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Short-range correlations in a two-dimensional electron gas

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Abstract

We construct a model for the value of the pair distribution function $g_{\uparrow\downarrow}(0)$ between antiparallel-spin electrons at contact in a two-dimensional electron gas with e^2/r interactions, as a function of the coupling-strength parameter r_s. The model involves an interpolation between the result of a low-r_s expansion, including the second-order direct and exchange contributions to the energy in the paramagnetic state, and the result of a partial-wave phase-shift analysis near Wigner crystallization. The interpolation formula is in excellent agreement with many-body calculations based on the ladder approximation. We further show through an STLS self-consistent calculation that $g_{\uparrow\downarrow}(0)$ is essentially independent of the state of spin polarization of the electron gas.

1. Introduction

Many of the electron–electron interaction effects in simple metals and semiconductors can be understood by reference to the interacting electron-gas model. Extensive studies of the three-dimensional (3D) electron gas have shown that short-range exchange and correlations play, especially at low density, a dominant role in determining the correlation energy and the electron-pair distribution function $g(r)$ at small separation r [1]. This function is a weighted mean of the functions $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$ for parallel-spin and antiparallel-spin electron pairs, where $g_{\uparrow\uparrow}(0)$ vanishes on account of the Pauli principle and $g_{\uparrow\downarrow}(0)$ directly reflects the electron–electron scattering events. Their treatment yields a cusp condition [2] relating the logarithmic derivative of $g_{\uparrow\downarrow}(r)$ at the origin $r = 0$ to the Bohr radius a_B. The importance of the electron–electron ladder diagrams in evaluating $g_{\uparrow\downarrow}(0)$ was first stressed by Yasuhara [3] and by Hede and Carbotte [4].

In this work we are concerned with the values taken by $g_{\uparrow\downarrow}(0)$ in a 2D electron gas with e^2/r interactions, first in the paramagnetic state with equal populations of the two spin orientations and then in magnetic states with an arbitrary degree of spin polarization. Many-body calculations of $g_{\uparrow\downarrow}(0)$ in the 2D paramagnetic electron gas have been carried out by Freeman [5] through a coupled-cluster summation of ladder diagrams and by Nagano *et al* [6] by solving the Bethe–Goldstone equation in the ladder approximation. Their results serve as a benchmark for the model of $g_{\uparrow\downarrow}(0)$ that we present and evaluate below.

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In section 2 we first calculate the leading term in the perturbation expansion for $g_{\uparrow\downarrow}(0)$ as a function of the coupling strength parameter $r_s = (\pi n a_B^2)^{-1/2}$, where n is the areal density of electrons. We then turn to the strong-coupling regime for an approximate evaluation of the leading term in the decay of $g_{\uparrow\downarrow}(0)$ to zero at large r_s and propose a simple interpolation formula between the two limits, that we test against the results of the many-body calculations. In section 3 we examine the dependence of $g_{\uparrow\downarrow}(0)$ on the degree of spin polarization within the so-called STLS self-consistent approximation [7]. Finally, section 4 gives our main conclusions.

2. Model for the pair distribution function at contact in the paramagnetic state

2.1. Weak-coupling limit

The pair distribution function $g(r)$ essentially is the Fourier transform of the structure factor $S(q)$,

$$g(r) = 1 + \frac{1}{N}\sum_{\boldsymbol{q}\neq\boldsymbol{0}}[S(q) - 1]\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}). \tag{1}$$

In turn the structure factor is the ground-state expectation value of an operator $\hat{S}(q)$ defined by

$$\hat{S}(q) = \frac{1}{N}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} a^{\dagger}_{\boldsymbol{k},\sigma} a^{\dagger}_{\boldsymbol{k}',\sigma'} a_{\boldsymbol{k}'-\boldsymbol{q},\sigma'} a_{\boldsymbol{k}+\boldsymbol{q},\sigma} \tag{2}$$

where the a and $a^{\dagger}$ are the usual fermion annihilation and creation operators. From equation (2) we see that the potential energy term in the 2D electron-gas Hamiltonian can be written as

$$\hat{H}_{pot} = \frac{N}{2}\sum_{\boldsymbol{q}\neq 0}[\hat{S}(q) - 1]v(q) \tag{3}$$

where in 2D we take $v(q) = 2\pi e^2/(q\Omega)$ as the Fourier transform of the interaction potential, with Ω the surface area. Hence, the Hellmann–Feynman theorem relates the structure factor to the ground-state energy E via a functional derivative,

$$S(q) - 1 = \frac{2}{N}\frac{\delta E}{\delta[v(q)]}. \tag{4}$$

As shown by Kimball [8] for the 3D electron gas, equation (4) is very well suited to obtain a weak-coupling expansion for the structure factor. Denoting by $\Delta S(q)$ the shift due to the interactions relative to the Hartree–Fock (ideal-gas) value, the corresponding shift $\Delta g(r)$ can then be obtained from equation (1) in 2D as

$$\Delta g(r) = 4\int_0^{\infty} y\,\mathrm{d}y\,\Delta S(y) J_0(2k_F r y). \tag{5}$$

Here $k_F = (2\pi n)^{1/2}$ is the Fermi wave number and $J_0(x)$ is the usual Bessel function of zeroth order.

For our purposes we need the structure factor only to first order in the coupling strength r_s, which from equation (4) implies calculating the second-order direct and exchange contributions to the ground state energy. The exchange term exactly cancels one-half of the direct term and the result is

$$\Delta S(q) = \frac{2m}{\hbar^2 N}\sum_{\boldsymbol{k},\sigma}\sum_{\boldsymbol{k}',\sigma'} v(q)\frac{f(k)f(k')[1 - f(|\boldsymbol{k}+\boldsymbol{q}|)][1 - f(|\boldsymbol{k}'-\boldsymbol{q}|)]}{k^2 + k'^2 - (\boldsymbol{k}+\boldsymbol{q})^2 - (\boldsymbol{k}'-\boldsymbol{q})^2} \tag{6}$$

where the f are ideal Fermi factors. Insertion in equation (5) and numerical integration yields

$$\lim_{r_s\to 0} g(0) = \tfrac{1}{2}\lim_{r_s\to 0} g_{\uparrow\downarrow}(0) = \tfrac{1}{2}[1 - 1.372 r_s]. \tag{7}$$

The corresponding numerical value for the coefficient of the linear term in 3D is 0.7315 [8], in accord with the well known fact that the role of the interactions weakens with increasing dimensionality.

The next term of the low-r_s expansion in 2D corrects equation (7) by a quadratic contribution, as already remarked by Kimball [8]. For reasons that will become clear in the following, we do not calculate the coefficient of the quadratic term by the perturbative approach but turn at this point to the strong-coupling regime.

2.2. Strong-coupling limit

Overhauser [9] has calculated $g(0)$ in the 3D electron gas by treating the two-electron scattering problem in a simple approximation. A pair of electrons with opposite spins form a singlet state whose radial wave function $R(r)$ is taken to satisfy the Schrödinger equation

$$-\frac{\hbar^2}{m}\left(\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right)+V(r)R(r)=ER(r). \tag{8}$$

$V(r)$ is an effective potential, which in Overhauser's 3D model is approximated with the potential of an electron at the centre of a sphere of radius r_sa_B and containing a uniformly distributed positive charge of amount $|e|$. The effective potential thus vanishes outside the sphere and the Schrödinger equation can be solved by setting $E=\hbar^2k^2/m$. The inner solution is obtained with sufficient accuracy by an iterative procedure and determines $g(0)$ through its value at the origin, while the outer solution defines the s-wave scattering length a_{sc} through its form $R_{out}(r)=1-a_{sc}/r$ at low energy.

In applying these ideas to the 2D electron gas one faces the difficulty that the effective potential due to an electron and a neutralizing disc of charge having radius r_sa_B does not vanish outside the disc. It is easily shown that the outer value of the electrical potential is determined by the multipole moments of the 2D charge density distribution $\sigma(r)$. Denoting by $\tilde{\sigma}(q)$ its Fourier transform, with

$$\tilde{\sigma}(q)=2\pi\int_0^\infty r\,\mathrm{d}r\,\sigma(r)J_0(qr) \tag{9}$$

the odd moments of the charge distribution vanish and its even moments are given by

$$M_{2\ell}=2\pi\left[\frac{\mathrm{d}^{2\ell}J_0(x)}{\mathrm{d}x^{2\ell}}\right]_{x=0}\int_0^\infty \mathrm{d}r\,\sigma(r)r^{2\ell+1}. \tag{10}$$

This implies a slow (r^{-3}) asymptotic decay of the outer potential, which is determined by the quadrupole moment of the 2D charge density.

We resolve this difficulty by adopting the model proposed by Nagy [10] in a variational calculation of the ground state energy of the 2D Wigner crystal. Nagy treats the radius of the disc (r_0, say) as a variational parameter and shows that, by setting to zero the outer potential, he obtains a lower bound for the ground state energy in correspondence to the value $r_0=\pi^{1/2}r_s/2$. This value is close to one-half of the first-neighbour distance in the triangular Wigner lattice.

Within this model the effective potential is

$$V(r)=\frac{e^2}{r}-\frac{2e^2r_0}{r_s^2a_B^2}\left[1-\frac{1}{4}\left(\frac{r}{r_0}\right)^2-\frac{3}{64}\left(\frac{r}{r_0}\right)^4\right] \tag{11}$$

for $r\leqslant r_0$ and zero otherwise. We use this expression in the 2D Schroedinger equation to treat the electron–electron scattering problem at strong coupling,

$$-\frac{\hbar^2}{mr}\frac{\mathrm{d}}{\mathrm{d}r}\left[r\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right]+V(r)R(r)=\frac{\hbar^2k^2}{m}R(r). \tag{12}$$

The inner solution of equation (12) tends to a constant value at the origin ($R_{in}(r \to 0) = \beta$, say), since we are treating scattering in the s-wave channel. With the notation $x = r/r_0$, an approximate solution of equation (12) is obtained by Overhauser's iterative method [9] as

$$R_{in}(r) = \beta\left\{1 + \frac{r_0}{a_B}\left[x - \left(\frac{r_0}{r_s a_B}\right)^2\left(\frac{1}{2}x^2 - \frac{1}{32}x^4 - \frac{1}{384}x^6\right)\right]\right\} \tag{13}$$

with its first derivative being given by

$$\frac{\mathrm{d}R_{in}(r)}{\mathrm{d}r} = \beta\frac{r_0}{a_B}\left[1 - \left(\frac{r_0}{r_s a_B}\right)^2\left(x - \frac{1}{8}x^3 - \frac{1}{64}x^5\right)\right]. \tag{14}$$

The value of β is obtained by matching the derivatives of the inner and outer solutions at the disc radius, the outer solution having the form $R_{out}(r) \propto \ln(r/a_{sc})$ at low energy. This yields

$$g(0) = \frac{2}{\pi r_s^2(1 - 55\pi/256)^2} \tag{15}$$

after using the Nagy value for the disc radius ($r_0 = \pi^{1/2}r_s/2$). Finally, we obtain the s-wave scattering length a_{sc} by matching the inner and outer solutions at the boundary, with the result

$$a_{sc} = \frac{\pi^{1/2}}{2}r_s \exp\left[-\frac{1 + (1 - 179\pi/1536)\pi^{1/2}r_s/2}{(1 - 55\pi/256)\pi^{1/2}r_s/2}\right]. \tag{16}$$

In view of the approximations made in the treatment of the scattering problem, these results are valid at strong coupling strength on the approach to Wigner crystallization.

2.3. Interpolation formula and cusp condition

The r_s^{-2} dependence of $g(0)$ predicted by equation (15) for the 2D electron gas at strong coupling becomes consistent with the linear plus quadratic dependence on r_s expected from the perturbation expansion at weak coupling if we adopt the simple interpolation formula $g(0) = \frac{1}{2}(1 + ar_s + br_s^2)^{-1}$. Explicitly, from equations (7) and (15) we have

$$g(0) = \frac{1/2}{1 + 1.372r_s + 0.0830r_s^2}. \tag{17}$$

Figure 1 compares the predictions of this interpolation formula with the results obtained by Freeman [5] and by Nagano *et al* [6] from many-body calculations within the electron–electron ladder approximation. Evidently, there is complete consistency between equation (17) and the available first-principles results for the paramagnetic state.

We also remark that the approximate 2D Schrödinger equation (12) can be generalized into an equation for the two-electron scattering problem having the form

$$-\frac{\hbar^2}{mr}\frac{\mathrm{d}}{\mathrm{d}r}\left[r\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right] + v(r)R(r) = \hat{E}R(r). \tag{18}$$

Here, $v(r)$ is the bare interaction potential and $\hat{E}$ is a complex operator accounting for all details of the scattering event. By imposing with Kimball [2] that $\hat{E}R(r)$ tends to a finite constant in the origin, we have $R(r) \to a_1 + a_2 r$ where $a_1/a_2 = a_B$ (compare with equation (13)). Hence, the cusp condition in 2D reads

$$\left[\frac{\mathrm{d}\ln g(r)}{\mathrm{d}r}\right]_{r=0} = \frac{2}{a_B}. \tag{19}$$

The factor 2 in equation (19) is at variance with the analogous result obtained by Kimball [2] in 3D.

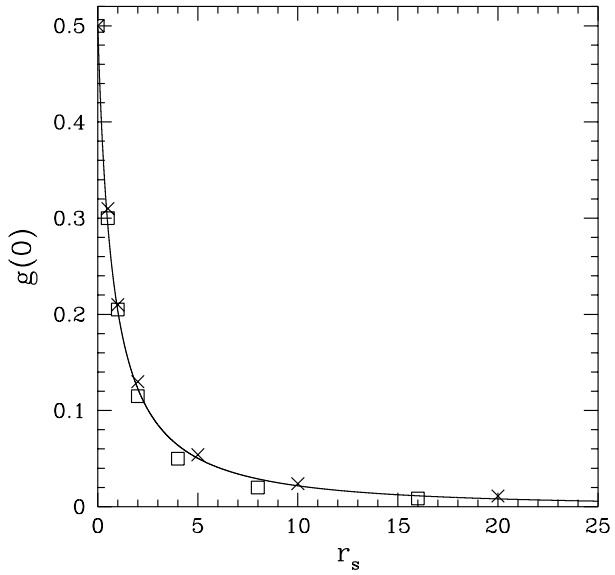

Figure 1. Electron-pair correlations $g(r = 0)$ as a function of coupling-strength parameter r_s in the 2D electron gas in the paramagnetic state, where $g(0) = g_{\uparrow\downarrow}(0)/2$. The results of equation (17) (full line) are compared with the many-body calculations of Freeman [5] (squares) and of Nagano *et al* [6] (crosses).

3. Dependence of short-range pair correlations on spin magnetization

The foregoing calculations have assumed that, at least in the strong-coupling regime, the calculation of short-range electron–electron correlations in the electron gas reduces in the limit $r \to 0$ to the solution of a two-body problem. This property is indeed to be expected in general, as a consequence of the divergence of the Coulomb potential in the origin [11]. One may expect, therefore, that the value of $g_{\uparrow\downarrow}(0)$ should be largely independent of the relative value of the two spin populations in the electron gas [12].

Figure 2 shows the extent to which this expectation is fulfilled in a 2D spin-polarized electron gas within the self-consistent STLS approach. The figure reports the values of $g_{\uparrow\downarrow}(0)$ at three values of r_s in the weak-coupling regime, as functions of a spin-polarization parameter ξ defined as $\xi = (n_\uparrow - n_\downarrow)/n$ where $n_\uparrow$ and $n_\downarrow$ are the mean areal densities of spin-up and spin-down electrons. It can also be seen from figure 2 that for the paramagnetic state ($\xi = 0$) these calculations yield values of $g(0) = g_{\uparrow\downarrow}(0)/2$ which are in agreement with the predictions made by equation (17).

We should briefly comment at this point on the theoretical approach leading to the results shown in figure 2 (a full account of the theory and of other calculated properties will be given elsewhere). We have studied the dielectric and magnetic response of a 2D electron gas in a state of arbitrary spin polarization ξ, as expressed through three local-field factors accounting for exchange and short-range correlations [12]. In an STLS approach [7] the local-field factors are determined self-consistently with the set of three structure factors describing correlations within and between the two spin components of the electron gas. The values of $g_{\uparrow\downarrow}(0)$ in figure 2 emerge from such a self-consistent treatment of fluid structure and linear response. Previous experience on 3D electron fluids (see for instance [1]) leads us to expect that these results should be fairly accurate.

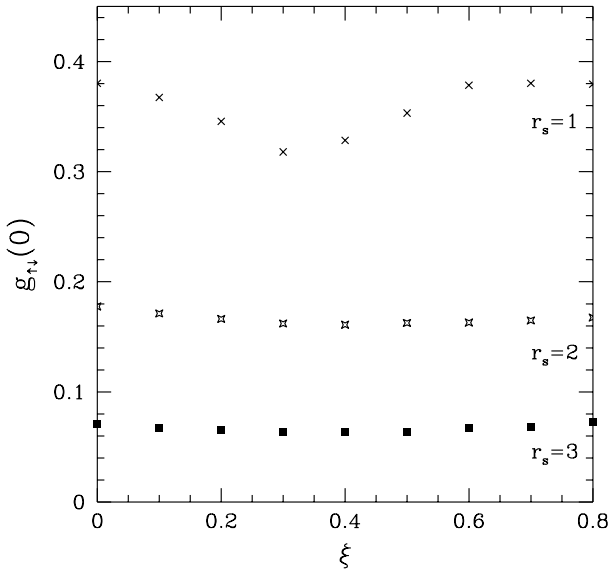

Figure 2. Electron-pair correlations $g_{\uparrow\downarrow}(r = 0)$ for antiparallel-spin electrons as functions of the spin-polarization parameter ξ at three values of the coupling strength parameter r_s.

4. Summary and conclusions

We have derived in this work a simple expression for short-range correlations in the 2D electron gas in a paramagnetic state by combining a perturbative expansion at weak coupling with an approximate treatment of electron–electron scattering processes at strong coupling. This physically transparent approach provides an accurate interpretation of the existing results from full many-body calculations. Quantitative data on short-range correlations, together with the appropriate cusp condition, are useful in providing tests for approximate solutions and for further modelling of the many-body problem. In this connection we have tested the predictions of an STLS approach to the paramagnetic electron gas and shown that in this approach the short-range correlation between spin-up and spin-down electrons are practically independent of the state of spin polarization of the many-electron fluid.

Acknowledgments

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