Phys. Rev. Letters 22, 807 (1969).
[61]D. A. Liberman, Phys. Rev. 171, 1 (1968).
[62]See, for example, A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Lattice Dynamics in the Harmonic Approximation* (Academic, New York, 1963), p. 24 2ff.
[63]C. B. Walker, Phys. Rev. 103, 547 (1956).

PHYSICAL REVIEW B VOLUME 3, NUMBER 10 15 MAY 1971

Momentum Distribution and Pair Correlation of the Electron Gas at Metallic Densities*

John Lam†
Division of Chemistry, National Research Council of Canada, Ottawa 7, Canada
(Received 11 December 1970)

The momentum-distribution and pair-correlation functions of the electron gas at metallic densities are calculated by means of an expression of the ground-state energy derived in a previous paper. Numerical studies of the momentum distribution show that even at metallic densities most of the electrons are still inside the Fermi sphere and that the Fermi surface persists. The effect of the exchange processes at metallic densities is found to pull the electrons back inside the Fermi sphere and to increase the discontinuity at the Fermi surface, which is the opposite effect to that at high density. The behavior of the pair-correlation functions indicates that at short distances the present results overestimate the correlation of antiparallel spins but underestimate that of parallel spins. On the whole, there is considerable improvement over the corresponding results in the random-phase approximation.

I. INTRODUCTION

In a previous paper[1] we formulated an approach to the correlation problem of the electron gas at metallic densities. The starting point of this approach is the transition from the paramagnetic fermion-state space to a boson-state space, by means of a transformation first introduced by Usui[2] to study the effect of exchange processes on the properties of a spinless electron gas at high density. Under this transformation, an electron-hole pair goes over into an ideal boson:

$$a^{\dagger}_{\vec{P}\sigma}\, a_{\vec{p}\sigma} \to C^{\dagger}_{\vec{p}\sigma}(\vec{P}-\vec{p}), \qquad P>p_F,\quad p<p_F\,. \tag{1.1}$$

The electron Hamiltonian H_F is mapped into a boson Hamiltonian of the form

$$H_B = H_0 + H_2 + H_3 + H_4\,. \tag{1.2}$$

Here H_0 is a c number identical to the ground-state energy in the Hartree-Fock approximation; H_2, H_3, and H_4 are, respectively, quadratic, cubic, and quartic in boson creation and annihilation operators. The ensuing calculations in Ref. 1 are based on two types of approximations. The first consists of the harmonic approximation in which H_3 and H_4 are assumed small and discarded. Then H_2 can be separated into two mutually independent parts describing the singlet and triplet states of an electron-hole pair:

$$H_2 = H^{(1)} + H^{(3)}\,. \tag{1.3}$$

The second type of approximation is employed to diagonalize these parts, and consists roughly in replacing the matrix elements of exchange processes by their averages. The result of these approximations is equivalent to taking as the singlet Hamiltonian the expression

$$H^{(1)} = \sum_{\vec{q}\vec{p}} \omega_{\vec{p}}(\vec{q})\, A^{\dagger}_{\vec{p}}(\vec{q})\, A_{\vec{p}}(\vec{q}) + \frac{1}{\Omega}\sum_{\vec{q}\vec{p}\vec{p}'} \{2F(\vec{q})\, A^{\dagger}_{\vec{p}}(\vec{q})\, A_{\vec{p}'}(\vec{q}) + G(\vec{q})[A^{\dagger}_{\vec{p}}(\vec{q})\, A^{\dagger}_{-\vec{p}'}(-\vec{q}) + \text{H.c.}]\}\,. \tag{1.4}$$

The notations in this paper are as in Ref. 1. In particular,

$$\omega_{\vec{p}}(\vec{q}) = \epsilon_{\vec{p}+\vec{q}} - \epsilon_{\vec{p}}\,,$$
$$F(\vec{q}) = V(\vec{q}) + f(\vec{q})\,,$$
$$G(\vec{q}) = V(\vec{q}) + g(\vec{q})\,. \tag{1.5}$$

Here $\epsilon_{\vec{p}}$ is the electron kinetic energy and $V(\vec{q})$ is the direct Coulomb potential. $f(\vec{q})$ and $g(\vec{q})$ are a pair of effective potentials expressible in terms of certain exchange matrix elements. They are defined in Eq. (5.7) and plotted in Fig. 2 of Ref. 1. The ground-state energy of $H^{(1)}$ is the singlet contribution to the correlation energy. It is given by

$$E^{(1)}_{\text{corr}} = \frac{1}{4\pi}\sum_{\vec{q}} \int_{-\infty}^{\infty} du\,[\ln\epsilon(\vec{q}, iu) - \Pi_1(\vec{q}, u)]\,, \tag{1.6}$$

where

$$\epsilon(\vec{q}, iu) = 1 + \Pi_1(\vec{q}, u) + \Pi_2(\vec{q}, u)\,,$$

$$\Pi_1(\vec{q}, u) = 4F(\vec{q})R(\vec{q}, u) ,$$

$$\Pi_2(\vec{q}, u) = 4[F^2(\vec{q}) - G^2(\vec{q})][R^2(\vec{q}, u) + I^2(\vec{q}, u)] ,$$

$$R(\vec{q}, u) + iI(\vec{q}, u) = \frac{1}{\Omega} \sum_{\substack{p<p_F \\ |\vec{p}+\vec{q}|>p_F}} \frac{1}{\omega_{\vec{p}}(\vec{q}) - iu} . \tag{1.7}$$

The Hamiltonian $H^{(3)}$ and the correlation energy $E_{\text{corr}}^{(3)}$ for the triplet state are obtained from (1.4) and (1.6) by replacing F and G with f and g. The random-phase approximation corresponds to setting f and g equal to zero.

In this work we present a calculation of the momentum-distribution and pair-correlation functions of the electron gas at metallic densities based on the above-mentioned approximation. The results are directly related to measurable quantities since the ground-state expectation values of one- and two-particle operators are expressible in terms of these functions. On the other hand, their behavior may give us an indication as to the validity of the assumptions made and the nature of the approximate solution. The momentum-distribution function was calculated by Daniel and Vosko[3] in the random-phase approximation. The spin-symmetric pair-correlation function was calculated in the same approximation by Brouers.[4] In a recent paper, Lobo, Singwi, and Tosi[5] calculated the pair-correlation functions for parallel and antiparallel spins by a self-consistent method using the Boltzmann equation. This last work also contains a summary of the results of several previous approximations.

In Secs. II–IV the analytical expressions for the momentum-distribution, pair-correlation, and spin-correlation functions are derived. In Sec. V numerical results are presented and compared with those obtained in the random-phase approximation. The difference roughly represents the effect of the exchange interaction. Finally, the results are briefly discussed in relation to the approximation introduced in Ref. 1.

II. MOMENTUM DISTRIBUTION

Let $|\Psi_0\rangle$ be the paramagnetic ground state of the electron gas. Then the momentum distribution can be obtained by functional differentiation of the ground-state energy E_{gr}:

$$n_{\vec{k}} = \langle \Psi_0 | a_{\vec{k}\sigma}^{\dagger} a_{\vec{k}\sigma} | \Psi_0 \rangle = \frac{1}{2} \left\langle \Psi_0 \left| \frac{\delta}{\delta \epsilon_{\vec{k}}} H_F \right| \Psi_0 \right\rangle = \frac{1}{2} \frac{\delta}{\delta \epsilon_{\vec{k}}} E_{gr} . \tag{2.1}$$

The last equality follows from the normalization of $|\Psi_0\rangle$. In our approximation

$$E_{gr} = E_{gr}^{\text{HFA}} + E_{\text{corr}}^{(1)} + E_{\text{corr}}^{(3)} , \tag{2.2}$$

where

$$E_{gr}^{\text{HFA}} = \sum_{\vec{p}\sigma} \epsilon_{\vec{p}} n_{\vec{p}}^0 + \frac{1}{2\Omega} \sum_{\substack{\vec{q}\vec{p}\vec{p}' \\ \sigma\sigma'}} V(\vec{q})[\delta(\vec{q}) - \delta_{\sigma\sigma'} \delta(\vec{p}+\vec{q}-\vec{p}')] n_{\vec{p}}^0 n_{\vec{p}'}^0 ,$$

$$n_{\vec{p}}^0 = \begin{cases} 1, & p < p_F \\ 0, & p > p_F \end{cases} \tag{2.3}$$

are the ground-state energy and momentum distribution in the Hartree-Fock approximation. Carrying out the functional differentiation, we obtain

$$\frac{\delta}{\delta \epsilon_{\vec{k}}} E_{\text{corr}}^{(1)} = \pm \frac{1}{\pi\Omega} \sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{du}{\epsilon(\vec{q}, iu)[\omega_{\vec{k}}^2(\vec{q}) + u^2]^2} \times (\{F(\vec{q}) + 2[F^2(\vec{q}) - G^2(\vec{q})]R(\vec{q}, u)\}[\omega_{\vec{k}}^2(\vec{q}) - u^2] + 4[F^2(\vec{q}) - G^2(\vec{q})]I(\vec{q}, u) u \omega_{\vec{k}}(\vec{q})) . \tag{2.4}$$

The ± sign corresponds to $k <$ or $> p_F$, respectively. For $k < p_F$, $\vec{q}$ is summed over the exterior of a sphere of radius p_F centered at $-\vec{k}$. For $k > p_F$, it is summed over the interior of a sphere of radius p_F centered at $\vec{k}$. As in all other instances, the corresponding result for the triplet state is obtained by replacing F and G with f and g.

As in Ref. 1, we introduce reduced momentum and energy variables x and y:

$$x = q/p_F , \quad y = u/E_F , \quad E_F = p_F^2/2m . \tag{2.5}$$

Integrating over the angles in (2.4) we finally obtain

$$n_{\vec{k}} = 1 - \frac{\gamma}{2\pi k} \left(\int_{1-k}^{1+k} x\,dx \int_0^{\infty} \frac{dy}{\epsilon(x, iy)} [P(x, y)\xi_1(x, y, k) + Q(x, y)\eta_1(x, y, k)] + \int_{1+k}^{\infty} x\,dx \times \int_0^{\infty} \frac{dy}{\epsilon(x, iy)} [P(x, y)\xi_2(x, y, k) + Q(x, y)\eta_2(x, y, k)] \right) - \text{triplet terms} , \qquad k < 1$$

$$= \frac{\gamma}{2\pi k} \int_{k-1}^{k+1} x\,dx \int_0^{\infty} \frac{dy}{\epsilon(x, iy)} [P(x, y)\xi_3(x, y, k) + Q(x, y)\eta_3(x, y, k)] + \text{triplet terms} , \qquad k > 1 , \tag{2.6}$$

where

$$\gamma=\frac{2}{\pi}\left(\frac{4}{9\pi}\right)^{1/3} r_s \simeq 0.332 r_s ,$$

$$P(x, y)=F(x)+\tfrac{1}{2}\gamma[F^2(x)-G^2(x)]R(x, y) ,$$

$$Q(x, y)=\tfrac{1}{2}\gamma[F^2(x)-G^2(x)]I(x, y) ,$$

$$\xi_1(x, y, k)=\frac{x(x+2k)}{x^2(x+2k)^2+y^2}-\frac{1-k^2}{(1-k^2)^2+y^2} ,$$

$$\eta_1(x, y, k)=\frac{y}{x^2(x+2k)^2+y^2}-\frac{y}{(1-k^2)^2+y^2} , \quad (2.7)$$

$$\xi_2(x, y, k)=\frac{x(x+2k)}{x^2(x+2k)^2+y^2}-\frac{x(x-2k)}{x^2(x-2k)^2+y^2} ,$$

$$\eta_2(x, y, k)=\frac{y}{x^2(x+2k)^2+y^2}-\frac{y}{x^2(x-2k)^2+y^2} ,$$

$$\xi_3(x, y, k)=\frac{x(2k-x)}{x^2(2k-x)^2+y^2}-\frac{k^2-1}{(k^2-1)^2+y^2} ,$$

$$\eta_3(x, y, k)=\frac{y}{x^2(2k-x)^2+y^2}-\frac{y}{(k^2-1)^2+y^2} .$$

In the limit of the random-phase approximation, we set f and g equal to zero and obtain

$$n_{\vec{k}}^{\mathrm{RPA}}=1-\frac{\gamma}{2\pi k}\left(\int_{1-k}^{1+k} x\,dx\int_0^\infty \frac{dy}{x^2\epsilon(x, iy)}\,\xi_1(x, y, k)\right.$$

$$\left.+\int_{1+k}^{\infty} x\,dx\int_0^\infty \frac{dy}{x^2\epsilon(x, iy)}\,\xi_2(x, y, k)\right) , \qquad k<1$$

$$=\frac{\gamma}{2\pi k}\int_{k-1}^{k+1} x\,dx\int_0^\infty \frac{dy}{x^2\epsilon(x, iy)}\,\xi_3(x, y, k) , \quad k>1 . \quad (2.8)$$

With a suitable change of variables this is identical to the result obtained by Daniel and Vosko by perturbation theory.

III. PAIR CORRELATION

Let $\psi_\sigma(\vec{r})$ be the electron field operator:

$$\psi_\sigma(\vec{r})=\Omega^{-1/2}\textstyle\sum_{\vec{p}} e^{i\vec{p}\cdot\vec{r}}\,a_{\vec{p}\sigma} . \quad (3.1)$$

Then the pair-correlation function is defined in general by

$$g_{\sigma\sigma'}(\vec{r})=\frac{4\Omega^2}{N^2}\langle\Psi_0|\psi_\sigma^\dagger(\vec{r})\psi_{\sigma'}^\dagger(0)\psi_{\sigma'}(0)\psi_\sigma(\vec{r})|\Psi_0\rangle$$

$$=\sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{r}}\,g_{\sigma\sigma'}(\vec{q}) , \quad (3.2)$$

where

$$g_{\sigma\sigma'}(\vec{q})=\frac{4}{N^2}\sum_{\vec{k}\vec{k}'}\langle\Psi_0|a_{\vec{k}+\vec{q}\sigma}^\dagger a_{\vec{k}'-\vec{q}\sigma'}^\dagger a_{\vec{k}'\sigma'}a_{\vec{k}\sigma}|\Psi_0\rangle . \quad (3.3)$$

The normalization in (3.2) is chosen to make $g_{\sigma\sigma'}(\vec{r})\to 1$ as $r\to\infty$. In the Hartree-Fock approximation, $|\Psi_0\rangle$ is the paramagnetic Fermi sphere and we easily obtain

$$g_{\sigma\sigma'}^{\mathrm{HFA}}(\vec{r})=1-\delta_{\sigma\sigma'}\,9\left(\frac{j_1(p_F r)}{p_F r}\right)^2 . \quad (3.4)$$

Since we have rotational invariance, $g_{\sigma\sigma'}=g_{\sigma'\sigma}$. We introduce the spin-symmetric combination

$$g_s(\vec{r})=\tfrac{1}{2}[g_{\uparrow\uparrow}(\vec{r})+g_{\uparrow\downarrow}(\vec{r})] . \quad (3.5)$$

Then the interaction energy, defined as the ground-state expectation value of the potential energy, is given by

$$E_{\mathrm{int}}=\frac{N^2}{2\Omega}\sum_{\vec{q}} V(\vec{q})g_s(\vec{q}) . \quad (3.6)$$

On the other hand, by the ground-state energy theorem,

$$E_{\mathrm{int}}=e^2\frac{\partial}{\partial e^2}E_{\mathrm{gr}} . \quad (3.7)$$

Combining (3.6) and (3.7), we obtain

$$g_s(\vec{q})=g_s^{\mathrm{HFA}}(\vec{q})-\frac{\Omega}{2\pi N^2 V(\vec{q})}$$

$$\times\int_{-\infty}^{\infty}\frac{du}{\epsilon(\vec{q}, iu)}\,[\Pi_1^2(\vec{q}, u)+\Pi_1(\vec{q}, u)\Pi_2(\vec{q}, u)$$

$$-2\Pi_2(\vec{q}, u)]-\text{triplet terms.} \quad (3.8)$$

Substituting (3.8) into (3.2), integrating over the angles, and going over to dimensionless variables, we finally obtain

$$g_s(\vec{r})=g_s^{\mathrm{HFA}}(\vec{r})-\frac{9\gamma}{8\pi}\int_0^\infty dx\,\frac{\sin p_F rx}{p_F rx}\int_0^\infty dy\,\frac{x^4}{\epsilon(x, iy)}$$

$$\times[\Pi_1^2(x, y)+\gamma\Pi_1(x, y)\Pi_2(x, y)-2\Pi_2(x, y)]$$

$$-\text{triplet terms.} \quad (3.9)$$

In the limit of the random-phase approximation this reduces to

$$g_s^{\mathrm{RPA}}(\vec{r})=g_s^{\mathrm{HFA}}(\vec{r})-\frac{9\gamma}{8\pi}\int_0^\infty dx\,\frac{\sin p_F rx}{p_F rx}$$

$$\times\int_0^\infty dy\,\frac{R^2(x, y)}{\epsilon(x, iy)} . \quad (3.10)$$

IV. SPIN CORRELATION

We consider the pair-correlation function for antiparallel spins

$$g_{\uparrow\downarrow}(\vec{q})=\frac{4}{N^2}\sum_{\vec{k}\vec{k}'}\langle\Psi_0|a_{\vec{k}+\vec{q}\uparrow}^\dagger a_{\vec{k}'-\vec{q}\downarrow}^\dagger a_{\vec{k}'\downarrow}a_{\vec{k}\uparrow}|\Psi_0\rangle . \quad (4.1)$$

The right-hand side can be reexpressed in terms of ground-state expectation values of boson oper-

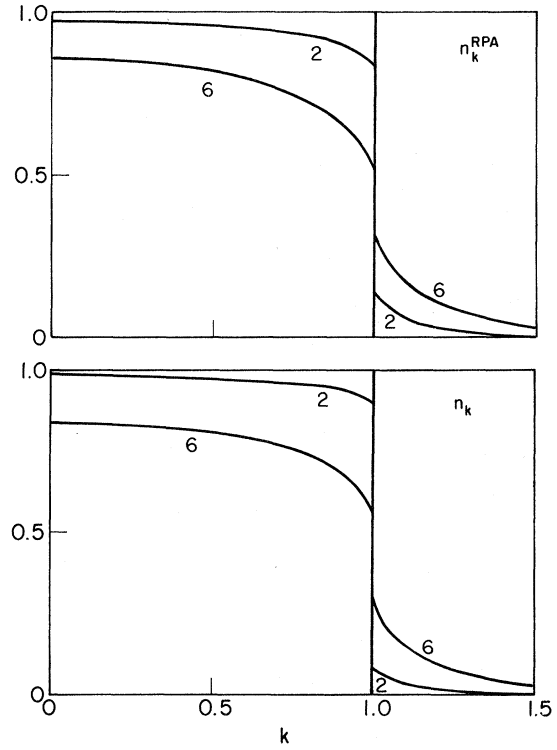

FIG. 1. Momentum distribution at $r_s = 2$ and 6.

ators by means of the transformation (1.1) as described in Ref. 1. After some amount of calculation, we obtain

$$g_{\uparrow\downarrow}(\vec{q}) = \delta(\vec{q}) + \frac{2}{N^2}\sum_{\vec{p}\vec{p}'}\langle\Psi_0|[2C^\dagger_{\vec{p}\uparrow}(\vec{q})C_{\vec{p}'\downarrow}(\vec{q}) + 2C^\dagger_{-\vec{p}\downarrow}(-\vec{q})C_{-\vec{p}'\uparrow}(-\vec{q}) + C^\dagger_{\vec{p}\uparrow}(\vec{q})C^\dagger_{-\vec{p}'\downarrow}(-\vec{q}) + C^\dagger_{-\vec{p}\downarrow}(-\vec{q})C^\dagger_{\vec{p}'\uparrow}(\vec{q}) + C_{-\vec{p}'\downarrow}(-\vec{q})C_{\vec{p}\uparrow}(\vec{q}) + C_{\vec{p}'\uparrow}(\vec{q})C_{-\vec{p}\downarrow}(-\vec{q})]|\Psi_0\rangle . \quad (4.2)$$

Terms beyond the quadratic have been discarded. Substituting (4.2) into (3.2) and expressing $C_\uparrow$ and $C_\downarrow$ in terms of the singlet and triplet operators, we obtain

$$g_{\uparrow\downarrow}(\vec{r}) = 1 + \frac{2}{N^2}\sum_{\vec{q}\vec{p}\vec{p}'}\cos\vec{q}\cdot\vec{r} \times\langle\Psi_0|[2A^\dagger_{\vec{p}}(\vec{q})A_{\vec{p}'}(\vec{q}) + A^\dagger_{\vec{p}}(\vec{q})A^\dagger_{-\vec{p}'}(-\vec{q}) + A_{-\vec{p}'}(-\vec{q})A_{\vec{p}}(\vec{q}) - \text{triplet terms}]|\Psi_0\rangle. \quad (4.3)$$

The ground-state expectation values can be obtained by functional differentiation of the correlation energy:

$$\frac{1}{\Omega}\sum_{\vec{p}\vec{p}'}\langle\Psi_0|2A^\dagger_{\vec{p}}(\vec{q})A_{\vec{p}'}(\vec{q})|\Psi_0\rangle = \frac{\delta}{\delta F(\vec{q})}E^{(1)}_{\rm corr},$$

$$\frac{1}{\Omega}\sum_{\vec{p}\vec{p}'}\langle\Psi_0|[A^\dagger_{\vec{p}}(\vec{q})A^\dagger_{-\vec{p}'}(-\vec{q}) + \text{H.c.}]|\Psi_0\rangle = \frac{\delta}{\delta G(\vec{q})}E^{(1)}_{\rm corr} \quad (4.4)$$

We finally obtain

$$g_{\uparrow\downarrow}(\vec{r}) = 1 - \frac{9\gamma}{8\pi}\int_0^\infty dx\,\frac{\sin p_F rx}{p_F rx}\int_0^\infty dy\,\frac{x^2}{\epsilon(x,iy)} \times\left(R(x,y)[\Pi_1(x,y) + \gamma\Pi_2(x,y)] - \frac{2}{F(x)+G(x)}\Pi_2(x,y)\right) + \text{triplet terms}. \quad (4.5)$$

In the limit of the random-phase approximation this reduces to

$$g^{\rm RPA}_{\uparrow\downarrow}(\vec{r}) = 1 - \frac{9\gamma}{8\pi}\int_0^\infty dx\,\frac{\sin p_F rx}{p_F rx}\int_0^\infty dy\,\frac{R^2(x,y)}{\epsilon(x,iy)}, \quad (4.6)$$

which agrees with the expression derived by Ueda.[6] Note that the integral in (4.6) is the same as that in (3.10).

The pair-correlation function for parallel spins can be obtained from (3.5).

V. NUMERICAL RESULTS

The integrals in (2.6) and (2.8) are evaluated numerically in the metallic density region: $r_s = 1$–6. We start out with a calculation using a ten-point Gaussian formula. The number of points is then increased and the calculation repeated until convergence to within 1% is achieved. For integrals over the range $1 + k < x < \infty$, convergence is improved by first subtracting from the integrand its asymptotic behavior at large y. The results of the calculation for $r_s = 2$ and 6 are plotted in Fig. 1 and a sample of those for $r_s = 4$ displayed in Table I.

Our results in the random-phase approximation are in apparent agreement with those of Daniel and Vosko, although the set of electron densities they consider is somewhat different from ours. The most noteworthy feature of the momentum-distribution function is the discontinuity at the Fermi level,

TABLE I. Momentum distribution at $r_s = 4$.

k	$n_{\vec{k}}$	$n^{\rm RPA}_{\vec{k}}$
0.1	0.930	0.917
0.4	0.921	0.902
0.6	0.905	0.878
0.8	0.872	0.826
0.9	0.840	0.776
1.0−	0.770	0.667
1.0+	0.155	0.225
1.1	0.080	0.113
1.2	0.048	0.066
1.4	0.020	0.026

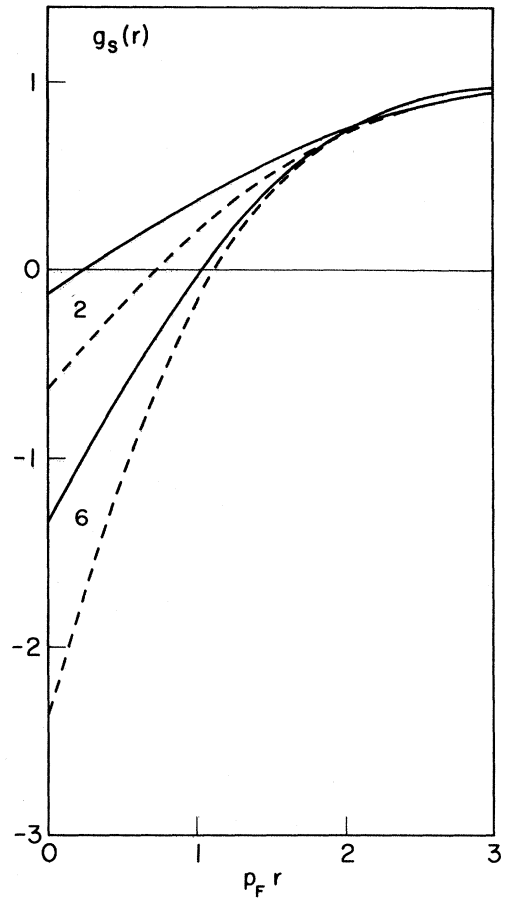

FIG. 2. Pair-correlation function $g_s(\vec{r})$ at $r_s = 2$ and 6. The broken curves are the corresponding results in the random-phase approximation.

so that the Fermi surface persists even at metallic densities—a fact supported by experiments. The magnitude of the discontinuity is of interest since it is equal to the quasiparticle renormalization constant Z. We list its values in Table II.

Comparing the results, we can say, in general, that at metallic densities the effect of the exchange processes is to pull the electrons back inside the Fermi surface and to increase the discontinuity at the surface. These findings are the opposite of those at high density, where the exchange interaction pushes the electrons from the Fermi sphere

TABLE II. Quasiparticle renormalization constant Z.

r_s	Z	Z^{RPA}
1	0.896	0.843
2	0.814	0.700
3	0.725	0.567
4	0.615	0.442
5	0.472	0.323
6	0.267	0.209

TABLE III. Pair-correlation functions at $r_s = 4$.

$p_F r$	$g_s(\vec{r})$	$g_s^{\mathrm{RPA}}(\vec{r})$	$g_{\uparrow\downarrow}(\vec{r})$	$g_{\uparrow\downarrow}^{\mathrm{RPA}}(\vec{r})$
0.0	−0.721	−1.561	−1.539	−1.061
0.5	−0.250	−0.678	−0.641	−0.202
1.0	0.170	−0.008	0.074	0.401
1.5	0.502	0.446	0.566	0.760
2.0	0.740	0.728	0.860	0.942
2.5	0.890	0.888	1.002	1.012
3.0	0.969	0.967	1.048	1.026
4.0	1.006	1.006	1.028	1.009

and lowers the discontinuity at the Fermi surface.[7] The explanation of this reversal of behavior is to be found in the fact that $f(q)$ is positive at small q.

The pair-correlation functions are again evaluated numerically by Gaussian quadrature for the metallic region. The x integrals are conveniently broken up into an infinite sum of terms over the periods of the sine function. For the special case $r = 0$, an appropriate period is arbitrarily assigned. Because of the rapid convergence of the integrands, only the

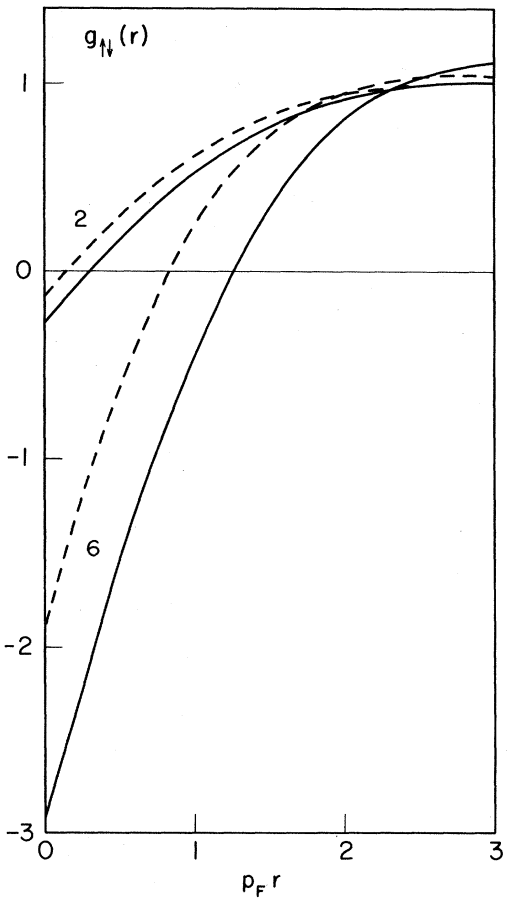

FIG. 3. Pair-correlation function $g_{\uparrow\downarrow}(\vec{r})$. The labeling is as in Fig. 2.

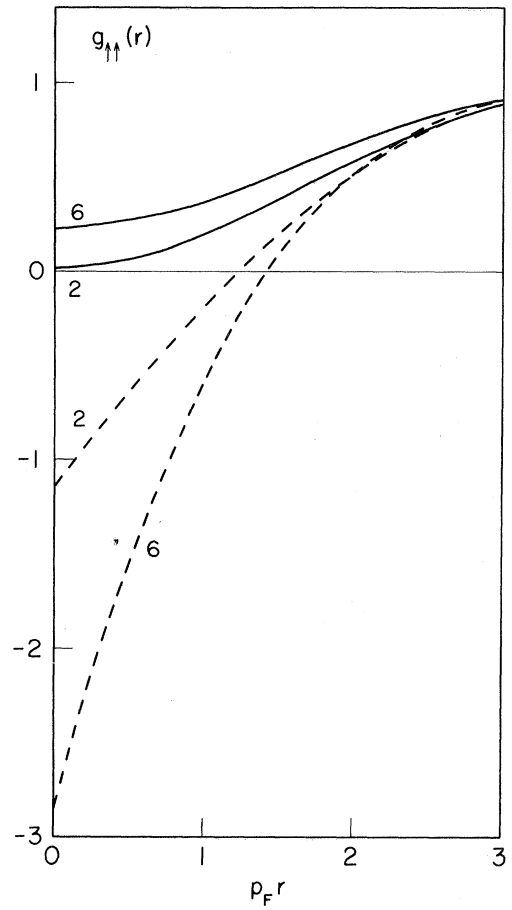

FIG. 4. Pair-correlation function $g_{\uparrow\uparrow}(\vec{r})$. The labeling is as in Fig. 2.

first few periods need be considered. Again, accuracy to within 1% is achieved. The results of the calculation for $r_s = 2$ and 6 are plotted in Figs. 2–4, and those for $r_s = 4$ displayed in Table III. Our random-phase results agree with those of Brouers, but differ slightly from those of Lobo, Singwi, and Tosi.

From very general considerations, it can be shown that the pair-correlation functions satisfy the constraints

$$g_{\sigma\sigma'}(\vec{r}) \geq 0, \quad g_{\uparrow\uparrow}(0) = 0 . \tag{5.1}$$

These are violated at short distances by the results of both the random-phase approximation and the present approximation in the metallic region. The severity of violation by our results is less than that by the random-phase results for $g_s(\vec{r})$ and more for $g_{\uparrow\downarrow}(\vec{r})$. This finding is common to many attempts to improve the random-phase approximation (see, for example, Fig. 4 of Ref. 5). However, the results are qualitatively the same in both approximations. This is not true for $g_{\uparrow\uparrow}(\vec{r})$: As r_s is increased, the random-phase curve is strongly depressed, while ours is slightly raised. Our results are also more in compliance with (5.1), indicating a better treatment of parallel-spin correlation in our approximation.

In conclusion, we wish to comment briefly on our results in relation to our approximation. As indicated in Fig. 1, even at metallic densities, most of the electrons are still inside the Fermi sphere. This lends support to the validity of the harmonic approximation. The anharmonic terms can be handled by perturbation theory in an improved calculation. From Figs. 3 and 4 we can conclude that at short distances, our approximation exaggerates the correlation between antiparallel spins and underestimates that between parallel spins. The net effect is to improve the results of the random-phase approximation, as shown in Fig. 2. However, we must caution against judging the merit of an approximation solely on short-range correlations; after all, many of the characteristic properties of the electron gas derive from the long-range nature of the Coulomb potential. We can readily cite two examples. In the Hartree-Fock approximation, the correlation functions behave impeccably; but this is known to be a poor approximation. Also, the correlation functions of a low-density electron gas, when extrapolated to the metallic region, behave better at short distances than those in the random-phase approximation, although the physical picture is completely misrepresented.

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. C. Mavroyannis for reading and commenting on the manuscript, and the National Research Council of Canada for its hospitality and the use of research facilities.

*Issued as National Research Council of Canada Report No. 11827.

†National Research Council Postdoctorate Fellow.

[1]J. Lam, Phys. Rev. B 3, 1910 (1971).

[2]T. Usui, Progr. Theoret. Phys. (Kyoto) 23, 787 (1960).

[3]E. Daniel and S. H. Vosko, Phys. Rev. 120, 2041 (1960).

[4]F. Brouers, Phys. Status Solidi 19, 867 (1967).

[5]R. Lobo, K. S. Singwi, and M. P. Tosi, Phys. Rev. 186, 470 (1969).

[6]S. Ueda, Progr. Theoret. Phys. (Kyoto) 26, 45 (1961).

[7]L. Mittag, *Lecture Notes on the Many-Body Problem from the First Bergen International School of Physics* 1961 (Benjamin, New York, 1962), p. 110.