$$I(s,s',k) \equiv \int d^3r \int d^3r' \mathfrak{N}(\vec{r}+s\vec{k}) \mathfrak{N}(\vec{r}'+s'\vec{k}) \times \frac{[(\vec{r}-\vec{r}')\cdot\vec{k}]^2}{|\vec{r}-\vec{r}'|^2}. \quad (A3)$$

By translation of the integration variable $\vec{r}$ into $\vec{r}+\vec{r}'$, the integral (A3) can be rewritten

$$I(s,s',k) = \int d^3r \frac{(\vec{r}\cdot\vec{k})^2}{r^2} T(\vec{r}+s\vec{k}, s'\vec{k}), \quad (A4)$$

where

$$T(\vec{a},\vec{b})\equiv\int d^3r'\,\mathfrak{N}(\vec{r}'+\vec{a})\mathfrak{N}(\vec{r}'+\vec{b})\,. \tag{A5}$$

If one introduces the new integration variable $\vec{r}-\frac{1}{2}(\vec{a}+\vec{b})$, the integral (A5) can easily be evaluated in cylindrical coordinates, giving

$$T(\vec{a},\vec{b})=\tfrac{4}{3}\pi\mathfrak{N}(\tfrac{1}{2}(\vec{a}-\vec{b}))[1-\tfrac{3}{2}|\tfrac{1}{2}(\vec{a}-\vec{b})|+\tfrac{1}{2}|\tfrac{1}{2}(\vec{a}-\vec{b})|^3]\,, \tag{A6}$$

and by inserting this result in (A4), we obtain

$$I(s,s',k)=8\frac{4\pi}{3}\int d^3r\left(\frac{\vec{r}\cdot\vec{k}}{r}\right)^2\times\mathfrak{N}(\vec{r}+\vec{t})(1-\tfrac{3}{2}|\vec{r}+\vec{t}|+\tfrac{1}{2}|\vec{r}+\vec{t}|^3)\,, \tag{A7}$$

where

$$\vec{t}=\tfrac{1}{2}(s-s')\vec{k}\,, \tag{A8}$$

and where the factor 8 preceding (A7) results from replacing the integration variable $\vec{r}$ in (A4) by $\frac{1}{2}\vec{r}$. Translating then the integration variable over $-\vec{t}$, and expressing the integral in spherical coordinates, (A7) becomes

$$I(s,s',k)=8\frac{4\pi}{3}\frac{k^2}{t^2}2\pi\int_0^1 r^2dr(1-\tfrac{3}{2}r+\tfrac{1}{2}r^3)\int_{-1}^1 du\frac{(rtu-t^2)^2}{r^2+t^2-2rtu}$$
$$=-8\frac{4\pi}{3}\frac{k^2}{t^2}\int_0^1 dr\left(r^4-\tfrac{3}{2}r^5+\tfrac{1}{2}r^7-3t^2(r^2-\tfrac{3}{2}r^3+\tfrac{1}{2}r^5)+\frac{1}{2t}(r-\tfrac{3}{2}r^2+\tfrac{1}{4}r^4)(r^2-t^2)^2\ln\left|\frac{r-t}{r+t}\right|\right). \tag{A9}$$

Although the further evaluation of (A9) is elementary, it is rather lengthy, and after a tedious calculation one eventually finds

$$I(s,s',k)=-8\frac{4\pi^2}{3}\frac{k^2}{t^2}\left[\frac{1}{2\times7\times9}-\frac{181t^2}{2\times3\times5\times7\times9}-\frac{71t^4}{2\times5\times7\times9}-\frac{2t^6}{5\times7\times9}+\frac{2t^6}{5\times7}\left(1-\frac{t^2}{9}\right)\ln\left|\frac{1-t^2}{t^2}\right|+\frac{1}{4t}\left(\frac{1}{7\times9}-\frac{3t^2}{5\times7}+\frac{t^4}{5}-\frac{t^6}{3}\right)\ln\left|\frac{1-t}{1+t}\right|\right], \tag{A10}$$

where t is given by (A8).

It is worthwhile to mention that, for small values of t, a Taylor-series expansion yields

$$I(s,s',k)\xrightarrow[t\to0]{}\pi^2k^2(\tfrac{16}{27}+\tfrac{32}{15}t^2+\cdots)\,. \tag{A11}$$

Inserting (A10) into (A2), and using (A8), one then finally obtains, with some algebra

$$G(k\,k_F,2\nu E_F/\hbar)\underset{|\nu|\gg|k^2/2\pm k|}{\simeq}-\frac{f(k,\nu)}{\nu^4}\frac{128\pi^2}{3}\left\{\frac{1}{2\times7\times9}-\frac{38}{3\times5\times7\times9}\left(\frac{k}{2}\right)^2-\frac{71}{2\times5\times7\times9}\left(\frac{k}{2}\right)^4-\frac{2}{5\times7\times9}\left(\frac{k}{2}\right)^6+\frac{2}{5\times7}\left(\frac{k}{2}\right)^6\left[1-\frac{1}{9}\left(\frac{k}{2}\right)^2\right]\ln\left|\frac{1-(\frac{1}{2}k)^2}{(\frac{1}{2}k)^2}\right|+\frac{1}{2k}\left[\frac{1}{7\times9}-\frac{3}{5\times7}\left(\frac{k}{2}\right)^2+\frac{1}{5}\left(\frac{k}{2}\right)^4-\frac{1}{3}\left(\frac{k}{2}\right)^6\right]\ln\left|\frac{2-k}{2+k}\right|\right\}. \tag{A12}$$

Using (A11) in (A2), the long-wavelength limit $k\to0$ can easily be found:

$$G(k\,k_F,2\nu E_F/\hbar)\xrightarrow[k\to0]{}\frac{f(k,\nu)}{\nu^4}\pi^2k^4\frac{8}{15}\,. \tag{A13}$$

From the definition (4) of $f(k,\nu)$, one therefore obtains in the long-wavelength limit, and, in the original units (q,ω) using (1),

$$G(q,\omega)\xrightarrow[q\to0]{}\frac{4}{15}\frac{q^2}{\omega^4}\frac{e^4k_F^4}{m^2\pi^2}\frac{1}{Q_0^2(q,\omega)}\simeq\frac{3}{20}\left(\frac{q}{k_F}\right)^2\,, \tag{A14}$$

which is exactly the result we obtained previously,[27] and from which it follows that the slope of the plasmon branch in the long-wavelength limit is lower by 10% to 20% compared to RPA in the range of metallic densities.

Finally, another interesting limit can be obtained from (A12). In the limit of very large k (but with a frequency still satisfying $|\nu|\gg|\frac{1}{2}k^2\pm k|$), a Taylor-series expansion in $1/k$ yields

$$G(k\,k_F,2\nu E_F/\hbar)\xrightarrow[\substack{|\nu|\gg|k^2/2\pm k|\\ k\to\infty}]{}\frac{f(k,\nu)}{\nu^4}\frac{32}{27}\times\pi^2k^2\left(1-\frac{4}{7}\frac{1}{k^2}+\cdots\right)\simeq\frac{1}{3}\left[1-\frac{4}{7}\left(\frac{k_F}{q}\right)^2\right]. \tag{A15}$$

This result will turn out to be very useful in paper II, when the third-moment sum rule will be discussed.

APPENDIX B: EVALUATION OF $A(a,b,c) \equiv \int_0^\infty d\xi (1/\xi) K_0(\xi a) J_1(\xi b) J_1(\xi c)$, $a>0,\ b>0,\ c>0$

Quite generally, this type of integral can be written as the fourth-type Appell hypergeometric function of two variables,[36] which in this case reduces to

$$A(a,b,c) = \frac{bc}{4a^2} F_4\left(1,1;2,2;-\frac{b^2}{a^2},-\frac{c^2}{a^2}\right). \quad \text{(B1)}$$

Because of the special values of the indices, it is possible to transform (B1) into an elementary function, by using the integral representation[37]

$$F_4(1,1;2,2;x-xy,y-xy) = \int_0^1 du \int_0^1 dv \frac{1-ux-vy}{(1-ux)^2(1-vy)^2}, \quad \text{(B2)}$$

which is valid if $|x| \leq \rho$, $|y| \leq \rho'$, where ρ and ρ' are some numbers, satisfying the conditions $\rho + \rho' < 1$ and $[\rho(1+\rho')]^{1/2} + [\rho'(1+\rho)]^{1/2} < 1$.

The fact that one has to consider the analytic continuation of (B1) and (B2), if these conditions are not fulfilled, makes it easier to follow another procedure, which is based on an integral representation for the product of two Bessel functions of the same order (Ref. 33, p. 367):

$$J_\nu(z)J_\nu(Z) = \frac{z^\nu Z^\nu}{2^\nu \Gamma(\nu+\frac{1}{2})\Gamma(\frac{1}{2})} \times \int_0^\pi d\varphi \sin^{2\nu}\varphi \frac{J_\nu((Z^2+z^2-2zZ\cos\varphi)^{1/2})}{(Z^2+z^2-2zZ\cos\varphi)^{1/2}}. \quad \text{(B3)}$$

The integral $A(a,b,c)$ then becomes

$$A(a,b,c) = \frac{bc}{\pi} \int_0^\pi d\varphi \frac{\sin^2\varphi}{(b^2+c^2-2bc\cos\varphi)^{1/2}} \times \int_0^\infty d\xi K_0(\xi a) J_1(\xi(b^2+c^2-2bc\cos\varphi)^{1/2}). \quad \text{(B4)}$$

As a function of ξ, the integrand is now a product of two Bessel functions, which by integration yields an ordinary hypergeometric function (Ref. 33, p. 410)

$$A(a,b,c) = \frac{bc}{\pi}\frac{1}{a^2}\int_0^\pi d\varphi \sin^2\varphi_2 \times F_1\left(1,1;2;-\frac{b^2+c^2-2bc\cos\varphi}{a^2}\right). \quad \text{(B5)}$$

By using a standard integral representation for the hypergeometric function, one obtains

$$A(a,b,c) = \frac{1}{4\pi}\int_0^1 dt \int_0^\pi d\varphi \sin^2\varphi \times \left(\frac{a^2+(b^2+c^2)t}{2bct} - \cos\varphi\right)^{-1}. \quad \text{(B6)}$$

The integral over φ can then be done by elementary methods:

$$A(a,b,c) = \frac{1}{4}\int_0^1 \frac{dt}{t}\left\{\frac{a^2+(b^2+c^2)t}{2bct} - \left[\left(\frac{a^2+(b^2+c^2)t}{2bct}\right)^2 - 1\right]^{1/2}\right\}. \quad \text{(B7)}$$

Finally performing the integration over t, one obtains

$$A(a,b,c) = \frac{1}{4bc}\left(\frac{1}{2}(W-a^2-b^2-c^2) + b^2 \ln\frac{b^2-c^2+a^2+W}{2a^2} + c^2\ln\frac{c^2-b^2+a^2+W}{2a^2}\right), \quad \text{(B8a)}$$

where

$$W = \{[a^2+(b-c)^2][a^2+(b+c)^2]\}^{1/2}. \quad \text{(B8b)}$$

Comparing (B8) with the result of Appendix D, we find the relation

$$\int_0^\infty \frac{d\xi}{\xi} K_0(\xi a) J_1(\xi b) J_1(\xi c) = \frac{1}{4bc}\frac{1}{\pi^2}\int_0^b \rho\, d\rho \int_0^c \rho'\, d\rho' \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \frac{1}{\rho^2+\rho'^2-2\rho\rho'\cos\varphi + a^2}. \quad \text{(B9)}$$

This transformation (B9) has been very useful in Sec. II for reducing the contribution of the second-order pole in $G(kk_F, 2\nu E_F/\hbar)$ to a single integral.

APPENDIX C: EVALUATION OF $F(b,a) = \int_0^\infty d\xi (\sin\xi/\xi)(d/d\xi)[J_1(a\xi)\sin b\xi]$ $a,b>0$

In Sec. II, the contribution to $G(kk_F, 2\nu E_F/\hbar)$ from the product of factors containing first-order poles, could be expressed as a double integral, because $F(b,a)$ can be expressed in terms of elementary functions (22)–(25).

Applying

$$\frac{d}{d\xi}J_1(a\xi) = \frac{a}{2}[J_0(a\xi) - J_2(a\xi)], \quad \text{(C1)}$$

the integral $F(b,a)$ can be written as

$$F(b,a)=\tfrac{1}{2}aF_0(b,a)+bF_1(b,a)-\tfrac{1}{2}aF_2(b,a)\,, \quad \text{(C2a)}$$

where

$$F_0(b,a)=\int_0^\infty d\xi\frac{1}{\xi}\sin\xi\sin b\xi\, J_0(a\xi)\,, \quad \text{(C2b)}$$

$$F_1(b,a)=\int_0^\infty d\xi\frac{1}{\xi}\sin\xi\cos b\xi\, J_1(a\xi)\,, \quad \text{(C2c)}$$

$$F_2(b,a)=\int_0^\infty d\xi\frac{1}{\xi}\sin\xi\sin b\xi\, J_2(a\xi)\,. \quad \text{(C2d)}$$

By expressing the product of trigonometric functions in (C2c) and (C2d) as a sum of trigonometric functions, both the integrals for $F_1(b,a)$ and $F_2(b,a)$ are sums of integrals of the Weber-Schaftheitlin type (Ref. 33, p. 405), yielding

$$F_1(b,a)=\frac{1}{2a}\left\{2-\Theta(a-|b+1|)(b+1)\left[1-\left(\frac{a}{1+b}\right)^2\right]^{1/2}-\Theta(a-|b-1|)(1-b)\left[1-\left(\frac{a}{1-b}\right)^2\right]^{1/2}\right\}, \quad \text{(C3)}$$

$$F_2(b,a)=-\frac{1}{2a^2}\left\{-4b+\Theta(a-|b+1|)(b+1)^2\left[1-\left(\frac{a}{1+b}\right)^2\right]^{1/2}-\Theta(a-|b-1|)(1-b)^2\left[1-\left(\frac{a}{1-b}\right)^2\right]^{1/2}\right\}, \quad \text{(C4)}$$

where the Θ function is defined as in (18). However, this procedure fails in evaluating $F_0(b,a)$ because both terms that would result from writing the product of trigonometric functions as a sum would diverge. We therefore use the integral

$$\frac{1}{\xi}\sin\xi\sin b\xi=\frac{1}{2}\int_{|1-b|}^{|1+b|}dy\,\sin\xi y \quad \text{(C5)}$$

to rewrite (C2b) as

$$F_0(b,a)=\frac{1}{2}\int_{|1-b|}^{|1+b|}dy\int_0^\infty d\xi\,\sin\xi y\, J_0(\xi a)\,. \quad \text{(C6)}$$

The integral over ξ is again of the Weber-Schaftheitlin type:

$$F_0(b,a)=\frac{1}{2}\int_{|1-b|}^{|1+b|}dy\,\Theta(a-y)\frac{1}{(y^2-a^2)^{1/2}}\,, \quad \text{(C7)}$$

and this integral can be done by elementary methods. Combining the result with (C4), (C3), and (C2a) one finally obtains

$$F(b,a)=\frac{1-b^2}{4a}\left\{\Theta(a-|1+b|)\left[1-\left(\frac{a}{1+b}\right)^2\right]^{1/2}-\Theta(a-|1-b|)\left[1-\left(\frac{a}{1-b}\right)^2\right]^{1/2}\right\}$$
$$+\frac{a}{4}\left\{\Theta(a-|1-b|)\ln\left|\frac{1+b+[(1+b)^2-a^2]^{1/2}}{|1-b|+[(1-b)^2-a^2]^{1/2}}\right|+\Theta(a-|1+b|)\Theta(|1-b|-a)\ln\frac{1+b+[(1+b)^2-a^2]^{1/2}}{a}\right\}. \quad \text{(C8)}$$

APPENDIX D: EVALUATION OF $J(a^2,b^2,c^2)=(\pi^2)^{-1}\int_0^b\rho\,d\rho\int_0^c\rho'd\rho'\int_0^{2\pi}d\varphi\int_0^{2\pi}d\varphi'(\rho^2+\rho'^2-2\rho\rho'\cos\varphi+a^2)^{-1}$ $a,b,c>0$

Because of the inequality $\rho^2+\rho'^2+a^2\geq 2\rho\rho'$, the integrations over φ and φ' are straightforward:

$$J(a^2,b^2,c^2)=4\int_0^b\rho\,d\rho\int_0^c\rho'\,d\rho'[(\rho^2+\rho'^2+a^2)^2-4\rho^2\rho'^2]^{-1/2}. \quad \text{(D1)}$$

The remaining double integral is not very difficult, if one introduces the new integration variables

$$\eta=\rho^2-\rho'^2,\quad \xi=\rho^2+\rho'^2\,, \quad \text{(D2)}$$

yielding

$$J(a^2,b^2,c^2)=\frac{1}{2}\int_{-c^2}^0 d\eta\int_{-\eta}^{\eta+2c^2}d\xi(\eta^2+2a^2\xi+a^4)^{-1/2}+\frac{1}{2}\int_0^{b^2}d\eta\int_\eta^{-\eta+2b^2}d\xi(\eta^2+2a^2\xi+a^4)^{-1/2}$$
$$-\frac{1}{2}\int_{b^2-c^2}^0 d\eta\int_{-\eta+2b^2}^{\eta+2c^2}d\xi(\eta^2+2a^2\xi+a^4)^{-1/2}. \quad \text{(D3)}$$

Performing the integrals over ξ, one obtains

$$J(a^2,b^2,c^2)=\frac{1}{2a^2}\left(\int_{-c^2}^{b^2-c^2}d\eta[(\eta+a^2)^2+4a^2c^2]^{1/2}-\int_{-c^2}^0 d\eta|\eta-a^2|+\int_{b^2-c^2}^{b^2}d\eta[(\eta-a^2)^2+4a^2b^2]^{1/2}-\int_0^{b^2}d\eta(\eta+a^2)\right), \quad \text{(D4)}$$

which again is rather elementary:

$$J(a^2, b^2, c^2) = \tfrac{1}{2}(W - a^2 - b^2 - c^2) + b^2 \ln \frac{c^2 - b^2 + a^2 + W}{2a^2} + c^2 \ln \frac{b^2 - c^2 + a^2 + W}{2a^2}, \tag{D5a}$$

where

$$W = [(b^2 - c^2)^2 + 2a^2(b^2 + c^2) + a^4]^{1/2}. \tag{D5b}$$

Comparing this result with the result (B8), one readily finds the relation

$$\frac{1}{\pi^2}\int_0^b \rho\, d\rho \int_0^c \rho'\, d\rho' \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \frac{1}{\rho^2 + \rho'^2 - 2\rho\rho' \cos\varphi + a^2} = 4bc \int_0^\infty d\xi \frac{1}{\xi} K_0(a\xi) J_1(b\xi) J_1(c\xi), \tag{D6}$$

which is used in Sec. II to calculate the contribution to $G(k k_F, 2\nu E_F/\hbar)$ from the poles of second order as a single integral.

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