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Variational Solution of Vertex Equation and Dielectric Function of an Interacting-Electron Gas

A. K. Rajagopal
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803
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It is shown that the static dielectric function computed from a variational solution of the appropriate vertex function obeys the compressibility sum rule and reaches the well-established limit for large $\vec{k}$. The vertex equation contains the self-energy contributions to the one-electron states as well as the exchange contributions. A comparison of the results with a recent scheme due to Toigo and Woodruff shows that the moment-conserving approximation used by these authors is correct for small wave vectors and incorrect for large wave vectors in contrast to the variational method.

Recently,[1] we calculated the dielectric function, the spin, and orbital susceptibilities of an interacting-electron gas using a variational solution of the appropriate vertex functions. In this note we wish to bring to attention the results of the static dielectric function[2] and compare it with a recent calculation of the same function by Toigo and Woodruff[3] who use a moment-conserving approximation scheme.

The expression for the dielectric function is[1]

$$\epsilon_L(\vec{q},\omega)=1+2V(q)I_\rho^2(\vec{q},\omega)/[I_\rho(\vec{q},\omega)-J_\rho(\vec{q},\omega)]\,, \tag{1}$$

where

$$I_\rho(\vec{q},\omega)=\int\frac{d^3k}{(2\pi)^3}\left(\frac{f_0(\vec{k}+\frac{1}{2}\vec{q})-f_0(\vec{k}-\frac{1}{2}\vec{q})}{\omega+i\eta-\vec{k}\cdot\vec{q}/m}\right)\,, \tag{2a}$$

$$J_\rho(\vec{q},\omega)=\iint\frac{d^3k\,d^3k'}{(2\pi)^6}\left(\frac{f_0(\vec{k}+\frac{1}{2}\vec{q})-f_0(\vec{k}-\frac{1}{2}\vec{q})}{\omega+i\eta-\vec{k}\cdot\vec{q}/m}\right)\times\left(\frac{f_0(\vec{k}'+\frac{1}{2}\vec{q})-f_0(\vec{k}'-\frac{1}{2}\vec{q}')}{\omega+i\eta-\vec{k}'\cdot\vec{q}/m}\right)\times\left(1-\frac{\omega+i\eta-\vec{k}'\cdot\vec{q}/m}{\omega+i\eta-\vec{k}\cdot\vec{q}/m}\right)\,. \tag{2b}$$

Here $V(\vec{q})=(4\pi e^2/q^2)$. $f_0(k)$ is the usual Fermi function.

Equation (1) can be recast into a more familiar form:

$$\epsilon_L(\vec{q},\omega)=1+Q_0(\vec{q},\omega)/[1-G_v(\vec{q},\omega)\,Q_0(\vec{q},\omega)]\,, \tag{3}$$

where

$$Q_0(\vec{q},\omega)=2V(q)I_\rho(\vec{q},\omega)\,, \tag{3a}$$

$$G_v(\vec{q},\omega)=J_\rho(\vec{q},\omega)/Q_0(\vec{q},\omega)I_\rho(\vec{q},\omega)\,. \tag{3b}$$

a. $\vec{q}\to 0$ limit. As in most calculations we take $\omega=0$ in G_v from now on. When $\omega=0$, the $\vec{q}\to 0$ limit of the integrals (2a) and (2b) has already been calculated in Ref. 1:

$$I_\rho(\vec{q},0)\to mk_F/2\pi^2\,, \tag{4a}$$

$$J_\rho(\vec{q},0)\to(mk_F/2\pi^2)(\alpha r_s/\pi)\,. \tag{4b}$$

Thus, we have

$$G_v(\vec{q},0)\to\tfrac{1}{4}(q^2/k_F^2) \tag{5}$$

and so,

$$\lim_{q\to 0}q^2\epsilon_L(\vec{q},0)=4(\alpha r_s/\pi)/[1-(\alpha r_s/\pi)]\,, \tag{6}$$

which expresses the compressibility sum rule (see Ref. 3 for instance). The same result was also obtained by Toigo and Woodruff.

b. $\vec{q}\to\infty$ limit. It is easy to show that for large $\vec{q}$,

$$I_\rho(\vec{q},0)\to(2m/q^2)(k_F^3/3\pi^2)\,. \tag{7}$$

To estimate J_ρ we first recast (2b) in the following form (take $\vec{q}$ long the z direction):

$$J_\rho(\vec{q},0)=\frac{4m^2}{q^4}\iint\frac{d^3k\,d^3k'}{(2\pi)^6}f_0(\vec{k})f_0(\vec{k}')\times\left(2V(\vec{k}-\vec{k}')\frac{(k_z-k_z')}{q}\left[\left(1-\frac{2k_z'}{q}\right)^{-1}\left(1-\frac{2k_z}{q}\right)^{-2}-\left(1+\frac{2k_z'}{q}\right)\left(1+\frac{2k_z}{q}\right)^{-2}\right]\right.$$
$$\left.+2V(\vec{k}-\vec{k}'+\vec{q})\left\{\left(1-\frac{2k_z'}{q}\right)^{-1}\left(1+\frac{2k_z'}{q}\right)^{-1}\left(1+\frac{k_z-k_z'}{q}\right)\left[\left(1+\frac{2k_z}{q}\right)^{-1}+\left(1-\frac{2k_z'}{q}\right)^{-1}\right]\right\}\right)\,.$$

In the large-$\vec{q}$ limit then, since $V(\vec{k}-\vec{k}'+\vec{q}) \to 4\pi e^2/q^2$, we obtain finally after expanding the terms in powers of $(1/q)$

$$J_\rho(\vec{q},0) \simeq \frac{4m^2}{q^4}\; 4\pi e^2 \frac{4}{q^2} \iint_{FS} \frac{d^3k\, d^3k'}{(2\pi)^6} \times \left(\frac{2}{|\vec{k}-\vec{k}'|^2} (k_z k_z' - k_z^2) + 1 \right) . \quad (8)$$

FS here stands for integration over the Fermi surface.

Using the expression

$$\frac{1}{|\vec{k}-\vec{k}'|^2} = \sum_{lm} \frac{4\pi}{2l+1} V^{(l)}(\vec{k},\vec{k}')\, Y_{lm}(\hat{k})\, Y^*_{lm}(\hat{k}') , \quad (9)$$

where $V^{(l)}(\vec{k},\vec{k}')$ is related to the associated Legendre function, all the angular integrals and the subsequent sums on (lm) can be performed (after scaling k, k' by k_F):

$$J_\rho(\vec{q},0) \simeq \frac{64m^2\pi e^2 k_F^6}{q^6} \int_0^1 \frac{x^2dx}{2\pi^2} \int_0^1 \frac{x'^2dx'}{2\pi^2} \times \{\tfrac{2}{3}[\tfrac{1}{3}xx'V^{(1)}(x;x') - x^2V^{(0)}(x;x')] + 1\} .$$

Now, we have

$$\{\cdots\} = \left[\left(\frac{x'^2-x^2}{4xx'} \right) \ln\left| \frac{x+x'}{x-x'} \right| - \frac{1}{3} + 1 \right] . \quad (10)$$

The first term in this is antisymmetric under the exchange of $\vec{k}$, $\vec{k}'$ and hence vanishes. We, thus, obtain the result

$$J_\rho(\vec{q},0) \simeq \frac{64m^2\pi e^2}{q^6} \left[\left(\frac{k_F^3}{6\pi^2} \right)^2 - \frac{1}{3}\left(\frac{k_F^3}{6\pi^2} \right)^2 \right] = \frac{32m^2e^2k_F^6}{27\pi^3q^6} . \quad (10')$$

The integral (8) can also be written as

$$J_\rho(\vec{q},0) \simeq \frac{64m^2e^2\pi}{q^6} \times \iint_{FS} \frac{d^3k\, d^3k'}{(2\pi)^6} \left(1 - \frac{(k_z-k_z')^2}{|\vec{k}-\vec{k}'|^2} \right) \quad (8')$$

after symmetrizing the integrand with respect to $(\vec{k},\vec{k}')$. The integration is straightforward because of the spherical symmetry of the intergration region as was pointed out by Geldart *et al.*[4] very recently.

Hence, we have

$$G_v(\vec{q},0) \simeq \tfrac{1}{3} \quad \text{for} \quad \vec{q} \to \infty . \quad (11)$$

The integral that Toigo and Woodruff encountered in their calculation has the same appearance as (2b) except for the absence of the factors $(\omega + i\eta - \vec{k}\cdot\vec{q}/m)^{-1}(\omega + i\eta - \vec{k}'\cdot\vec{q}/m)^{-1}$ in the integrand in (2b). The above procedure then yields a plus sign in (8′) and (10′), and hence their integral can also be done exactly and differs from the result they quote. The same point has just been made by Geldart *et al.* also.[4] The above result (11) agrees with the static Hartree-Fock value for $G(q)$ derived by Geldart *et al.*,[4] in contrast to that of Toigo and Woodruff.

The "reduced" vertex function used in the above calculation is[1]

$$\tilde{\Gamma}_\rho(\vec{k};\vec{q}) = 1 + \int \frac{d^3k'}{(2\pi)^6} V(\vec{k}-\vec{k}') \times \left[\frac{f_0(\vec{k}'+\frac{1}{2}\vec{q}) - f_0(\vec{k}'-\frac{1}{2}\vec{q})}{\omega + i\eta - \vec{k}'\cdot\vec{q}/m} \right] \times \left(\tilde{\Gamma}_\rho(\vec{k}';\vec{q}) - \frac{\omega + i\eta - \vec{k}'\cdot\vec{q}/m}{\omega + i\eta - \vec{k}\cdot\vec{q}/m} \tilde{\Gamma}_\rho(\vec{k};\vec{q}) \right). \quad (12)$$

The variational solution

$$\tilde{\Gamma}_{\rho v}(\vec{k};\vec{q}) = I_\rho(\vec{q})/(I_\rho - J_\rho) \quad (13)$$

minimizes the density-density response function. In (12) the exchange processes and the self-energy contribution to the one-electron states are represented by the last two terms. This is the linearized form of the nonlinear vertex equation in the Ladder-Bubble scheme, where the equation explicitly contains also the dynamically screened exchange contributions. (See Ref. 5, for example.)

In trying to resolve the various intriguing problems associated with the calculation of the dielectric function of this system, Singwi *et al.*[6] proposed a very attractive and successful ansatz. Its relation to the usual many-body formalism (mbf) has remained a mystery. Instead of trying to understand the ansatz from the mbf, one, therefore, must resort to finding equivalent approximation schemes within the mbf and this resulted in the elegant moment conserving scheme of Toigo and Woodruff. The relation of our own earlier studies of the vertex function formalism and the new scheme of Toigo and Woodruff seems to be now clear. We may conclude that the Toigo-Woodruff scheme is exact in the small-$\vec{k}$ limit but not for large-$\vec{k}$ values, whereas our solution is exact in the small-$\vec{k}$ limit and approaches the static Hartree-Fock theory in the large-$\vec{k}$ limit. At present, we are studying (in collaboration with Rath) other correlations in the system using the Toigo-Woodruff formalism and will report the conclusions of this in the light of our recent work.

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