Spin-resolved pair-distribution functions in an electron gas: A scattering approach based on consistent potentials

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The spin-resolved pair-functions $g_{\uparrow\downarrow}(r)$ and $g_{\uparrow\uparrow}(r)$ of an interacting unpolarized electron gas are calculated. The calculations are based on geminal representations of two-electron states and physically motivated model potentials, $V_{\uparrow\downarrow}(r)$ and $V_{\uparrow\uparrow}(r)$, in the scattering Schrödinger equations for relative movements. The proper normalization conditions for the pair functions, as natural constraints, are used to obtain consistent effective potentials. Good agreement with data of quantum Monte Carlo treatment on the pair-distribution functions is established. Possible applications of the potentials in other two- and one-particle characteristics are briefly discussed.

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I. INTRODUCTION

The uniform interacting electron gas is a prototype many-body model. This model is of great interest from important points of view: It provides an approximation to describe Fermi liquids in metals. It is the basic ingredient of practical density-functional approximations, both at the local-density level and beyond.

The pair-distribution function $g(r)$ of this system is a typical two-body quantity. This important quantity is related to the average density of electrons at r when an electron is at the origin $r=0$. With spin resolution, one has $g(r)=(1/2) \times [g_{\uparrow\downarrow}(r)+g_{\uparrow\uparrow}(r)]$ for an unpolarized system, and the normalizations for the spin-antiparallel and spin-parallel components are¹

$$\frac{n_0}{2} \int_0^\infty 4\pi r^2 [1 - g_{\uparrow\downarrow}(r)] dr = 0, \quad (1)$$

$$\frac{n_0}{2} \int_0^\infty 4\pi r^2 [1 - g_{\uparrow\uparrow}(r)] dr = 1, \quad (2)$$

where n_0 is the given density. These pair functions are the diagonal elements of the two-body density matrix. The $g_{\uparrow\uparrow}(r)$ of Eq. (2) describes *both* exchange and Coulomb correlations among equal-spin electrons, while $g_{\uparrow\downarrow}(r)$ of Eq. (1) describes Coulomb correlation among electrons of opposite spin.

The wave function of a noninteracting homogeneous system is described by a Slater determinant of one-particle plane-wave states, whose occupation function is the Fermi-Dirac one. These characterize the one-body matrix. In this ideal [$g_{\uparrow\downarrow}^0(r)=1$] case, the well-known expression for $g^0(r)$ is

$$g^0(r) = 1 - \frac{1}{2} \left[\frac{3}{x} j_1(x) \right]^2, \quad (3)$$

in which $j_1(x)=(\sin x - x \cos x)/x^2$, $x=k_F r$, and $k_F=(3\pi^2 n_0)^{1/3}$ (atomic units are used throughout).

This $g^0(r)$ is usually derived² via the Fourier transform of the one-particle ideal momentum distribution function. Of course, the $g_{\uparrow\downarrow}^0(r)$ and $g_{\uparrow\uparrow}^0(r)$ components satisfy the normalization conditions. The form of the noninteracting $g^0(r)$ of Eq. (3) is prescribed *solely* by the Pauli exclusion principle.

The constraints in Eqs. (1) and (2) should be useful in modeling and understanding the details of spin-resolved effective interactions in an interacting system. The present paper deals with this particular problem and rests on a natural factorization, via $V_{\uparrow\downarrow}(r)$ and $V_{\uparrow\uparrow}(r)$, to satisfy the normalization constraints.

The next section, Sec. II, contains a theoretical background, the physically motivated potentials, and our results with detailed comparisons. The last section, Sec. III, is devoted to a short summary.

II. THEORY AND RESULTS

One of the key quantities that provides a link between one- and two-matrix characteristics of an ideal system is the normalized probability, $P^0(k)$, of finding *two* electrons with relative momentum $\mathbf{k}=(\mathbf{k}_1-\mathbf{k}_2)/2$; $k \in [0, k_F]$. This probability is given by³

$$P^0(k) = 24 \frac{k^2}{k_F^3} \left[1 - \frac{3}{2} \frac{k}{k_F} + \frac{1}{2} \left(\frac{k}{k_F} \right)^3 \right]. \quad (4)$$

Two free electrons have $\varepsilon_k^0=k^2/2\mu$ energy in their center-of-mass system ($\mu=1/2$ is the reduced mass), and its average value (averages are denoted by $\langle \cdots \rangle$) is

$$\langle \varepsilon_k^0 \rangle = \int_0^{k_F} dk P^0(k) \frac{k^2}{2\mu} = \frac{3}{5} \frac{1}{2} k_F^2. \quad (5)$$

The other important step is the use of two-electron wave functions (geminals) in partial-wave representation^{4,5} for the spatial parts. The mutual scattering of two particles, which interact by central forces does not alter the center-of-mass

wavevector $\mathbf{K}=\mathbf{k}_1+\mathbf{k}_2$. It is unaffected by the scattering process, so that one can view the scattering in the rest frame where $\mathbf{K}=0$.

By weighting the *noninteracting* probability amplitudes of triplet and singlet states (at a given k) with the above $P^0(k)$, one gets,⁵ for Eq. (3), the following:

$$g^0(r) = \frac{3}{2} \sum_{\substack{\text{odd } l \\ l=1}}^{\infty} (2l+1) \langle j_l^2(kr) \rangle + \frac{1}{2} \sum_{\substack{\text{even } l \\ l=0}}^{\infty} (2l+1) \langle j_l^2(kr) \rangle. \quad (6)$$

The spin-resolved components are, therefore,

$$g_{\uparrow\downarrow}^0(r) = \sum_{l=0}^{\infty} (2l+1) \langle j_l^2(kr) \rangle \equiv 1, \quad (7)$$

$$g_{\uparrow\uparrow}^0(r) = 2 \sum_{\substack{\text{odd } l \\ l=1}}^{\infty} (2l+1) \langle j_l^2(kr) \rangle \equiv 1 - \left[\frac{3}{x} j_1(x) \right]^2, \quad (8)$$

in which the previously defined x variable is used.

Notice that only the triplet part (first term) of Eq. (6) and the $g_{\uparrow\uparrow}^0(r)$ component rest on the *same* (odd) partial waves. The $g_{\uparrow\downarrow}^0(r)$ component is characterized by all partial waves, similar to the scattering of distinguishable particles. The quite logical approximation for the case of an *interacting* system may rest on the radial solutions, $R_l(kr)$, of the scattering Schrödinger equation with *certain* effective potentials. Effective potentials that shape the geminals have received great theoretical interest recently.⁴⁻⁸ Sum rules for phase shifts, based on a generalized Hartree-Fock treatment by using the true one-particle momentum distribution function, have also been derived.⁹

In our paper, the averages, $\langle R_l^2(kr) \rangle$, will still be defined with $P^0(k)$, the ideal occupation of geminals. This treatment to a two-body quantity is partly motivated by the success of the Kohn-Sham auxiliary-orbital treatment with Fermi-Dirac occupation numbers. In such a treatment, one gets optimized ground-state densities¹⁰ in density-functional theory. Therefore, in our case, the effective potentials are those which result in normalized distribution functions, as prescribed by Eqs. (1) and (2). This goal is achieved via the auxiliary $\langle R_l^2(kr) \rangle$ terms in places of $\langle j_l^2(kr) \rangle$ in Eqs. (7) and (8) for the $g_{\uparrow\downarrow}(r)$ and $g_{\uparrow\uparrow}(r)$ components of $g(r)$ of an interacting system.

The potentials, $V_{\uparrow\downarrow}(r)$ and $V_{\uparrow\uparrow}(r)$, are modeled by the following forms:

$$V_{\uparrow\downarrow}(r) = \frac{1}{r} e^{-\lambda_{\uparrow\downarrow} r} \cos(\lambda r), \quad (9)$$

$$V_{\uparrow\uparrow}(r) = \frac{1}{r} e^{-\lambda_{\uparrow\uparrow} r} \cos(\lambda r). \quad (10)$$

The potentials have the Coulombic singularity. We fix their first zero by the intrinsic lengthscale of the system $r_s = [3/(4\pi n_0)]^{1/3}$ by using $\lambda = (\pi/2)/r_s$. Due to their oscillat-

FIG. 1. Numerically determined consistent screening parameters to Eqs. (9) and (10), as a function of the Fermi momentum (density parameter). The dashed-dotted lines are based on linear fitting, see Eqs. (12) and (13).

ing nature, these potentials can yield positive and negative phase shifts, depending on the value of l . Their Fourier transforms ($ij = \uparrow\downarrow$ or $\uparrow\uparrow$):

$$V_{ij}(q) = 4\pi \frac{q^2 + \lambda_{ij}^2 - \lambda^2}{[\lambda_{ij}^2 + (q + \lambda)^2][\lambda_{ij}^2 + (q - \lambda)^2]}, \quad (11)$$

at the forward ($q=0$) limit are useful in estimating *kinetic* energy changes using the $(n_0/2)V(q=0)$ perturbative expression.¹¹ It is this quantity which competes with the potential-energy gain due to the interaction.

It is to be noted that, in our problem, one is dealing with a kind of distortion by going from the noninteracting pair functions to the interacting ones. The electrons are inherent constituents of the Fermi system, i.e., no excess state is generated by their interaction.⁹ A lower-energy state is due to rearrangement contributions. In field-theoretical approximations for an effective interaction, the consideration of virtual-pair excitations together with the Pauli constraint yields to the Bethe-Goldstone equation.¹²

In order to determine the $\lambda_{\uparrow\downarrow}$ and $\lambda_{\uparrow\uparrow}$ parameters, as a function of k_F , we compute the $R_l(kr)$ functions using the above potentials in the center-of-mass wave equation. Their averages, $\langle R_l^2(kr) \rangle$, are used in the component equations [see, Eqs. (7) and (8)]. Finally, we constrain [see Eqs. (1) and (2)] the *volume* integrals of the $[g_{\uparrow\downarrow}(r) - g_{\uparrow\downarrow}^0(r)]$ and $[g_{\uparrow\uparrow}(r) - g_{\uparrow\uparrow}^0(r)]$ differences to be zero. The resulting $\lambda_{\uparrow\downarrow}(k_F)$ and $\lambda_{\uparrow\uparrow}(k_F)$ consistent parameters are plotted in Fig. 1, and are denoted by solid squares and circles, respectively. The linear fitting results in the simple

$$\lambda_{\uparrow\downarrow} = 0.07 + 0.86k_F, \quad (12)$$

$$\lambda_{\uparrow\uparrow} = 0.016 + 1.6k_F, \quad (13)$$

practical expressions for the $r_s \in [1, 10]$ most important

FIG. 2. The $r_s g(r=0)$ function as a function of the density parameter r_s . The solid curve (solid squares) is the present result. The dashed-dotted curve refers to the analytic expression of Overhauser. The dotted and dashed curves are based on the exact high-density expression and ladder approximation, respectively. Solid triangles are the results of numerical solution of an effective Euler-Lagrange equation.

range. The $\lambda_{\uparrow\downarrow} < \lambda_{\uparrow\uparrow}$ relation holds and, thus, $V_{\uparrow\downarrow}(r) > V_{\uparrow\uparrow}(r)$ in the investigated range of r_s . This observation is in accord with earlier physical statements.¹³

The value of $g(0, r_s)$ at a given density reflects most clearly the effect of Coulomb correlation since $g_{\uparrow\uparrow}(0, r_s) = 0$ due to the Pauli principle. Figure 2 contains the relevant information, as a function of the density parameter. Our results are plotted by solid squares on the solid curve. The dashed-dotted curve corresponds to the analytic expression⁴ of Overhauser (Ov): $g^{Ov}(0, r_s) = 32/(8 + 3r_s)^2$ obtained by using a Wigner-Seitz-type, fixed-range potential in the Schrödinger equation and treating the scattering in an approximate first iteration. The dashed curve is based on the well-known ladder approximation¹⁴ for the on-top $g(0, r_s)$ values. This last result is in perfect agreement with recent ones (not shown in Fig. 2), obtained by solving (numerically) the geminal-based scattering problem with the Wigner-Seitz⁵ and Hulthen-type⁸ potentials.

The dotted curve reflects the limited applicability of the high-density expression $2g(0, r_s) = 1 - 0.732r_s$ which is asymptotically exact.^{15,16} Our results in Fig. 2 can be numerically fitted to the expression $2g(0, r_s) = 1 - 0.62r_s$ in this limit. Let us mention that a one-parametric version of Eq. (9), i.e., using only a common (c) λ_c , could give perfect agreement with the asymptotic expression with $\lambda_c = 0.766k_F$. On the other hand, by this choice one *cannot* (similar to an asymptotic expansion¹⁶) satisfy the normalization conditions simultaneously.

The solid triangles denote the numerical results obtained from a zero-energy Schrödinger-type equation¹⁷ for the probability amplitude $\sqrt{g(r)}$. In this case, the common effective potential consists of the Coulombic, a bosonic reference, and a fermionic correction term. There is good agreement with our results. Similar Euler-Lagrange equations, with other type of effective interactions, were also investigated^{18,19} for the pair-correlation problem.

FIG. 3. Pair-correlation functions at $r_s = 1$, as a function of the (r/r_s) -variable. Solid squares, up triangles, and down triangles refer to Monte Carlo data.

In Figs. 3 and 4 we exhibit the $g_{\uparrow\downarrow}(r)$ and $g_{\uparrow\uparrow}(r)$ functions, together with their arithmetic mean $g(r)$, for $r_s = 1$ and $r_s = 5$, respectively. The increasing effect of Coulomb correlation at lower densities is clearly visible. There is a tendency to the *classically* optimal electrostatic limit: $g_{\uparrow\downarrow}(r) \approx g_{\uparrow\uparrow}(r) \rightarrow 0$ for $(r/r_s) \leq 1$. The data²⁰ of diffusion quantum Monte Carlo calculations are denoted by solid squares [$g(r)$], up triangles [$g_{\uparrow\uparrow}(r)$], and down triangles [$g_{\uparrow\downarrow}(r)$]. A remarkable agreement is clearly visible, which supports the reliability of the consistently optimized simple potentials. The physically motivated model [see Eqs. (9) and (10)] is capable of providing useful information in a broad range of densities of an interacting system.

A mathematically self-consistent field (SCF) approximation would require explicit connections between modulated density distributions and effective screening. Clearly, in our problem, a Poisson-equation-based connection⁶ (Hartree-type treatment) could cover the physics only partly; for a

FIG. 4. The same as in Fig. 3, at the $r_s = 5$ density parameter.

recent comparative discussion see Ref. 19. SCF attempts in the geminal-based construction for a two-particle quantity are inherently difficult, and need further investigations. The application of a $P(k)$ interacting normalized probability⁹ seems to be the first logical step in the present framework.

The consistent potentials obtained may be useful in scattering T -matrix construction and, thus, in retarded single-particle self-energy $\Sigma(\mathbf{k}_1)$ calculation.² Furthermore, transport characteristics involving scattering processes of electrons in different relative-spin states, can be easily modeled by the $V_{\uparrow\downarrow}(q)$ and $V_{\uparrow\uparrow}(q)$ consistent potentials. Effective spin-dependent interactions^{21,22} are needed in calculations related to the superconductivity problem, too.^{23,24}

Experimentally, in double-photoelectron emission from solids, one deals with a pair of electrons simultaneously.²⁵ The geminals may provide a consistent “initial state” to a detailed theory on this tool for electronic-correlation imaging. The couplings needed in the theory can be modeled by the spin-resolved potentials. Theoretical understanding of this problem should give important information beyond those obtained by using the “one-particle in a dielectric medium” concept.

III. SUMMARY

In the present paper, we have investigated the role of exchange and Coulomb correlations in the spin-resolved pair functions of an unpolarized interacting electron gas. The theoretical approach rests on the effective-potential concept and uses geminal representation for two-electron states. The level of consistency between potentials and pair functions is achieved by using the normalization conditions, as constraints, on the calculated pair functions. The consistent potentials give pair-distribution functions which are in good agreement with Monte Carlo data.

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