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Dynamical exchange effects in the dielectric function of jellium from perturbative and variational methods

F. Brosens
Physics Department, University of Antwerp (Universitaire Instelling Antwerpen), Universiteitsplein 1, B-2610 Wilrijk, Belgium

J. T. Devreese
Physics Department, University of Antwerp (Universitaire Instelling Antwerpen), Universiteitsplein 1, B-2610 Wilrijk, Belgium,
Institute of Applied Mathematics, University of Antwerp (Rijksuniversitair Centrum Antwerpen), Groenenborgerlaan 171, B-2020 Antwerpen, Belgium,
and Eindhoven University of Technology, 5600-MB Eindhoven, The Netherlands
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The dielectric function of the electron gas with dynamical exchange effects, obtained from a variational treatment of the equation of motion for the Wigner distribution function, is compared with the expansion of the proper polarizability to first order in the electron-electron interactions. The latter dielectric function turns out to be the expansion of the variational one to first order in the exchange effects. Furthermore, the diagrammatic approach shows finite regions in the particle-hole continuum, where the imaginary part of the perturbative dielectric function is negative.

In an earlier paper,[1] a variational method was proposed to include dynamical exchange effects in the dielectric function of the homogeneous electron gas, via a complex and frequency-dependent "local-field correction" $G(q,\omega)$. In this procedure, a variational principle was used to obtain the dielectric function from the equation of motion for the Wigner distribution function, which was considered to first order in the applied external fields and decoupled according to the Hartree-Fock (HF) prescription.

As a result, the dielectric function was obtained in the form

$$\epsilon^{\mathrm{var}}(q,\omega)=1+\frac{Q_0(q,\omega)}{1-G^{\mathrm{var}}(q,\omega)Q_0(q,\omega)}\,, \tag{1}$$

where $Q_0(q,\omega)$ is the Lindhard function[2]

$$Q_0(q,\omega)=\frac{4\pi e^2}{q^2}\int d^3p\,\frac{N_{\vec{q}}(\vec{p})}{\omega^+-\vec{p}\cdot\vec{q}/m}\,, \tag{2}$$

with

$$\hbar N_{\vec{q}}(\vec{p})=f^0(\vec{p}+\hbar\vec{q}/2)-f^0(\vec{p}-\hbar\vec{q}/2)\,, \tag{3}$$

$f^0(\vec{p})$ is the equilibrium distribution function, assumed to be homogeneous in space, and for which in the actual calculations, the paramagnetic Fermi-Dirac distribution at zero temperature was taken. For the exchange correction $G^{\mathrm{var}}(q,\omega)$ the following expression was obtained:

$$G^{\mathrm{var}}(q,\omega)=\frac{4\pi e^2}{q^2}\frac{2\pi e^2\hbar^2}{Q_0^2(q,\omega)}\int d^3p\int d^3p'\,\frac{N_{\vec{q}}(\vec{p})N_{\vec{q}}(\vec{p}\,')}{|\vec{p}-\vec{p}\,'|^2}\frac{1}{\omega^+-\vec{p}\cdot\vec{q}/m}\left[\frac{1}{\omega^+-\vec{p}\,'\cdot\vec{q}/m}-\frac{1}{\omega^+-\vec{p}\cdot\vec{q}/m}\right]. \tag{4}$$

Some preliminary frequency-dependent results for $G^{\mathrm{var}}(q,\omega)$ were already given in Ref. 3, and also the outline of a method to reduce (4) to a numerically tractable twofold integral. A more elaborate study of the analytical methods involved is given in Ref. 4, and in Ref. 5 we give a quite extensive overview of the numerical results and of the sum rules and consistency requirements which are satisfied.

It should be noted that several other attempts[6–11] have been made to account for dynamical exchange effects via a complex frequency-dependent function $G(q,\omega)$, although in most of these treatments the actual evaluation was restricted to some limiting cases. The relation between these approximations is discussed in Ref. 12 and lies beyond the scope of the present paper. The treatment of dynamical exchange effects by Holas, Aravind, and Singwi[11] (hereafter referred to as HAS) leads to a dielectric function which is closely related to our variational result $G^{\mathrm{var}}(q,\omega)$. They obtain

$$\epsilon^{\mathrm{HAS}}(q,\omega)=1+Q_0(q,\omega)[1+G^{\mathrm{var}}(q,\omega)Q_0(q,\omega)]\,. \tag{5}$$

If (5) is written in the more familiar form

$$\epsilon^{\mathrm{HAS}}(q,\omega)=1+\frac{Q_0(q,\omega)}{1-G^{\mathrm{HAS}}(q,\omega)Q_0(q,\omega)} \tag{6}$$

the relation between $G^{\mathrm{var}}(q,\omega)$ and $G^{\mathrm{HAS}}(q,\omega)$ is obviously

$$G^{\mathrm{var}}(q,\omega)=\frac{G^{\mathrm{HAS}}(q,\omega)}{1-G^{\mathrm{HAS}}(q,\omega)Q_0(q,\omega)}\,. \tag{7}$$

Since HAS included dynamical-exchange effects by a diagrammatic expansion of the proper polarizability to first order in the electron-electron interaction, it is not surprising that their result $G^{\mathrm{HAS}}(q,\omega)$ is the dominant term in the expansion of $G^{\mathrm{var}}(q,\omega)$ if exchange effects are assumed to be relatively small. Similarly, the dielectric function $\epsilon^{\mathrm{HAS}}(q,\omega)$ is obtained by expanding $\epsilon^{\mathrm{var}}(q,\omega)$ to first order in the exchange correction.

The close relation between both approaches is also manifest from the equation of motion for the Wigner distribution function with dynamical exchange decoupling. As is discussed in Ref. 12, $\epsilon^{\mathrm{HAS}}(q,\omega)$ can be obtained from this equation of motion by iterating to first order, treating the exchange term as a first-order perturbation.

It should be emphasized that both the perturbative and the variational approaches give fairly similar results in many aspects. Most of the consistency requirements that have been checked do not favor one of both approaches, except for the compressibility sum rule. Indeed, the compressibility as obtained from $\epsilon^{\mathrm{HAS}}(q,\omega)$ turns out to be the expansion of the HF compressibility to first order in the electron-electron interaction, whereas $\epsilon^{\mathrm{var}}(q,\omega)$ is consistent with the HF compressibility. This phenomenon is closely related to the fact that $G^{\mathrm{var}}(q,\omega)$ is a universal function of q/k_F and $\hbar\omega/2E_F$ for all densities. The perturbative result $G^{\mathrm{HAS}}(q,\omega)$, however, explicitly depends on the density, even as a function of q/k_F and $\hbar\omega/2E_F$.

A detailed discussion of the general properties of $\epsilon^{\mathrm{var}}(q,\omega)$ and $\epsilon^{\mathrm{HAS}}(q,\omega)$ can be found in Refs. 5 and 12. But it is remarkable that neither of these properties gives some decisive insight concerning the validity of the approximations considered. Interesting conclusions should be obtained from the explicit evaluation of the ground-state energy, the static structure factor and the pair-correlation function from the dielectric function. Although HAS claim to have performed this calculation (slightly favoring their perturbative approach), we must

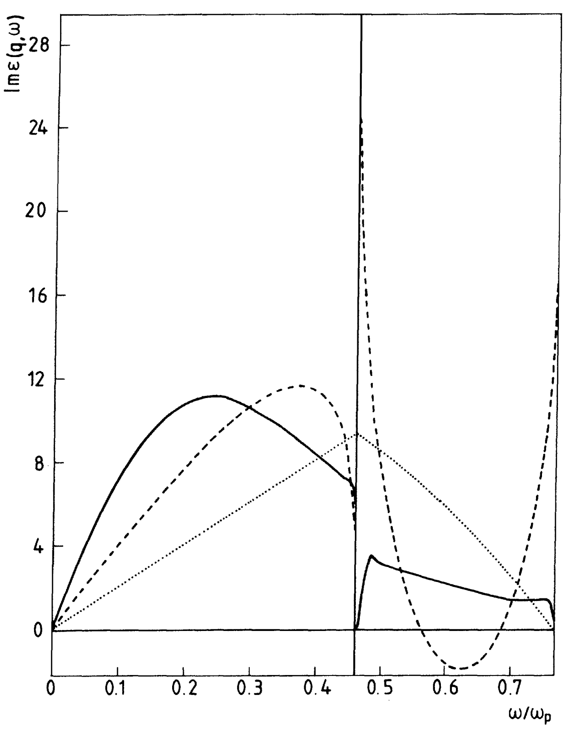

FIG. 2. Same as Fig. 1, but for $r_s=3$.

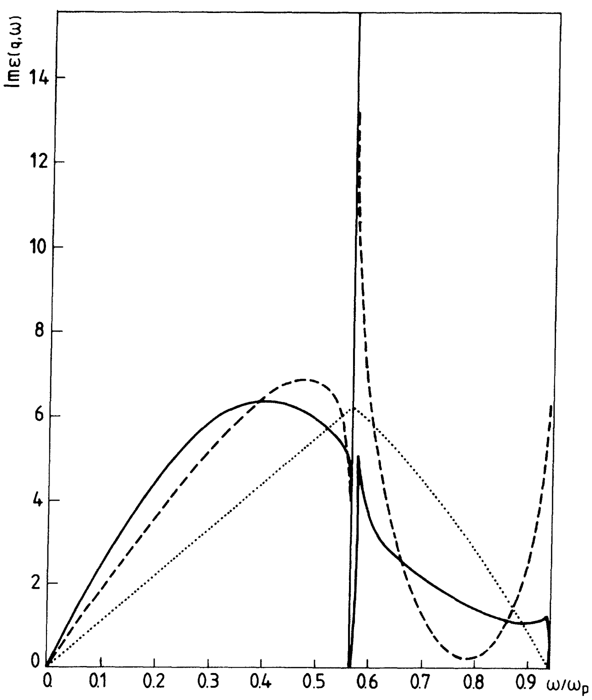

FIG. 1. Imaginary part of the variational (solid line) and perturbative (dashed line) dielectric function with dynamical exchange effects, compared to random-phase approximation (RPA) (dotted line), as a function of frequency for $q=k_F/2$ and $r_s=2$.

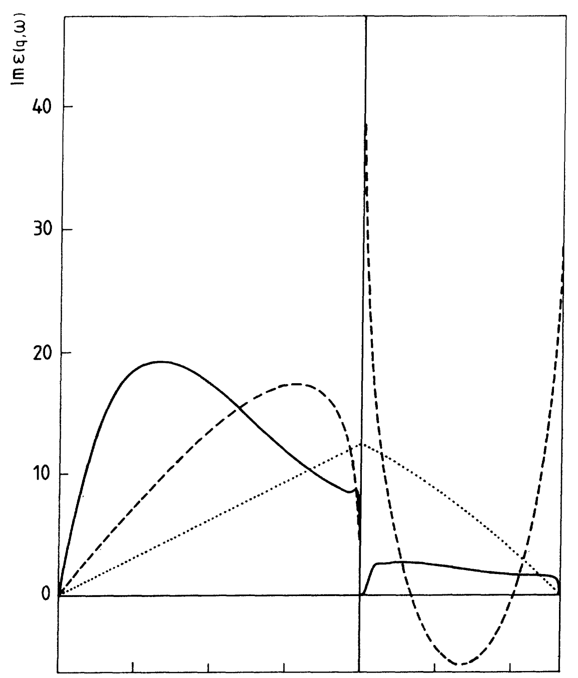

FIG. 3. Same as Fig. 1, but for $r_s=4$.

confess that we were unable to reproduce their results. Up to now, we did not succeed in developing an algorithm with sufficient accuracy to handle the rather singular dielectric function, including dynamical exchange effects.

However, another rather straightforward condition is that the imaginary part of the dielectric function should be positive. It is surprising that a direct evaluation of $\epsilon^{\text{HAS}}(q,\omega)$, starting from the tables in Ref. 5, and using (5) or (7) and (6), shows appreciable regions in the (q,ω) plane where its imaginary part turns out to be negative for sufficiently low density. This is shown in Figs. 1–3, where $\text{Im}\epsilon^{\text{HAS}}(q,\omega)$ is plotted as a function of ω/ω_p (ω_p is the plasma frequency) for $q=k_F/2$ and for the three values $r_s=2,3,4$ of the Wigner-Seitz radius r_s. For reference, the corresponding results of the random-phase approximation (RPA) and of the variational method are also given.

A major difference between $\epsilon^{\text{var}}(q,\omega)$ and $\epsilon^{\text{HAS}}(q,\omega)$ is that $\text{Im}\epsilon^{\text{HAS}}(q,\omega)$ has pronounced discontinuities at the parabolas $\nu=|k^2/2-k|$ and $\nu=k^2/2+k$ with

$$\nu=\hbar\omega/2E_F\ , \tag{8}$$

$$k=q/k_F\ . \tag{9}$$

These parabolas define distinct regions in the particle-hole continuum. In contrast, $\text{Im}\epsilon^{\text{var}}(q,\omega)$ tends to zero at these parabolas. This fact is related to the logarithmic singularities in $G^{\text{var}}(q,\omega)$, as discussed in Ref. 5. Since the perturbative approach is supposed to describe sufficiently small r_s, it is not completely unexpected that $\text{Im}\epsilon^{\text{HAS}}(q,\omega)$ becomes negative for larger r_s. However, a rather surprising problem occurs in the region $\nu>|k^2/2-k|$ for $k>2$ where $\text{Im}\epsilon^{\text{HAS}}(q,\omega)$ turns out to be negative, independent of r_s. This behavior can be derived from the following analytical considerations.

It has been shown (see, e.g., Ref. 4) that $G^{\text{var}}(q,\omega)$ can be written as

$$G^{\text{var}}(kk_F;2\nu E_F/\hbar)=\frac{2\pi^2}{k^2}f(k,\nu)R(k,\nu)\ , \tag{10a}$$

$$R(k,\nu)=k\int_{-1}^{1}dz\,T(z,k)\left[\frac{1}{\nu^+-k^2/2-kz}-\frac{1}{\nu^++k^2/2-kz}\right], \tag{10b}$$

with

$$f(k,\nu)=\frac{1}{2\pi^4a_0^2k^2k_F^2Q_0^2(q,\omega)}\ , \tag{11}$$

where a_0 is the Bohr radius, and where $T(z,k)$ is explicitly given in Ref. 4. From (5), (10), and (11) one readily derives

$$\text{Im}\epsilon^{\text{HAS}}(q,\omega)=\text{Im}Q_0(q,\omega)+\frac{\text{Im}R(k,\nu)}{\pi^2a_0^2k_F^2k^4}\ . \tag{12}$$

It is well known, as follows from (2), that

$$\text{Im}Q_0(kk_F,2\nu E_F/\hbar)=\begin{cases}\dfrac{2\nu}{a_0k_Fk^3}, & 0<\nu<k-k^2/2\\[2ex] \dfrac{k^2-(k^2/2-\nu)^2}{a_0k_Fk^5}, & |k-k^2/2|<\nu<k^2/2+k\ .\end{cases} \tag{13}$$

Furthermore, it follows from (10b) that

$$\text{Im}R(k,\nu)=\begin{cases}-\pi[T(\nu/k-k/2,k)-T(-\nu/k-k/2,k)], & 0<\nu<k-k^2/2\\ -\pi T(\nu/k-k/2,k), & |k-k^2/2|<\nu<k^2/2+k\ .\end{cases} \tag{14}$$

The lowest-frequency limit of the particle-hole continuum for $k>2$ corresponds to $\nu=k^2/2-k$, and thus involves $T(-1,k)$, which is given by (see Ref. 4)

$$T(\pm1,k)=-k\frac{k\pm2}{k\pm1}\ln\left|\frac{2\pm k}{k}\right|\ . \tag{15}$$

Since $T(-1,k)>0$ for $k>2$, and $\text{Im}Q_0(q,\omega)=0$ at the boundary of the continuum under consideration, it clearly follows from (12)–(15) that $\text{Im}\epsilon^{\text{HAS}}(q,\omega)<0$ in a finite region of the particle-hole continuum (which broadens with increasing r_s), even for arbitrary small r_s. These analytical considerations confirm the numerical evaluation. A very careful analysis to second order in the deviation from the boundary of the continuum leads to the same conclusion.

A similar analysis was performed for the variational result. Because in $\epsilon^{\text{var}}(q,\omega)$ both the imaginary and the real parts of $Q_0(q,\omega)$ and $G^{\text{var}}(q,\omega)$ must be included, the algebra involved is rather tedious, although straightforward. This analysis revealed that $\text{Im}\epsilon^{\text{var}}(q,\omega)$ does not present the problems which occur in $\epsilon^{\text{HAS}}(q,\omega)$, except possibly in an infinitesimally small interval for $k<2$ and $\nu\approx k-k^2/2$. Owing to the combination of logarithmic singularities from $G^{\text{var}}(q,\omega)$ and the discontinuity in the slope of $Q_0(q,\omega)$, we could not yet handle this region with sufficient reliability. Also, the numerical evaluation turns out to be rather inaccurate in the immediate neighborhood of this parabola.

In conclusion, we stress that both the perturbative and the variational approach for treating dynamical exchange effects have in many aspects the same merits and disadvantages. There are, however, a few properties which seem to favor the use of the variational dielectric function. In the first place, $\epsilon^{\text{HAS}}(q,\omega)$ is to be considered as the expansion of $\epsilon^{\text{var}}(q,\omega)$ to first order in the exchange effects. Furthermore, the imaginary part of the perturbative dielectric function $\epsilon^{\text{HAS}}(q,\omega)$ becomes negative in a finite region of the particle-hole continuum. The variational treatment of dynamical exchange seems not to suffer from this disadvantage, except possibly in an extremely small region, which up to now could not be handled accurately enough by analytical or numerical methods.

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