Short-range correlation in a two-dimensional electron gas

I. Nagy
Quantum Theory Group, Institute of Physics, Technical University of Budapest, H-1521 Budapest, Hungary
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Short-range correlation between electrons with antiparallel spins is considered for a two-dimensional electron gas. A model for the effective electron-electron interaction is constructed using a pseudo-linear-response treatment. This treatment rests on a parametric Thomas-Fermi-Weizsäcker approximation for screening. The parameter is constrained by the electronic cusp condition for the induced hole. Comparison with results obtained by means of the ladder approximation for the effective interaction is presented. A remarkable agreement for the pair-correlation functions at zero interparticle separation is established.

In a paramagnetic electron gas, the pair distribution function $g(r)$ is an arithmetic average of the spin-parallel distribution function $g^{\uparrow\uparrow}(r)$ and the spin-antiparallel one, $g^{\uparrow\downarrow}(r)$. The only fixed rule for $g(r)$ is that it may not be negative, since it is a probability.[1] The spin-parallel distribution function vanishes at zero interparticle separation $g^{\uparrow\uparrow}(0)=0$, due to the exclusion principle. Because of this restriction, the function $g^{\uparrow\uparrow}(r)$ at short distances is little affected by inclusion of the electrostatic Coulomb interaction. On the other hand, the interaction between two electrons of antiparallel spins in the presence of a filled Fermi sea plays a determining role in calculations of $g^{\uparrow\downarrow}(0)$. In the Hartree-Fock approximation $g^{\uparrow\downarrow}(0)=1$, deviations form this value signal the importance of correlation effects in an interacting electron liquid.[2] This polarization is related to deviations from plane-wave states, i.e., the wave function of two electrons with antiparallel spins is deformed at small separations by the short-range part of the effective potential.

The problem of $g^{\uparrow\downarrow}$ at short distances is essentially the two-particle-scattering problem in the medium. In the standard diagrammatic approach, one calculates the short-range part of the effective interaction by solving the Bethe-Goldstone integral equation[3] within the ladder approximation. In this case, the effective interaction (the particle-particle ladder vertex) satisfies an integral equation with bare Coulomb interparticle potential.[4–6] The kernel of the integral equation contains the Fermi factors that restrict the allowed states of a scattering pair in the filled Fermi sea.

The long-range correlations in an electron system reduce the Coulomb potential to a screened one. Using the physically appealing picture of impurity (with charge Z) screening, one can determine the induced hole and thus $g^{\uparrow\downarrow}(0)$ within an effective mean-field approximation. To our knowledge, such a treatment of the problem has not been discussed for a two-dimensional (2D) electron gas. Our basic framework is the Thomas-Fermi-Weizsäcker classical density-functional theory (TFW-λ), which relies directly on electron-density distributions and does not involve explicit electronic wave functions. We use Hartree atomic units throughout this report.

The energy functional of the TFW-λ theory for a D-dimensional electron gas with $V(D,r)$ common one-body potential is the following:[7]

$$E(D)=\int d^D r\left[t_{\mathrm{TF}}(D,n)+\frac{\lambda}{8}\frac{(\nabla n)^2}{n}+V(D,r)n\right], \tag{1}$$

where n is the density, λ is the Weizsäcker parameter, and t_{TF} is the Thomas-Fermi kinetic-energy density,

$$t_{\mathrm{TF}}(D,n)=\frac{2\pi D}{D+2}\left[\frac{1}{2}\Gamma\left[\frac{D+2}{2}\right]\right]^{2/D} n^{(D+2)/D}. \tag{2}$$

By variational principle, E is stationary with respect to small variation of the ground-state density, thus it is easy to obtain the relevant Euler equation. Next, we *linearize*[8] our Euler equation by using the $n(D,r)=n_0+\delta n(D,r)$ and $\delta n(D,r)=2\sqrt{n_0}w_L(D,r)+O(w_L^2)$ expressions, where n_0 is the unperturbed host density in dimension D. Finally, we arrive at the following equation for the determination of w_L:

$$\left[-\frac{\lambda}{2}\nabla^2+P(D,n_0)\right]w_L(D,r)+\sqrt{n_0}V(D,r)=0, \tag{3}$$

where

$$P(D,n_0)=2n_0\frac{\partial^2}{\partial n_0^2}t_{\mathrm{TF}}(D,n_0).$$

We can solve Eq. (3) by Fourier transformation; the result reads

$$w_L(D,q)=-\frac{\sqrt{n_0}}{(\lambda q^2/2)+P(D,n_0)}V(D,q). \tag{4}$$

The one-body potential in our mean-field approximation is *specified* as

$$V(D,q)=-v(D,q)[Z-\delta n(D,q)], \tag{5}$$

in which $v(D,q)=A(D)/q^{D-1}$ (here we exclude the $D=1$ case; see Ref. 9) is the Fourier transform of the Coulomb potential $v(r)=1/r$, and $A(D)$ is given by

$$A(D)=2^{D-1}\pi^{(D-1)/2}\Gamma[(D-1)/2].$$

By substituting Eq. (5) into Eq. (4) we obtain for the (linear) density change $\delta n(D,q)$,

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$$\delta n(D,q)=\frac{2Zn_0v(D,q)}{(\lambda q^2/2)+P(D,n_0)+2n_0v(D,q)} . \quad (6)$$

Considering the short-range part ($r\to 0$) of Eq. (3) we can deduce

$$\delta n'(D,r=0)=-\frac{4Zn_0}{\lambda(D-1)} \quad (7)$$

for the derivative of δn at the origin.

From this step we restrict ourselves to the $D=2$ and $Z=-1$ (i.e., electron) case. The induced hole density at zero interparticle separation ($r=0$) is given by

$$\delta n(2,r=0)=\frac{1}{2\pi}\int_0^\infty dq\, q\,\delta n(2,q) . \quad (8)$$

Introducing the variable $a=(4\pi n_0/\lambda)$, after straightforward integration one obtains [$P(2,n_0)=2\pi n_0$ and $v(2,q)=2\pi/q$] from Eq. (8) with Eq. (6),

$$\delta n(2,0)=-\frac{1}{2\pi}\frac{\alpha}{3-\alpha}\left[\frac{1}{2}\alpha\ln\left[\frac{\alpha^3}{2a}\right]+\frac{\alpha^3+4a}{\alpha}\frac{1}{\sqrt{\beta}}\times\left[\frac{\pi}{2}+\tan^{-1}\frac{\alpha}{\sqrt{\beta}}\right]\right] , \quad (9)$$

in which α and β are the following:

$$\alpha=[a+\sqrt{a^2+(a/3)^3}]^{1/3}+[a-\sqrt{a^2+(a/3)^3}]^{1/3} ,$$

$$\beta=a(6+\alpha)/\alpha .$$

From now on we keep Eq. (6) in view as the defining expression of a *pseudolinear* response treatment. In such a treatment, we transfer the problem of nonlinearity into the determination of λ, by using Eqs. (7) and (9), via the (representation-independent) electronic cusp condition[10]

$$\left.\frac{n'(D,r)}{n(D,r)}\right|_{r=0}=-\frac{4Z\mu}{D-1} , \quad (10)$$

in which μ is the two-body reduced mass; $\mu=\frac{1}{2}$ for electron-electron interaction ($Z=-1$), and $n(D,r)=n_0+\delta n(D,r)$ in *our* case. This condition is related to a general property of Coulombic systems and prescribes the proper derivative of configurational eigenfunctions or densities at the singularity point $r=0$. For high density of the system $n(D,r)\to n_0$, the parameter λ tends to a fixed value $\lambda\to\mu^{-1}$. The spin-antiparallel distribution function at zero interparticle separation is defined as follows:

$$g^{\uparrow\downarrow}(0)=1+\frac{\delta n(2,r=0)}{n_0} , \quad (11)$$

where $n_0=(\pi r_s^2)^{-1}$ is the host density and r_s is the usual density parameter.

In the following, we present results obtained for $g^{\uparrow\downarrow}(0)$ as a function of r_s. The solid curve in Fig. 1 is based on our approximation. The small solid circles refer to Ref. 6, in which the standard diagrammatic approach was used. By comparison we can establish a remarkable agreement over a very broad range of the electron density. An approximate solution of Ref. 6 is as follows:

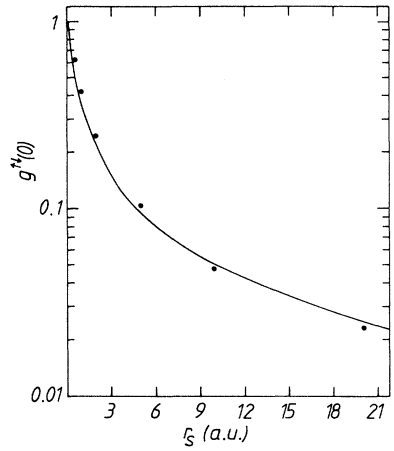

FIG. 1. Spin-antiparallel distribution function of a 2D electron gas at zero interparticle separation $g^{\uparrow\downarrow}(0)$, as a function of the density parameter r_s. The solid curve is the result of the present calculation while the small solid circles are results of Ref. 6, which is based on the diagrammatic method.

$$g^{\uparrow\downarrow}(0)=\left[1+\frac{\pi}{2}L_1(x)-\frac{\pi}{2}L_0(x)\frac{I_1(x)}{I_0(x)}\right]^2 , \quad (12)$$

where $x=(2\sqrt{2}r_s)^{1/2}$, L_0 and L_1 are modified Struve functions of order 0 and 1, I_0 and I_1 are modified Bessel functions of the first kind of order 0 and 1, respectively. For the very dilute limit ($r_s\to\infty$), Eq. (12) gives

$$g^{\uparrow\downarrow}(0)\to\frac{1}{x^2}\cong\frac{0.35}{r_s} .$$

In our formulation, the corresponding asymptotic result is

$$g^{\uparrow\downarrow}(0)\to\frac{B}{\mu r_s} ,$$

in which $B=(3\sqrt{3}/\pi)^{3/2}/8\cong 0.27$ and $\mu=\frac{1}{2}$ for electron-electron interaction. Our asymptotic expression gives accurate numerical values [in comparison with Eq. (11)] for $r_s>2$, in practice. It is worth mentioning that without constraining the values of λ (i.e., using only the value of $\lambda=\mu^{-1}$) the unmodified linear approximation results in $g^{\uparrow\downarrow}(0)\le 0$ for $r_s\ge 0.73$, which is unphysical.

In summary, we have calculated the spin-antiparallel distribution function at zero interparticle separation for a two-dimensional electron gas. We constructed a model for the induced hole using the impurity concept, via a pseudo-linear-response treatment based on a parametric Thomas-Fermi-Weizsäcker approximation. We applied a general constraint to determine the free parameter of the von Weizsäcker term. Application of this nonperturbative constraint in our model yields accurate values for $g^{\uparrow\downarrow}(0)$. The presented method might be useful to construct reliable screening densities and effective one-body scattering potentials for ions of different charge-sign moving in a 2D electron gas. A recently developed

theory of stopping power for two dimensions requires these potentials as input quantities.[11] Ideas of a similar nature were successfully applied to various problems in three dimensions also.[12]

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