Pair densities at contact in the quantum electron gas

R. Asgari$^{1,2}$, M. Polini$^1$, B. Davoudi$^{1,2}$, and M. P. Tosi$^1$

$^1$NEST-INFM and Classe di Scienze, Scuola Normale Superiore, I-56126 Pisa, Italy
$^2$Institute for Studies in Theoretical Physics and Mathematics, Tehran, P.O.Box 19395-5531, Iran

Abstract

The value of the pair distribution function $g(r)$ at contact ($r = 0$) in a quantum electron gas is determined by the scattering events between pairs of electrons with antiparallel spins. The theoretical results for $g(0)$ as a function of the coupling strength $r_s$ in the paramagnetic electron gas in dimensionality $D = 2$ and $3$, that have been obtained from the solution of the two-body scattering problem with a variety of effective scattering potentials embodying many-body effects, are compared with the results of many-body calculations in the ladder approximation and with quantum Monte Carlo data.

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*Corresponding author: tosim@sns.it
The equilibrium pair distribution function \( g(r) \) in a quantum electron gas describes the so-called Pauli and Coulomb hole which on average surrounds each electron from many-body exchange and Coulomb correlations. This function, which has an important role in the development of non-local density functional theories [1], is a weighted mean of the functions \( g_{\uparrow \uparrow}(r) \) and \( g_{\uparrow \downarrow}(r) \) for pairs of electrons with parallel or antiparallel spins. On account of the Pauli principle, \( g_{\uparrow \uparrow}(r) \) vanishes at contact \((r = 0)\) while \( g_{\uparrow \downarrow}(0) \) is wholly determined by scattering events between electron pairs. The value of \( g_{\uparrow \downarrow}(0) \) enters to determine the asymptotic values of the local field factors at large momenta and thus has a specific role in describing exchange and short-range correlation effects in the linear response properties of the electron gas (see e.g. [2] and references given therein).

Although the value of \( g_{\uparrow \downarrow}(0) \) results strictly from two-body collisional events, as noted above, the many-body aspects of the interactions between electrons in the quantum Coulomb gas affect the pair wave functions in a profound way. Two main theoretical approaches have been followed in the literature for evaluating \( g_{\uparrow \downarrow}(0) \). The first is based on many-body diagrammatic techniques and the second involves the direct calculation of the pair wave function from an appropriate Schrödinger equation. The main purpose of this Letter is to compare the results that have been obtained by these two methods in the paramagnetic fluid state over a broad range of values of the coupling strength appropriate Schrödinger equation. The main emphasis will be on results for the electron gas in dimensionality \( D = 2 \), where the many-body effects at any given \( r_s \) are comparatively more important. A discussion will also be given, however, for the 3D case.

A brief presentation of the two theoretical approaches will be useful. The approach first proposed by Yasuhara [3] and by Hede and Carbotte [4] for the 3D electron gas evaluates the ladder diagrams representing the virtual processes in which two electrons are excited from the unperturbed Fermi sphere leaving two holes behind and repeat their mutual interactions via the Coulomb potential to finally be scattered back into their initial momentum states. The calculation of these diagrams leads to an effective interaction between the two electrons which is to be determined from the solution of a Bethe-Goldstone integral equation. A simple analytic expression is obtained for \( g_{\uparrow \downarrow}(0) \) in terms of a modified Bessel function when the kernel of the integral equation is approximated to include the screening effects in a somewhat crude way. Further work on the electron-electron interactions in \( D = 3 \) from the Bethe-Goldstone equation was carried out by Lowy and Brown [5], who were able to establish a close connection between the diagrammatic approach and the self-consistent method of Singwi et al. [6].

The alternative method for the evaluation of pair distribution functions in the electron gas is based on the solution of the Schrödinger equation for the electron-pair wave function with the use of an effective scattering potential embodying many-body effects. This approach was initiated in the work of Overhauser [7], who constructed a simple model for the scattering potential in 3D as the electrostatic potential of an electron surrounded by a Wigner-Seitz sphere of neutralizing background. This potential vanishes outside the sphere, allowing simple analytic expressions to be obtained in this way for \( g_{\uparrow \downarrow}(0) \) and for the s-wave scattering length [7]. Later refinements have involved an accurate numerical solution of Overhauser’s two-body Schrödinger equation [8] and a self-consistent Hartree model for the scattering potential [9].

In the pair-scattering approach the value of \( g_{\uparrow \downarrow}(0) \) is determined by the square modulus of the s-wave component of the pair wave function \( \Phi_{k,\ell}^{(\uparrow \downarrow)}(r) \), averaged over the probability \( p(k) \) of finding two electrons with given relative momentum \( k \): that is,

\[
g_{\uparrow \downarrow}(0) = \frac{1}{\pi} \langle |\Phi_{k,\ell=0}^{(\uparrow \downarrow)}(0)|^2 \rangle_{p(k)} \tag{1}
\]

in \( D = 2 \). Here, \( \Phi_{k,\ell=0}^{(\uparrow \downarrow)}(r) \) is the solution of the Schrödinger equation

\[
\left\{ -\frac{\hbar^2}{m} \frac{d^2}{dr^2} - \frac{\hbar^2}{4m} \right\} \Phi_{k,\ell=0}^{(\uparrow \downarrow)}(r) + \frac{\hbar^2 k^2}{m} \Phi_{k,\ell=0}^{(\uparrow \downarrow)}(r) = \frac{\hbar^2 k^2}{m} \Phi_{k,\ell=0}^{(\uparrow \downarrow)}(r)
\]

where \( V_{KS}^{(\uparrow \downarrow)}(r) \) has been shown to be the Kohn-Sham effective potential associated with the local inhomogeneity in the density of electrons with given spin surrounding an electron of opposite spin [10]. The function \( p(k) \) can be evaluated from the free-electron momentum distribution, the result obtained by Ziesche et al. [11] for the 2D electron gas being...
related to the spin-resolved pair distribution functions by v proposed in Ref. [10]. That is, the results that we have obtained from Eq. (2) for a first-neighbour shell already at relatively low values of the coupling strength in this case [14]. We report in Figure 1 of exchange and correlation through a spin-dependent scattering potential is needed to account for the emergence of (formulae in Refs. [17,18]. Finally, the functions Sσσ′(q) in Eq. (4) are the partial liquid structure factors, which are related to the spin-resolved pair distribution functions by

\[ S_{\sigma\sigma'}(q) = \delta_{\sigma\sigma'} + \frac{n}{2} \int d^2r \left[ g_{\sigma\sigma'}(r) - 1 \right] \exp(-i\mathbf{q} \cdot \mathbf{r}). \]

The dependence of the scattering potentials in Eq. (4) on the pair distribution functions requires a self-consistent solution of the effective two-body Schrödinger equations for both \( g_{\uparrow\downarrow}(r) \) and \( g_{\uparrow\downarrow}(r) \) (see Ref. [10]).

Figure 1 plots the quantity \( r_s g(0) = r_s g_{\uparrow\downarrow}(0)/2 \) as a function of the coupling strength \( r_s \), as a device for emphasizing the large-\( r_s \) region where \( g_{\uparrow\downarrow}(0) \) is becoming very small at the expense of the low-\( r_s \) region where \( g_{\uparrow\downarrow}(0) \) can be calculated perturbatively [12]. Together with our present results we report those calculated by Isawa and Yasuhara [19] and by Nagano et al. [20,21] in the ladder approximation and those obtained in a QMC study by Dr. S. Moroni (private communication). The agreement between these two basic theoretical approaches with each other and with the QMC data is quite remarkable. It is also worth noticing from Figure 1 that the use of the Hartree model in the scattering approach [9] leads to results of good quantitative value for \( g_{\uparrow\downarrow}(0) \).

Figure 1 reports also some other theoretical results, which appear to be rather different from the evidence discussed just above. These are (i) the results reported by Freeman [22] from a coupled-cluster summation of ladder diagrams; (ii) the results obtained by representing the scattering potential in 2D through simple electrostatic models [12, 13]; and (iii) the results taken up to \( r_s \simeq 5 \) from the work of Bulutay and Tanatar [23], who used a classical-map hypernetted chain (CHNC) model proposed by Dharma-wardana and Perrot [24].

A similar examination of theoretical values for \( r_s g_{\uparrow\downarrow}(0) \) as a function of \( r_s \) in the 3D electron gas is displayed in Figure 2. While in this case the lack of data on local-field factors has prevented a self-consistent calculation including exchange and correlation in the scattering potentials, Figure 2 shows that the Hartree model results [9] are again in quite good agreement with those obtained by the evaluation of ladder diagrams [3] and from the QMC study of Ortiz and Ballone [25]. Figure 2 also reports the results obtained with Overhauser’s electrostatic model for the scattering potential [7, 8], which in the 3D case are in good agreement with the other evidence discussed just above. There are appreciable discrepancies, however, with the predictions given by an interpolation formula reported by Gori-Giorgi et al. [26] from unpublished QMC work by Ortiz and coworkers.

In summary, we have discussed the status of various theoretical approaches to the calculation of the pair distribution function at contact in the electron gas. In view of the demonstrated sensitivity of this quantity to the details of the
theory and to the role of exchange and short-range correlations, especially in the case $D = 2$, further accurate studies by quantum simulation techniques would be useful.

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FIG. 1. The pair distribution function $g(0)$ as a function of $r_s$ in the 2D electron gas (multiplication of $g(0)$ by $r_s$ enhances the strong-coupling regime). The present results are shown as dots and the QMC data as crosses. The meaning of the other symbols is as follows: PSDT and MM from Ref. [12] and [13], respectively; CHNC, from Ref. [23]; Hartree, from Ref. [9]; IY, NSO from Refs. [19-21]; Freeman, from Ref. [22]. The present results for $r_s g(0)$, as well as the QMC and Hartree ones, involve an extrapolation of the values of $g_{↑↓}(0)$ to $r = 0$, that we have carried out with the help of the cusp-condition law, $g_{↑↓}(r) = g_{↑↓}(0)[1 + \sqrt{2} r_s (r k_F) + ...]$. 
FIG. 2. The pair distribution function $r_s g(0)$ as a function of $r_s$ in the 3D electron gas. The QMC data from Ref. [25] are shown as crosses. The meaning of the other symbols is as follows: Overhauser and GP from Refs. [7] and [8], respectively; Hartree, from Ref. [9]; Y from Ref. [3]; GSB, from Ref. [26]. The cusp-condition law in 3D is $g_{\uparrow\downarrow}(r) = g_{\uparrow\downarrow}(0)[1 + (9\pi/4)^{-1/3} r_s (r k_F) + ...]$. 