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Pair distribution function in a two-dimensional electron gas

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Abstract

We calculate the pair distribution function, $g(r)$, in a two-dimensional electron gas and derive a simple analytical expression for its value at the origin as a function of r_s . Our approach is based on solving the Schrödinger equation for the two-electron wavefunction in an appropriate effective potential, leading to results that are in good agreement with quantum Monte Carlo data and with the most recent numerical calculations of $g(0)$ (Bulutay and Tanatar 2002 *Phys. Rev. B* **65** 195116). We also show that the spin-up spin-down correlation function at the origin, $g_{\uparrow\downarrow}(0)$, is mainly independent of the degree of spin polarization of the electronic system.

1. Introduction

There has recently been a growth of interest in studying the pair distribution function, $g(r)$, in electron gas models [1–4], caused mainly by its relevance in non-local density functional theories [5–7]. The zero inter-electronic distance value, $g(r = 0)$, also appears in the large wavevector and the high-frequency limits of the electronic charge and spin response functions [8, 9]. The importance of $g(r)$ lies in its connection with the electronic exchange and correlation of the electron gas model. Moreover, theoretical calculations of the pair distribution function can be directly compared with material properties since $g(r)$ is the Fourier transform of the static structure factor.

The pair distribution function is the probability of finding a pair of electrons at a distance r from each other. Therefore, the average number of electrons in a spherical shell centred on a given electron is $ng(r)\Omega_D r^{D-1} dr$, where $\Omega_D r^{D-1} dr$ is the volume of the D -dimensional shell and $n = N/V$ is the uniform electron density. At large distances, $g(r)$ approaches 1, whereas near the origin, where the electron charge is depleted, it is small on account of the Pauli exclusion principle and the exchange and correlation effects associated with the Coulomb interaction.

The subject of this paper is an analysis of the dependence of the pair correlation function on the inter-electronic distance and electron density in a two-dimensional, interacting, spin-polarized electron system. Earlier approaches to the calculation of this quantity using the

random phase approximation, the Hubbard approximation or the self-consistent Singwi–Tosi–Land–Sjölander approximation [10–12] were inadequate leading to divergences and negative values of the pair correlation function near the origin. Calculations of $g(r)$ in a two-dimensional paramagnetic electron gas have also been reported by Freeman [13] and Nagano *et al* [14] within the ladder approximation, by Tanatar and Ceperley [15] using the diffusion quantum Monte Carlo method (QMC) and, more recently, by Bulutay and Tanatar [16] using the hypernetted-chain approximation (CHNC). Moreover, an analytical expression of $g(0)$ has previously been derived by Polini *et al* [4].

In order to calculate $g(r)$, we follow the approach developed in three-dimensional systems by Overhauser [17] and further refined in [18] and [3]. This method is based on the relation between $g(r)$ and the two-electron scattering problem in an appropriately chosen effective potential which will be discussed in detail in the following sections. In addition to obtaining the variation of the pair distribution function as a function of the coupling strength, r_s , and of the spin polarization, we also derive an analytic expression for $g(0)$:

$$g(0) = \frac{1}{2} \frac{1}{[1 + 0.6032r_s + 0.07263r_s^2]^2}. \quad (1)$$

This expression is found to agree very well with the results of the most recent numerical calculations [15, 16]. We also compare our results with the expression derived in [4].

2. Effective model for the pair distribution function

A spin-polarized electron gas is characterized, in equilibrium, by two parameters: the electronic density, or its equivalent r_s , and the polarization, $\zeta = (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow)$, where n_\uparrow and n_\downarrow are the spin-up and spin-down electron densities. For this system, the pair distribution function is given by

$$g(\rho) = \frac{1}{4}[(1 + \zeta)^2 g_{\uparrow\uparrow}(\rho) + 2(1 - \zeta^2) g_{\uparrow\downarrow}(\rho) + (1 - \zeta)^2 g_{\downarrow\downarrow}(\rho)], \quad (2)$$

where $g_{\sigma\sigma'}$ are the spin-resolved pair distribution functions. Following Overhauser [18], $g_{\sigma\sigma'}$ can be related to the two-electron wavefunctions by [3]:

$$g_{\uparrow\downarrow}(\rho) = \frac{1}{2} \langle |\Psi_{\text{singlet}}(\rho)|^2 \rangle_{p_{\uparrow\downarrow}(k)} + \frac{1}{2} \langle |\Psi_{\text{triplet}}(\rho)|^2 \rangle_{p_{\uparrow\downarrow}(k)}, \quad (3)$$

$$g_{\uparrow\uparrow}(\rho) = \langle |\Psi_{\text{triplet}}(\rho)|^2 \rangle_{p_{\uparrow\uparrow}(k)}, \quad (4)$$

$$g_{\downarrow\downarrow}(\rho) = \langle |\Psi_{\text{triplet}}(\rho)|^2 \rangle_{p_{\downarrow\downarrow}(k)}, \quad (5)$$

where $\Psi_{\text{singlet}}(\rho)$ and $\Psi_{\text{triplet}}(\rho)$ are, respectively, the two-electron wavefunction for the singlet and triplet states and $\langle \dots \rangle_{p_{\sigma\sigma'}(k)}$ denotes the average over the probability of finding two electrons with relative momentum k and spins σ and σ' [3].

The wavefunction of an electron pair, $\Psi(\rho)$, verifies an effective Schrödinger equation:

$$-\frac{\hbar^2}{2m^*} \left(\frac{\partial^2 \Psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \Psi}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 \Psi}{\partial \phi^2} \right) + V(\rho) \Psi = E \Psi, \quad (6)$$

where $V(\rho)$ is the effective potential, $m^* = m/2$ is the reduced mass and E is the energy of the electron pair, which is approximated by $\hbar^2 k^2 / (2m^*)$. Since the solution to this equation can be written as $\Psi = \sum_m \cos(m\phi) \Psi_m(\rho)$, the spin-resolved pair distribution functions become

$$g_{\uparrow\downarrow}(\rho) = \langle |\Psi_0(\rho)|^2 \rangle_{p_{\uparrow\downarrow}(k)} + 2 \sum_{m=1}^{\infty} \langle |\Psi_m(\rho)|^2 \rangle_{p_{\uparrow\downarrow}(k)}, \quad (7)$$

$$g_{\uparrow\uparrow}(\rho) = 4 \sum_{m \text{ odd}} \langle |\Psi_m(\rho)|^2 \rangle_{p_{\uparrow\uparrow}(k)}. \quad (8)$$

Overhauser’s method relies on the appropriate selection of an effective potential capturing the short-range correlation effects of the Coulomb interaction. In three dimensions, Overhauser chose the electrical potential created by an electron and a neutralizing sphere of uniform charge with radius r_s surrounding it [17, 18]. The effective potential is expected to mimic the true one when the relative distance between electrons verifies $r < r_s$. When $r > r_s$ the potential vanishes and is not expected to be close to the true potential felt by an electron moving in a uniform electron gas. This approach is equivalent to assuming that the probability of finding three electrons in a sphere of radius r_s is exactly zero [3]. Numerical estimates of this probability for a three-dimensional interacting electron gas [19] have shown that is indeed small and we expect the same result to hold in two dimensions.

Following this procedure, in two dimensions, we might approximate the screened Coulomb potential by the potential of an electron surrounded by a circle of radius r_s uniformly filled with screening charge density $ne = e/(\pi r_s^2)$. For convenience, we introduce dimensionless variables, $x = \rho/r_s$ and $V(x) = V(\rho)/(e^2/r_s)$, where r_s is measured in units of Bohr radius ($a_B = \hbar^2/me^2$),

$$V(x) = \begin{cases} \frac{1}{x} - \frac{4}{\pi}E(x), & x \leq 1 \\ \frac{1}{x} - \frac{4}{\pi}x \left[E\left(\frac{1}{x}\right) - \left(1 - \frac{1}{x^2}\right)K\left(\frac{1}{x}\right) \right], & x \geq 1 \end{cases} \quad (9)$$

where $K(x)$ and $E(x)$ are, respectively, the complete elliptic integral of first and second kind. The screened potential of a uniformly charged disc of radius r_s with an electron at its centre does not vanish, but it has an attractive long-range tail, $V(x \rightarrow \infty) \rightarrow -1/(8x^3)$. Since we are interested in obtaining an analytical expression for $g(0)$, a further simplification of the effective potential is needed. Since Overhauser’s effective potential is not reliable outside the disc of radius r_s , the most reasonable simplification is to make it zero outside this disc. To avoid a discontinuity in the effective potential and considering that $V(x)$ is arbitrary to the extent that a constant can be added to it, we subtract from the potential in the region where $x \leq 1$ its value at $x = 1$, $V_0 = 1 - (4/\pi)$. Thus, our effective potential is:

$$V_{\text{eff}}(x) = \begin{cases} \frac{1}{x} - \frac{4}{\pi}E(x) + \frac{4}{\pi} - 1, & x \leq 1 \\ 0, & x \geq 1. \end{cases} \quad (10)$$

Figure 1 displays the initial effective potential from equation (9) together with our election of effective potential, equation (10), and the choice of Polini *et al* [4], which was based on a previous variational calculation [20]. The main difference between the effective potential used in [4] and ours is that the former has a discontinuity at $\rho = \sqrt{\pi}r_s/2$ while ours is always continuous.

Using equation (10) for the electronic potential, the Schrödinger equation becomes:

$$\begin{aligned} \frac{d^2\Psi_m}{dx^2} + \frac{1}{x} \frac{d\Psi_m}{dx} + \left(q^2 - \frac{m^2}{x^2} \right) \Psi_m(x) &= 0, & x \geq 1, \\ \frac{d^2\Psi_m}{dx^2} + \frac{1}{x} \frac{d\Psi_m}{dx} + \left(q^2 - \frac{m^2}{x^2} \right) \Psi_m(x) & \\ - r_s \left(\frac{1}{x} - \frac{4}{\pi}E(x) + \frac{4}{\pi} - 1 \right) \Psi_m(x) &= 0, & x \leq 1, \end{aligned} \quad (11)$$

where the relative momentum is also renormalized, $q = kr_s$. The general solution for $x \geq 1$ is given by $\Psi_m(x) = J_m(qx) + B_m(q, r_s)N_m(qx)$, where J_m is the Bessel function of order m and N_m is the corresponding Neumann function. The coefficient $B_m(q, r_s)$ can be written as

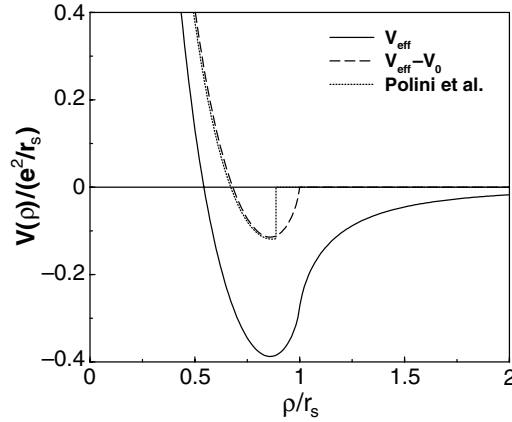


Figure 1. Normalized effective potential, $V(\rho)/(e^2/r_s)$, as function of ρ/r_s . The potential from equation (9) (solid curve) and our choice of effective potential, equation (10) (dashed curve) are displayed. The effective potential used by Polini *et al* [4] is also shown (dotted curve).

$B_m(q, r_s) = \cot(\delta_m(q, r_s))$, where $\delta_m(q, r_s)$ is the wavefunction phase shift due to the presence of the scattering potential¹.

To find the solution inside the circle of radius unity we make a Taylor expansion of the pair wavefunction: $\Psi_m(x) = \sum_{n=m}^{\infty} \alpha_{m,n} x^n$. We arrive at the following recurrent relation between the coefficients:

$$(n^2 - m^2)\alpha_{m,n} = r_s \left\{ \alpha_{m,n-1} + \left(\frac{4}{\pi} - 3 \right) \alpha_{m,n-2} + \sum_r \mathcal{A}(r) \alpha_{m,n-2r-2} \right\} - q^2 \alpha_{m,n-2}, \quad (12)$$

where $\mathcal{A}(r) = 2 \left[\frac{(2r-1)!!}{2^r r!} \right]^2 \frac{1}{2r-1}$. As a consequence of this recurrent relation, every $\alpha_{m,n}$ is proportional to $\alpha_{m,m}$ and a function of r_s and q , $\alpha_{m,n} = \alpha_{m,m} F_n(r_s, q)$.

In order to solve equation (11) we match $\Psi_m(x)$ and its derivative at $x = 1$:

$$\alpha_{m,m} G_m(r_s, q) = J_m(q) + B_m(q, r_s) N_m(q) \quad (13)$$

$$\alpha_{m,m} \tilde{F}_m(r_s, q) = q J'_m(q) + B_m(q, r_s) q N'_m(q) \quad (14)$$

where $G_m(r_s, q) = \sum_{n=m}^{\infty} F_n(r_s, q)$ and $\tilde{F}_m(r_s, q) = \sum_{n=m}^{\infty} n F_n(r_s, q)$. For a given momentum transfer and coupling strength the parameters $\alpha_{m,m}$ and $\delta_m(q, r_s)$ become

$$\alpha_{m,m}(q, r_s) = \frac{J_m(q) + \cot(\delta_m(q, r_s)) N_m(q)}{G_m(r_s, q)}, \quad (15)$$

and

$$\cot(\delta_m(q, r_s)) = \frac{\tilde{F}_m(r_s, q) J_m(q) - G_m(r_s, q) q J'_m(q)}{G_m(r_s, q) q N'_m(q) - \tilde{F}_m(r_s, q) N_m(q)}. \quad (16)$$

The pair wavefunctions $\Psi_m(x)$ are computed for any value of q and r_s using equations (15) and (16) and the spin-resolved pair distribution functions are calculated using equations (7) and (8) and an appropriate choice for the distribution of the relative momentum of an electron pair. For simplicity, we use the probability distribution of a free Fermi gas. For the unpolarized electron system, the probability of a pair with momentum q is independent of the spin

¹ At large distances the two-electron wavefunction can be written as: $\Psi_m(x) \rightarrow \sqrt{2/\pi q x} [\cos(qx - m\pi/2 - \pi/4) + \cot(\delta_m(q, r_s)) \sin(qx - m\pi/2 - \pi/4)] = [1/\sin \delta_m(q, r_s)] \sqrt{2/\pi q x} \sin[qx - m\pi/2 - \pi/4 + \delta_m(q, r_s)]$.

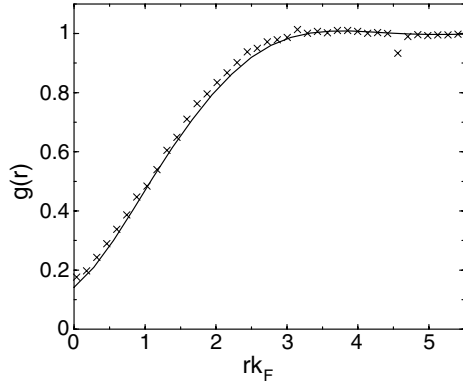


Figure 2. Pair distribution function of the unpolarized electron gas at $r_s = 1$ as a function of rk_F . Our approximation (solid curve) is compared with the quantum Monte Carlo data of [15] (crosses).

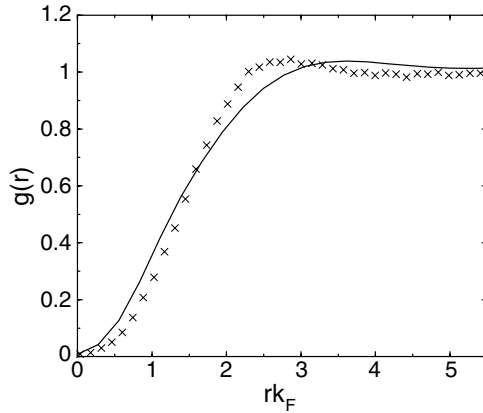


Figure 3. Pair distribution function of the unpolarized electron gas at $r_s = 5$ as a function of rk_F . Our approximation (solid curve) is compared with the quantum Monte Carlo data of [15] (crosses).

orientation and proportional to the overlap between two circles of radius k_F displaced by $2q$ [19],

$$p_{\sigma\sigma'}(q) = \frac{16q}{\pi k_F^2} \left[\arccos\left(\frac{q}{k_F}\right) - \left(\frac{q}{k_F}\right) \sqrt{1 - \left(\frac{q}{k_F}\right)^2} \right]. \tag{17}$$

Figures 2 and 3 display our results for the pair distribution function of the unpolarized system at $r_s = 1$ and 5 respectively. We have used seven ($m_{\max} = 7$) partial waves and up to $n = 50$ terms for the expansion of $\Psi_m(x)$ in the internal disc. We have checked that this choice of parameters is consistent with the charge neutrality condition, $2 \int_0^\infty x dx [g(x) - 1] = -1$, for small values of r_s . Our results at moderate coupling strengths agree quite well with the QMC data [15]. However, at larger values of r_s our method is unable to reproduce the strong quantum oscillations of the numerical results and tends to slightly overestimate the value of $g(r)$. This discrepancy is expected and shared by previous calculations using a self-consistent Hartree scheme [1]. With decreasing dimensionality the role of exchange and correlations becomes more important and a screened Coulomb potential is insufficient to completely capture this

physics. The use of self-consistent spin-dependent effective potentials has proved able to reproduce more closely the numerical results in this range of densities [2].

3. Pair distribution function at the origin

At zero distance, $g_{\uparrow\uparrow}(\rho = 0)$ vanishes on account of the Pauli exclusion principle, while $g_{\uparrow\downarrow}(\rho = 0)$ is determined by the $m = 0$ component of the two-body wavefunction,

$$g_{\uparrow\downarrow}(\rho = 0) = \langle |\Psi_0(\rho = 0)|^2 \rangle_{p_{\uparrow\downarrow}(k)} = \langle |\alpha_{0,0}|^2 \rangle_{p_{\uparrow\downarrow}(k)}. \quad (18)$$

Since the distribution of the relative momentum of an electron pair is a smooth function, a good estimate of $\langle |\alpha_{0,0}|^2 \rangle_{p_{\uparrow\downarrow}(k)}$ is obtained by making an expansion around the momentum where the distribution reach its maximum as:

$$\alpha_{0,0} \sim \frac{1}{G(r_s)}, \quad (19)$$

where the momentum dependence of G has been dropped. Using the recurrent relation (12), we obtain a series expansion of $G(r_s)$:

$$\begin{aligned} G(r_s) = & 1 + r_s \left\{ a_1 + \sum_{m=1}^{\infty} \frac{\mathcal{A}(m)}{(2m+2)^2} \right\} + r_s^2 \left\{ a_2 + \sum_{m=1}^{\infty} \mathcal{A}(m) \left[\frac{1}{(2m+3)^2} \left(1 + \frac{1}{(2m+2)^2} \right) \right. \right. \\ & + \left. \left(\frac{1}{\pi} - \frac{3}{4} \right) \frac{1}{(2m+4)^2} \left(1 + \frac{4}{(2m+2)^2} \right) \right. \\ & \left. \left. + \sum_{n=1}^{\infty} \mathcal{A}(n) \frac{1}{(2n+2)^2(2n+2m+4)^2} \right] \right\} + O(r_s^3) \\ & \sim (1 + 0.6032r_s + 0.07263r_s^2) \end{aligned} \quad (20)$$

where $a_1 = \frac{1}{4} + \frac{1}{\pi}$ and $a_2 = \frac{5}{9\pi} - \frac{1}{6} + \frac{1}{4} \left(\frac{1}{\pi} - \frac{3}{4} \right)^2$.

We can obtain $g(0)$ at any order in the expansion on the parameter r_s since $g(\rho = 0) = \frac{1}{2} g_{\uparrow\downarrow}(0) = \frac{1}{2} \frac{1}{G(r_s)^2}$. To first order in the expansion of $G(r_s)$ the pair distribution is:

$$g(\rho = 0) = \frac{1}{2} \frac{1}{[1 + 0.6032 r_s]^2}. \quad (21)$$

To second order we recover equation (1). Our approximation procedure also allows us to sum all the orders as:

$$g(\rho = 0) = \frac{1}{2} \left(\sum_{n=0}^{\infty} \frac{\alpha_{0,n}}{\alpha_{0,0}} \right)^{-2}. \quad (22)$$

Finally, we also calculate $g(0)$ performing the average over the distribution of relative momenta:

$$g(0) = \frac{1}{2} g_{\uparrow\downarrow}(0) = \frac{1}{2} \int_0^{k_F} p(q) |\alpha_{0,0}(q, r_s)|^2 dq \quad (23)$$

where $\alpha_{0,0}(q, r_s)$ is given by equations (15) and (16) and $p(q)$ by (17).

Figure 4 displays the pair distribution function of a two-dimensional unpolarized electron gas at the origin as a function of the coupling strength r_s . We display the quantity $r_s g(0)$ instead of $g(0)$ to emphasize the large r_s region where $g(0)$ becomes very small. Results of the first order in the analytic expansion on r_s , equation (21), the second order, equation (1), and the infinite-order solution, equation (22), together with the momentum average results, equation (23), are displayed. In addition, the numerical and analytical results of Nagano *et al* [14], the numerical calculation of Bulutay and Tanatar [16] and the recent estimate by

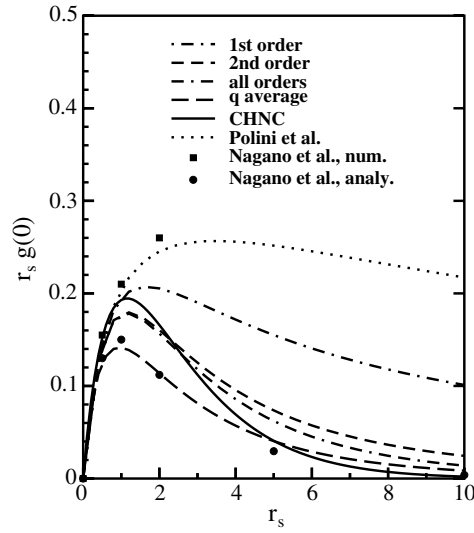


Figure 4. Two-particle distribution functions at the origin ($g(0)$ have been multiplied by r_s) as a function of r_s . Results of the analytical expansion to first order given by equation (21) (dot-dashed curve), second order by equation (1) (dashed curve) and infinite order (equation (22)) (dot-double-dashed curve), and the average over the distribution of relative momentum (equation (23)) (long-dashed curve) are displayed. The numerical (black squares) and analytical (black circles) results of Nagano *et al* [14], the numerical results of Bulutay and Tanatar [16] (solid curve) and the interpolation results of Polini *et al* [4] (dotted curve) are also displayed.

Polini *et al* [4] are also included for comparison. Several conclusions can be made. By adding additional terms in the analytical expansion on r_s we are able to closely approach the numerical results [16] in the low-density regime. Note that equation (1) is already a reliable analytical expression for $g(0)$. Figure 4 also shows that the results of the momentum average approach, equation (23), are slightly below Bulutay and Tanatar’s results for small r_s , but become even closer to the numerical curve in the low-density regime. The momentum average results are also very close to the analytical estimates of [14]. In this regime, the analytical expression obtained on [4] displays much larger values of $g(0)$ than the available numerical data [15, 16].

The contact value of the pair distribution function changes when the electron gas is polarized. The spin polarization directly appears on the expression for $g(0)$, $g(0) = \frac{1-\zeta^2}{2}g_{\uparrow\downarrow}(0)$. In addition, the polarization modifies the distribution of momenta of the electron pair and, as a consequence, the value of $g_{\uparrow\downarrow}(0)$. We calculate the spin-resolved pair distribution function as:

$$g_{\uparrow\downarrow}(\zeta, \rho = 0) = \int_0^{k_+} p_\zeta(q) |\alpha_{0,0}(q, r_s)|^2 dq \tag{24}$$

where $p_\zeta(q)$ is the distribution of relative momentum in the polarized electron gas:

$$p_\zeta(q) = \begin{cases} \frac{8q}{\max(k_{F\uparrow}^2, k_{F\downarrow}^2)} & (\text{for } 0 \leq q \leq k_-) \\ \frac{8q}{\pi k_{F\uparrow}^2 k_{F\downarrow}^2} [k_{F\uparrow}^2 (\arccos(x) - x\sqrt{1-x^2}) + k_{F\downarrow}^2 (\arccos(y) - y\sqrt{1-y^2})] & (\text{for } k_- \leq q \leq k_+) \end{cases} \tag{25}$$

where $x = (q + [(k_{F\uparrow}^2 - k_{F\downarrow}^2)/4q])/k_{F\uparrow}$, $y = (q - [(k_{F\uparrow}^2 - k_{F\downarrow}^2)/4q])/k_{F\downarrow}$ and $k_- = |k_{F\uparrow} - k_{F\downarrow}|/2$, $k_+ = (k_{F\uparrow} + k_{F\downarrow})/2$. The Fermi momentum for the spin-up (spin-down) population is related with the polarization and the Fermi momentum of the unpolarized gas (k_F) by $k_{F\uparrow} = k_F\sqrt{1 + \zeta}$ and $k_{F\downarrow} = k_F\sqrt{1 - \zeta}$.

Our results show that $g_{\uparrow\downarrow}(\zeta, \rho = 0)$ is largely unaffected by the degree of spin polarization. The difference between $g_{\uparrow\downarrow}(\zeta = 1, 0)$ and its unpolarized counterpart $g_{\uparrow\downarrow}(\zeta = 0, 0)$ is, at most, a few per cent for any given value of r_s . The absence of a significant dependence on the spin polarization was also found in previous calculations [4]. Moreover, given that the momentum dependence of our results is rather weak, we do not expect important changes if the free Fermi momentum distributions, equations (17) and (25), are replaced by the interacting ones.

4. Conclusions

We have calculated the pair distribution function in a two-dimensional interacting electron gas, following an approach originally developed in three dimensions by Overhauser [18]. Within this framework, the short-range correlations of the Coulomb interaction are replaced by an effective potential, and the calculation of $g(\rho)$ is reduced to solving the corresponding two-electron scattering problem and averaging over the probability distribution of the momentum of the electron pair. Our results for $g(r)$ at moderate coupling strengths agree well with the numerical data [15]. At larger values of r_s , however, this approximation is unable to reproduce the strong quantum oscillations of the numerical results.

The analytic expression for $g(0)$ as a function of r_s , equation (1), derived in this context compares very favourably with the complete solution of the effective potential, equation (23), and with recent numerical calculations [15, 16]. We believe that the discrepancy between the present results and the analytical expression obtained in [4] is essentially due to the different choice of effective potential (see figure 1). Besides, while we have used the same approach for all values of the electronic density and polarization, Polini *et al* use an interpolating scheme between the results of a perturbative expansion at high density and Overhauser's treatment of scattering processes in the low-density limit.

We have also studied the dependence of $g(0)$ with the spin polarization of the electron gas. We have found that the spin-up spin-down correlation function, $g_{\uparrow\downarrow}(0)$, is basically independent of the degree of polarization. Therefore, the polarization modifies $g(0)$ only through its dependence on the density, $g(0) = \frac{2n_{\uparrow}n_{\downarrow}}{n^2}g_{\uparrow\downarrow}(0)$.

Within this approach, further study of how the choice of the effective potential modifies the pair distribution function can provide valuable insight into the short-range electronic correlations in real materials.

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