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Simple physical picture of the Overhauser screened electron-electron interaction

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As shown by Overhauser and others, the pair-distribution function $g(r)$ of a many-electron system may be found by solving a two-electron scattering problem with an effective screened electron-electron repulsion $V(r)$. We propose a simple physical picture in which this screened repulsion is the "dressed-dressed" interaction between two neutral objects, each an electron surrounded by its full-coupling exchange-correlation hole. For the effective interaction between two electrons of antiparallel spin in a high-density uniform electron gas of arbitrary spin polarization, we confirm that this picture is qualitatively correct. In contrast, the "bare-dressed" interaction is too repulsive, and does not have the expected symmetry $V_{\uparrow\downarrow}(r)=V_{\downarrow\uparrow}(r)$. The simple original Overhauser model interaction, independent of the relative spin polarization ζ, does not capture the ζ dependence of the correlation contribution to $g(r=0)$.

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I. INTRODUCTION

The quantum-mechanical many-electron problem is notoriously hard if all its degrees of freedom are taken into account. For both practical computational and conceptual purposes, however, it can often be replaced by a one- or two-electron problem with an effective external potential or electron-electron interaction, respectively. The effective potential that shapes the orbitals of the one-electron problem in Kohn-Sham density-functional theory[1,2] has been intensively explored, but the effective screened interaction that shapes the geminals of the two-electron problem[3–8] has received less attention. Here we propose and provide some support for a physically appealing "dressed-dressed" picture based upon the interaction between two neutral objects, each being an electron dressed by its surrounding exchange-correlation hole. In this picture, the "bare-bare" Coulomb repulsion $1/r$ is strongly screened out over the Wigner-Seitz radius r_s.

Overhauser[7] showed that the singlet geminals of an effective two-electron scattering problem can be used to estimate the on-top pair-distribution function $g(0)$ in a spin-unpolarized $(\zeta=0)$ three-dimensional electron gas of uniform density

$$\overline{n}=3/4\pi r_s^3. \tag{1}$$

(We use Hartree atomic units where $\hbar=m=e^2=1$.) Overhauser used an effective "bare-dressed" interaction between a bare electron and a neutral object composed of another electron and a concentric sphere of positive background charge of density $\overline{n}$ and radius r_s. Gori-Giorgi and Perdew[9,10] used the same effective interaction, but solved the Overhauser model exactly and found a pair-distribution function $g(r)$ in close agreement with that of Quantum Monte Carlo calculations over the whole short-range region $r\lesssim r_s$ for the physical density regime $1\lesssim r_s\lesssim 10$. For the high-density $(r_s\to 0)$ limit, they found good agreement with the exact[11,12] $g(r)$ to order r_s. Since then, there have been many related studies for the three- or two-dimensional electron gas,[13–17] sometimes using constructions of self-consistent effective interactions following the general bare-dressed picture of Overhauser.[3,7] Sum rules for the scattering phase shifts have also been derived.[18]

In this work, we consider a three-dimensional uniform electron gas with relative spin polarization

$$\zeta=(\overline{n_\uparrow}-\overline{n_\downarrow})/\overline{n}, \tag{2}$$

where $\overline{n}=\overline{n_\uparrow}+\overline{n_\downarrow}$ is the total density of Eq. (1). The pair-distribution function is then

$$g(r)=\left(\frac{1+\zeta}{2}\right)^2 g_{\uparrow\uparrow}(r)+\left(\frac{1-\zeta}{2}\right)^2 g_{\downarrow\downarrow}(r)+\frac{(1-\zeta^2)}{2}g_{\uparrow\downarrow}(r), \tag{3}$$

where only $g_{\uparrow\downarrow}$ contributes at $r=0$ because of the Pauli principle. $\overline{n}g(r)$ is the average density of electrons at r when an electron is at the origin, and $\overline{n}[g(r)-1]$ is the density of the exchange-correlation hole at full coupling strength, which carries a charge equal and opposite to that of the electron it surrounds:[10]

$$\int_0^\infty dr\, 4\pi r^2\overline{n}[g(r)-1]=-1, \tag{4}$$

with the same equation for $\overline{n_\uparrow}[g_{\uparrow\uparrow}(r)-1]$ and $\overline{n_\downarrow}[g_{\downarrow\downarrow}(r)-1]$. We focus on the effective interaction $V_{\uparrow\downarrow}(r)$ between two electrons of opposite spin in the high-density $(r_s\to 0)$ limit, since in this case correlation can be neglected and the interaction is purely electrostatic. Thus we can evaluate the bare-dressed and dressed-dressed models exactly and compare the predictions of both to the exact pair-distribution function[11,12,19] whose short-ranged part is dominated by $V_{\uparrow\downarrow}(r)$. We do not explicitly discuss the electron-electron scattering effects on transport properties, which are a second important application of the effective two-electron problem.[3,4,6,17] We note, however, that the expected symmetry $V_{\uparrow\downarrow}=V_{\downarrow\uparrow}$ of the effective interaction for $\zeta\neq 0$ is only achieved by the dressed-dressed picture, not by the bare-dressed one.

II. SPIN-UNPOLARIZED GAS

In the Overhauser approach[7,9] to electronic correlation in the unpolarized ($\zeta=0$) uniform gas, the many-electron problem is reduced to a scattering event between two electrons in a suitable effective potential $V(r,r_s)$, with a corresponding radial Schrödinger equation

$$\left[\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}-V(r,r_s)+k^2\right]u_\ell=0,$$

$$u_\ell=kr\,R_\ell(r,k,r_s). \quad (5)$$

The presence of the other electrons is taken into account in two ways: (i) via $V(r,r_s)$, (ii) via an average over the possible relative momentum $k=\frac{1}{2}|\mathbf{k}_1-\mathbf{k}_2|$ of the scattering event. The exchange symmetry between the two electrons is ensured via a proper summation over the partial waves ℓ; the resulting spin-resolved pair-distribution functions are then[9]

$$g_{\uparrow\downarrow}(r,r_s)=\left\langle\sum_{\ell=0}^{\infty}(2\ell+1)R_\ell^2(r,k,r_s)\right\rangle, \quad (6)$$

$$g_{\uparrow\uparrow}(r,r_s)=2\left\langle\sum_{\substack{\ell=1\\ \text{odd }\ell}}^{\infty}(2\ell+1)R_\ell^2(r,k,r_s)\right\rangle, \quad (7)$$

where the symbol $\langle\cdots\rangle$ denotes the average over the probability $p(k)$ (obtained from the momentum distribution of the ideal Fermi gas[9]). Overhauser's original choice[7] for $V(r,r_s)$ was the potential of an electron surrounded by a Wigner-Seitz sphere of uniformly distributed positive charge:

$$V(r,r_s)=\begin{cases}\frac{1}{r_s}\left(\frac{1}{s}+\frac{s^2}{2}-\frac{3}{2}\right) & (r\leq r_s)\\ 0 & (r>r_s),\end{cases} \quad (8)$$

where

$$s=r/r_s \quad (9)$$

is a scaled variable. As said, this simple potential gave surprisingly accurate results[9] for the short-range ($r\lesssim r_s$) part of the unpolarized-gas $g(r)$, at metallic and lower electron densities. The result for the high-density ($r_s\to 0$) limit was also quite accurate: the form of the screened Overhauser potential ensures that the correction to the noninteracting gas for $r_s\to 0$ is of first order in r_s, as in the exact perturbative result:[11]

$$g_{\sigma\sigma'}(s,r_s\to 0)=g^{(0)}_{\sigma\sigma'}(s)+r_s g^{(1)}_{\sigma\sigma'}(s)+o(r_s), \quad (10)$$

where $g^{(0)}$ is the pair-distribution function of the noninteracting gas. [Eq. (10) is valid for $r\ll\sqrt{r_s}$.] In particular, for the value of the $\uparrow\downarrow$ pair-correlation function at contact ($r=0$), the solution of the Overhauser model gives[9] $g_{\uparrow\downarrow}(r=0,r_s\to 0)=1-0.694\,r_s+o(r_s)$, in reasonable agreement with the exact result[12] $1-0.732\,r_s+o(r_s)$. Nagy *et al.*[17] have shown that the high-density form $g_{\uparrow\downarrow}(r=0,r_s\to 0)=1-\lambda\,r_s+o(r_s)$ is guaranteed when Eqs. (5)–(7) employ a screened potential with screening length $\propto r_s$. For finite r, the $r_s\to 0$ form of Eq. (10) is satisfied, within the Overhauser approach, if the potential $V(r,r_s)$ is such that

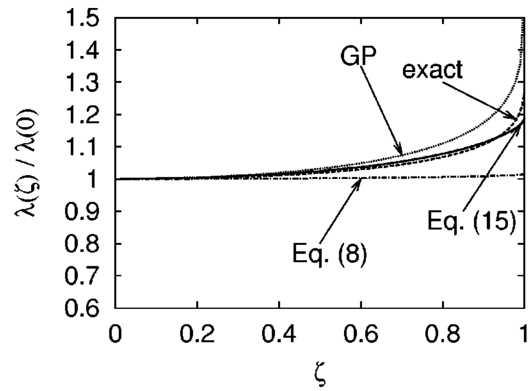

FIG. 1. ζ dependence of the high-density ($r_s\to 0$) correction to the on-top value $\lambda(\zeta)/\lambda(0)$ [see Eq. (12)]. The result from the dressed-dressed potential of Eq. (15) [$\lambda(0)=0.83$] is compared with the exact calculation[11,19] [$\lambda(0)=0.732$], with the result obtained from the original Overhauser potential of Eq. (8) [$\lambda(0)=0.694$], and with the scaling relation proposed in Ref. 9 (GP).

$$V(r,r_s\to 0)=\frac{1}{r_s}U(s). \quad (11)$$

The Overhauser potential of Eq. (8) fulfills Eq. (11) at all r_s.

III. SPIN-POLARIZED GAS

In the original formulation of the Overhauser model,[7] information on the spin-polarization state of the electron gas only enters through the probability distribution for the relative momentum k. The potential, purely based on classical electrostatic arguments, is independent of ζ. The probability functions $p_\zeta^{\sigma\sigma'}(k)$ are given in Eqs. (42)–(44) of Ref. 9, where, however, the calculations for the Overhauser model with $\zeta\neq 0$ have not been carried out. Instead, a scaling relation has been proposed.

Here, we carry out the calculations for the high-density limit with the correct $p_\zeta^{\uparrow\downarrow}(k)$, and we find a very weak ζ dependence of the first-order correction $\lambda(\zeta)$ to the on-top value,

$$g_{\uparrow\downarrow}(r=0,r_s\to 0,\zeta)=1-\lambda(\zeta)r_s+o(r_s), \quad (12)$$

as shown in Fig. 1. This is due to the weak[7] k dependence of the short-range part of the s-wave radial wave function $R_0(r\to 0,k,r_s)$ of Eq. (5). An explicit dependence on ζ in the effective potential is thus needed in order to reproduce the correct behavior[11,19] of the short-range part of $g(r)$ in the spin-polarized electron gas. Moreno and Marinescu[16] have recently applied the Overhauser model to the two-dimensional electron gas, finding an extremely weak ζ dependence of the on-top value. Figure 1 suggests that their result could be an artifact of their ζ-independent effective interaction.

IV. EFFECTIVE INTERACTION FOR OPPOSITE-SPIN ELECTRONS

In the high-density limit, a simple physically motivated effective potential for antiparallel-spin interactions, which depends on ζ and has the symmetry $\uparrow\downarrow=\downarrow\uparrow$, can be obtained in the following way. Consider two electrons of opposite spin in a uniform electron gas in the high-density limit. Each electron induces around itself an exchange hole, forming a neutral object. The effective potential can be approximated with the electrostatic interaction between two neutral or dressed objects. When $\zeta=0$, each electron is surrounded by a compact exchange hole, leading to effective screening of the Coulomb repulsion. But as ζ approaches 1, the exchange hole around the minority spin will become shallow and broad, so the Coulomb repulsion will be less well screened.

The two charge distributions are then

$$\rho_1(\mathbf{x})=\delta(\mathbf{x})+\overline{n_\uparrow}[g_x^{\uparrow\uparrow}(\mathbf{x})-1], \tag{13}$$

$$\rho_2(\mathbf{x})=\delta(\mathbf{x}-\mathbf{r})+\overline{n_\downarrow}[g_x^{\downarrow\downarrow}(\mathbf{x}-\mathbf{r})-1], \tag{14}$$

and the corresponding electrostatic potential is given by

$$V(r,r_s,\zeta)=\int d\mathbf{x}\int d\mathbf{x}'\frac{\rho_1(\mathbf{x})\rho_2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{15}$$

$V(r,r_s,\zeta)$ can be computed analytically: its Fourier transform $\tilde{V}(k,r_s,\zeta)$ is equal to

$$\tilde{V}(k,r_s,\zeta)=\frac{4\pi}{k^2}+v_1(k,r_s,\zeta)+v_2(k,r_s,\zeta)+v_3(k,r_s,\zeta),$$

with

$$v_1=[S_x^{\uparrow\uparrow}(k,r_s,\zeta)-1]\frac{4\pi}{k^2}, \tag{16}$$

$$v_2=[S_x^{\downarrow\downarrow}(k,r_s,\zeta)-1]\frac{4\pi}{k^2}, \tag{17}$$

$$v_3=[S_x^{\uparrow\uparrow}(k,r_s,\zeta)-1][S_x^{\downarrow\downarrow}(k,r_s,\zeta)-1]\frac{4\pi}{k^2}, \tag{18}$$

where $S_x^{\sigma\sigma}$ are the exchange-only static structure factors

$$S_x^{\sigma\sigma}=\begin{cases}\frac{3}{4}\frac{k}{k_F^\sigma}-\frac{1}{16}\left(\frac{k}{k_F^\sigma}\right)^3 & (k\leq 2k_F^\sigma)\\ 1 & (k>2k_F^\sigma),\end{cases} \tag{19}$$

with $k_F^\sigma=[1+\mathrm{sgn}(\sigma)\zeta]^{1/3}k_F$, $k_F=(9\pi/4)^{1/3}r_s^{-1}$, and $\mathrm{sgn}(\sigma)=+1$ for spin-$\uparrow$ and -1 for spin-$\downarrow$ electrons. The exchange-only pair-distribution function g_x only depends on r_s through the scaled variable $s=r/r_s$. This ensures that $V(r,r_s,\zeta)=(1/r_s)U(s,\zeta)$, as required by Eq. (11). The dimensionless potential $U(s,\zeta)$ is screened for $s\gtrsim 1$, and goes to zero, when $s\to\infty$, as s^{-4}. Its ζ dependence is the one expected from the qualitative arguments given above, as shown in Fig. 2: when $\zeta\to 1$ the potential is less and less screened; for ζ exactly equal to 1 (but only in this case) $U(s\to\infty,\zeta=1)$ goes to zero as s^{-2}.

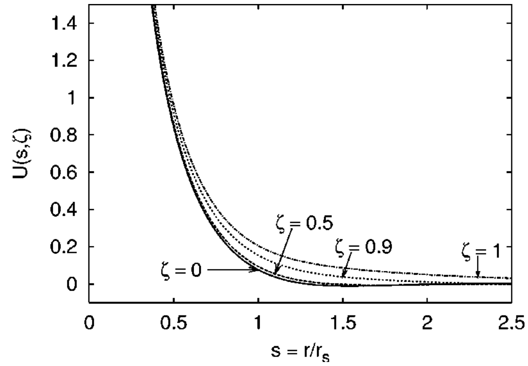

FIG. 2. ζ dependence of the dimensionless dressed-dressed potential $U(s,\zeta)$ calculated from Eq. (15).

Using the effective potential $U(s,\zeta)$ in the Overhauser scheme, we calculated the $\uparrow\downarrow$ high-density pair-correlation functions $g_{\uparrow\downarrow}^{(1)}$ for different values of the spin polarization ζ. They are shown in Fig. 3. The qualitative behavior is very similar to the exact one of Fig. 1 of Rassolov *et al.*[11] This is more evident in Fig. 1, where the function $\lambda(\zeta)/\lambda(0)$ is compared with the exact result.

While the ζ dependence of $g_{\uparrow\downarrow}^{(1)}(s,\zeta)$ obtained from the simple potential $U(s,\zeta)$ is rather good, the quantitative agreement with the exact result when $\zeta=0$ is less accurate than the result obtained with the original Overhauser potential. [In particular, we find $\lambda(0)=0.83$ in Eq. (12) for comparison with the original Overhauser and exact coefficients given after Eq. (10).] This is shown in Fig. 4: we see that for small *s*, $g_{\uparrow\downarrow}^{(1)}$ obtained with $U(s,\zeta)$ of Eq. (15) is too deep, while the original Overhauser potential of Eq. (8) gives a result which is slightly less deep than the exact one. This means that the original Overhauser potential of Eq. (8) is

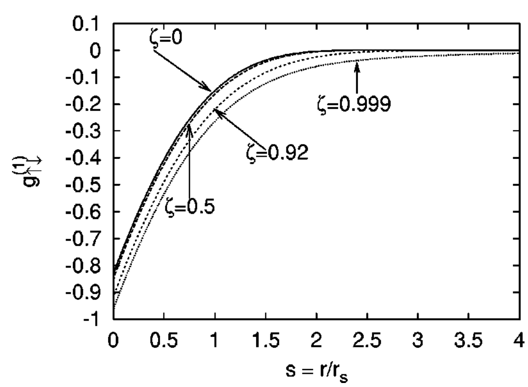

FIG. 3. High-density ($r_s\to 0$) $\uparrow\downarrow$ correlation holes computed from the dressed-dressed potential of Eq. (15) for different values of the spin polarization ζ.

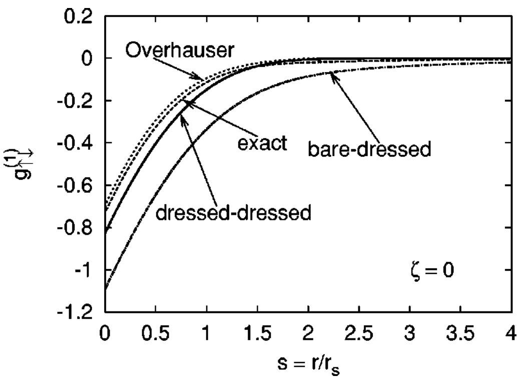

FIG. 4. High-density ($r_s \to 0$) ↑↓ pair-correlation function for the $\zeta=0$ gas obtained from different screened interactions: the dressed-dressed potential of Eq. (15), the original Overhauser potential of Eq. (8), and the bare-dressed potential of Eq. (20). The exact calculation of Rassolov *et al.*[11] is also reported.

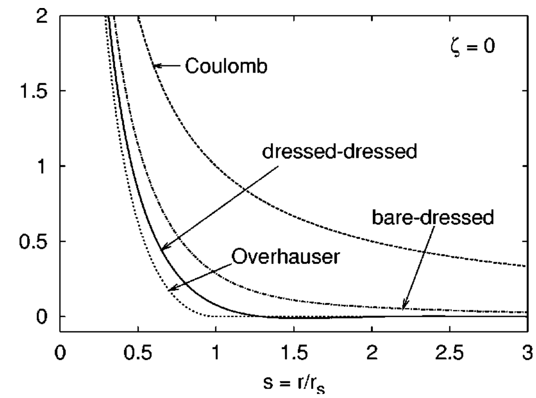

FIG. 5. Comparison of the bare Coulomb potential with different simple screened potentials for the $\zeta=0$ gas in the high-density ($r_s \to 0$) limit: the bare-dressed potential of Eq. (20), the dressed-dressed potential of Eq. (15), and the original Overhauser potential of Eq. (8). All curves have been multiplied by r_s.

slightly too screened in the $r_s \to 0$ limit, while $U(s,\zeta=0)$ of Eq. (15) is not screened enough in the same limit. The "exact" effective potential for the high-density limit should thus lie in between the two curves "Overhauser" and dressed-dressed of Fig. 5. In the same figure we also show the bare Coulomb potential, and the bare-dressed potential (obtained from the interaction of a bare electron with a dressed electron, i.e., surrounded by its exchange hole), whose Fourier transform $\tilde{V}_1(k,r_s,\zeta)$ is

$$\tilde{V}_1(k,r_s,\zeta)=\frac{4\pi}{k^2}+v_1(k,r_s,\zeta), \tag{20}$$

where v_1 is given in Eq. (16). The bare-dressed potential is "philosophically" closer to the original picture of Overhauser[3,7] and to the high-density limit of the self-consistent Hartree approximation of Davoudi *et al.*[14] We see that the bare-dressed potential is much less screened that the dressed-dressed one and thus corresponds to a deeper (i.e., further from the exact result) $g^{(1)}_{\uparrow\downarrow}$, as shown in Fig. 4.

The bare-dressed potential encounters severe problems for the calculation of $\lambda(\zeta)/\lambda(0)$ of Fig. 1. When $\zeta \to 1$, each majority ↑ electron dresses itself in an exchange hole deeper and more short-ranged than for $\zeta=0$, while each minority ↓ electron undresses. So the interaction between a bare ↓ and a dressed ↑ becomes *less* repulsive as ζ increases from 0, reducing $\lambda(\zeta)/\lambda(0)$. If we try to symmetrize using the interaction of a hypothetical bare ↑ with a dressed ↓, we find that this interaction tends to the unscreened $1/r$ as $\zeta \to 1$.

V. CONCLUSIONS

We have proposed a simple dressed-dressed picture for the effective screened electron-electron interaction that shapes the geminals and thus the pair distribution function of a many-electron system. In this picture, the interaction is between two neutral objects, each an electron dressed by its exchange-correlation hole. For two electrons of opposite spin in a high-density electron gas of arbitrary spin polarization, where the dressed-dressed and bare-dressed interactions can be evaluated exactly, we have shown that the dressed-dressed picture is qualitatively correct. In future work, it may be possible to construct the dressed-dressed $V_{\sigma\sigma'}(r)$ for all r_s and ζ, using density-functional theory[1,2] to describe the additional exchange-correlation terms that arise when $\sigma'=\sigma$ or $r_s \gg 0$.

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