Screening of interparticle interaction and local field effects in a system of spin-polarized electrons

S. V. Ivliev and V. N. Sobakin

Moscow Engineering Physics Institute

(Received 10 April 1990; resubmitted 23 October 1990)
Zh. Eksp. Teor. Fiz. **98**, 2000–2010 (December 1990)

The screening properties of a system of interacting spin-polarized electrons are investigated. An exact closed equation is derived in the many-particle approach for the vertex function and the principal contribution arising in the ladder approximation with respect to the generalized screened potential is found. The local field correction, which is strongly dependent on the electron density, is calculated; this correction ensures positive compressibility across a broad range of electron densities.

1. INTRODUCTION

The need to incorporate many-particle effects consistently and the lack of explicit small parameters have lead to the development of a new direction in condensed-matter theory (see, for example, Refs. 1–3 and the work they cite) devoted to the formulation and analysis of the permittivity function of an interacting electron gas. A variety of techniques are employed to obtain a great variety of expressions for the permittivity in which the Coulomb interaction effects between electrons are taken into account in one form or another.[4–11] However virtually all of the proposed approaches have limited applicability and require at least partial additional substantiation.

In the present paper we propose a method of describing the screening properties of a system of interacting electrons with a positive neutralizing background, based on an approximate solution of the equation for the vertex function. The exact equation for the vertex is formally obtained in closed form using functional derivatives.

The primary result of this study is the weakening of interelectron correlations due to screening of the interaction. This is directly manifested as a reduction in the local field correction at low momenta in the intermediate range of electron densities characterized, as usual, by the dimensionless parameter r_s. This entire analysis corresponds to values of r_s where the electronic system takes the form of a homogeneous gas or liquid, since no fundamental rearrangement of the one-particle spectrum has yet occurred.

It is demonstrated that we can utilize an approximate equation for the vertex to first order in a certain generalized potential for a spin-polarized electron gas; the potential is the product of the interelectron screened interaction and the vertex function. This is due to the cancellation of higher-order contributions accounting for the screening of interparticle interaction. The region where this potential is effectively small also determines the range of r_s for which the analysis is valid. Analysis of this particular system is made even more interesting by the fact that a wide range of experimental and theoretical results have already been obtained for a number of Fermi systems of this type.[12,13] We assume $T = 0$ and $\hbar = 1$ throughout the analysis below.

2. SELF-CONSISTENT INTERPARTICLE INTERACTION OF ELECTRONS

We consider a system of interacting electrons superposed on a background of homogeneous positive neutralizing charge. Then including the external field $U(r, t)$, the Hamiltonian of this system takes the standard form in the second quantization representation:

$$H = \int d^3r\,\Psi^+(\mathbf{r},t)\left[-\frac{\nabla^2}{2m} - \mu + U(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$
$$+\frac{1}{2}\int d^3r\,d^3r_1\,\Psi^+(\mathbf{r},t)\,\Psi(\mathbf{r}_1,t)\,V_{ee}(\mathbf{r}-\mathbf{r}_1)\,\Psi(\mathbf{r}_1,t)\,\Psi(\mathbf{r},t). \tag{1}$$

Introducing in the usual manner the one-particle Green's function

$$G(x, x_1) = -i\langle T\Psi(\mathbf{r}, t)\,\Psi^+(\mathbf{r}_1, t_1)\rangle$$

together with the effective field

$$V(x) = U(x) + \int d^3r_1\,V_{ee}(\mathbf{r}-\mathbf{r}_1)\,\langle\Psi^+(\mathbf{r}_1,t)\,\Psi(\mathbf{r}_1,t)\rangle,$$

using the formalism proposed in Ref. 14 we obtain the closed equation

$$\left(i\frac{\partial}{\partial t}+\frac{\nabla^2}{2m}\right)G(x,x_1) - \int dx_2\,\Sigma(x,x_2)\,G(x_2,x_1) = \delta(x-x_1). \tag{2}$$

Here we introduce the electron self-energy part

$$\Sigma(x,x_1) = -i\int dx_2\,dx_3\,\frac{\delta G^{-1}(x_2,x_1)}{\delta V(x_3)}\,G(x,x_2)\,W(x_2,x_3), \tag{3}$$

defined through the total effective interelectron interaction potential

$$W(x_1,x_2) = \int d^3r_3\,V_{ee}(\mathbf{r}_1-\mathbf{r}_3)\,\varepsilon^{-1}(\mathbf{r}_3,t_1;x_2). \tag{4}$$

This potential is essentially a screened two-particle potential in which all screening effects are described by the permittivity function

$$\varepsilon(x_1,x_2) = \delta(x_1-x_2) + \int d^3r_3\,V_{ee}(\mathbf{r}_1-\mathbf{r}_3)\,\Pi(\mathbf{r}_3,t_1;x_2). \tag{5}$$

0038-5646/90/121125-06$03.00

Here the permittivity is given by the polarization operator

$$\Pi(x_1,x_2)=-\frac{\delta\langle\Psi^+(x_1)\Psi(x_1)\rangle}{\delta V(x_2)}$$

$$=i\int dx_3\,dx_4\,G(x_1,x_3)G(x_4,x_1)\Gamma(x_3,x_4,x_2) \quad (6)$$

and the vertex function

$$\Gamma(x_1,x_2,x_3)=-\frac{\delta G^{-1}(x_1,x_2)}{\delta V(x_3)}. \quad (7)$$

It is the study of the vertex function that is of primary interest in investigating the role of many-particle effects in a system of interacting electrons. A qualitative analysis of the contribution of various diagrams to the vertex has been provided in Ref. 14. It was noted in this study that no consistent strategy for selecting the most important diagrams exists, since the Coulomb interelectron interaction is not small at real electron densities.

The present paper demonstrates how, by deriving a consistent rigorous equation for the vertex function and then solving it approximately, we can identify the main contributions to the vertex. It is therefore possible to obtain rather simple equations in explicit form without using the variational procedure (see, for example, Refs. 15, 16) for the vertex and the corresponding permittivity of the interacting electron gas.

In the simplest approximation, that of noninteracting electrons, we assume

$$\Gamma(x_1,\ x_2,\ x_3)\approx\Gamma_0=\delta(x_1-x_2)\,\delta(x_1-x_3).$$

Including interactions results in a self-consistent redefinition of the vertex:

$$\Gamma(x_1,x_2,x_3)=\delta(x_1-x_2)\,\delta(x_1-x_3)+\int dx_4\,dx_5\,dx_6\,dx_7$$

$$\cdot\frac{\delta\Sigma(x_1,x_2)}{\delta G(x_4,x_5)}G(x_4,x_6)G(x_7,x_5)\Gamma(x_6,x_7,x_3). \quad (8)$$

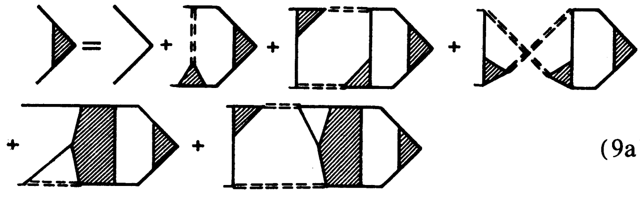
We obtain an exact closed equation for the vertex function (the arguments are dropped from the functions to simplify the notation) from straightforward calculation of the functional derivatives with respect to the Green's function of the self-energy part and the generalized potential:

$$\Gamma=\Gamma_0+\int GG(W\Gamma)\Gamma+\int GGGG(W\Gamma)(W\Gamma)\Gamma$$

$$+\int GG(W\Gamma)GG(W\Gamma)\Gamma$$

$$+i\int GGG\left(W\frac{\delta\Gamma}{\delta G}\right)\Gamma+i\int GGG(W\Gamma)GG\left(W\frac{\delta\Gamma}{\delta G}\right)\Gamma. \quad (9)$$

In graphical form this equation appears as



(9a)

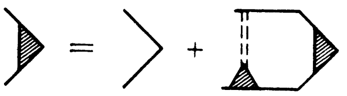
Here the solid lines correspond to the electron Green's functions $G(x_1,x_2)$, while the double dashed lines correspond to the screened effective potential $W(x_1,x_2)$, with the shaded triangles referring to the vertices $\Gamma(x_1,x_2,x_3)$ and the pentagon representing the block $\delta\Gamma(x_1,x_2,x_3)/\delta G(x_4,x_5)$.

Equations (1)–(6), (9) are applicable for describing an arbitrary state of an interacting electronic system, including a Wigner crystal. The possible approximate solutions are determined by the selection of the corresponding zeroth approximation and the expansion parameter.

It directly follows from Eq. (9) that it is precisely this screened interaction W that determines the many-particle properties of the electron system. As a rule incorporation of screening effects weakens the potential. Formally treating W as a small quantity we can transform this equation by writing it as an expansion in powers of the effective potential. The resulting expression does not yet contain functional derivatives of the vertex function. To first order in the potential W Eq. 10 takes the form

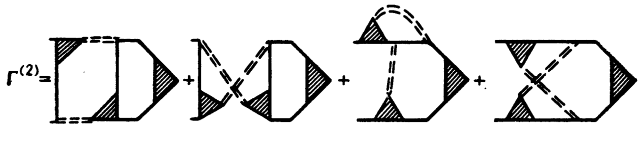
$$\Gamma=\Gamma_0+\int GG(W\Gamma)\Gamma. \quad (10)$$

This result corresponds to the approximation



(11)

To second order in W it is necessary to retain the contributions of the third and fourth terms in Eq. (9) and also to evaluate $\delta\Gamma/\delta G$ from Eq. (10) and then substitute it into the expression $\int GGG(W\delta\Gamma/\delta G)\Gamma$. We then have the following graphical representation for the contribution to the vertex:



(12)

The analytical expression for $\Gamma^{(2)}$ is already cumbersome and is not provided here. In this way it is possible to obtain terms of any order in W. This procedure can be formalized so that analytical programming techniques (such as REDUCE) can be used up to any term in the series.

The primary result from analyzing this expansion is that the actual parameter of the expansion is the quantity $\widetilde{W}=W\Gamma$ which functions as a characteristic "generalized interaction potential" in this system. The function $\widetilde{W}(x_1,x_2,x_3)$, as we see by the definition, is nonlocal in the general case even if the initial electron system is spatially uniform.

Below we use the so-called "local vertex" approximation[15] to carry out a consistent and transparent analysis. Here the solution of Eq. (9) is sought in the function class

$$\Gamma(x_1,\ x_2,\ x_3)=\delta(x_1-x_3)\,\Gamma(x_2-x_3),$$

which corresponds to a dependence of the vertex on momentum only.

As we demonstrate below, this choice is equivalent to describing the interaction in terms of corrections to the local field.

The function $\widetilde{W}$ is therefore dependent solely on a single momentum and in fact becomes a local pair interaction potential. According to the definition (4) this is a screened potential and, consequently, it has a limited radius in a charged liquid or gas system. An important property of the series (9) obtained for the vertex is the partial cancellation of the contributions of the diagrams to all orders in $\tilde{W}$, beginning with the second order. This is most clearly manifested for the short-range potentials. Indeed the first and third as well as the second and fourth terms have opposite signs in Eq. (12) and taking into account the effective short-range action of $\tilde{W}$ we see that these graphs become topologically equivalent. For an unpolarized electron gas the first and second terms contain an additional summation over spin, so the cancellation is incomplete. In the case of a spin-polarized gas the additional summation is absent and these four diagrams cancel one another in a pairwise manner. This same effect occurs for higher order terms in $\tilde{W}$.

This cancellation can be explained physically by noting that the Pauli principle forbids particles to approach one another and, consequently, directly sense the short-range potential. Hence all correlation effects corresponding to second or higher order diagrams become insignificant, and the first-order exchange diagram (12) makes the primary contribution to the vertex. Strictly speaking, correlation effects are present in this diagram as well, since the effective potential $\tilde{W}$ differs substantially from the Coulomb potential due to screening.

Equation (10) therefore determines the principal behavorial characteristics of the vertex function for a spin-polarized system of electrons. At higher densities it is valid simply because the quantity $\tilde{W}$ itself is small compared to the kinetic energy with reasonably small r_s. Generally speaking dense spin-polarized systems are unlikely to exist, so the problem of describing their properties in the limit $r_s \ll 1$ is of purely academic interest. The approximate equation (10) is also valid in the intermediate density range $r_s \geqslant 1$, since screening results in a progressively weaker dependence of the potential on momentum in the range $q \leqslant 2k_F$ with increasing r_s, which is the condition for cancellation of the higher-order diagrams.

Taking this into account we use this same approach to describe a system of spin-polarized interacting electrons. We note that this method may be rather effective for an unpolarized gas due to the partial cancellation of the corresponding diagrams and, as we shall see, the numerical smallness of $\tilde{W}$, even for $r_s \geqslant 1$.

In principle another method has also been proposed (see Ref. 13) for transformating the functional differential equations by the substitution $\delta\tilde{W}/\delta G \to d\tilde{W}/dp$ in Eq. (8). However this requires separate treatment

3. PROPERTIES OF THE PERMITTIVITY OF A SPIN-POLARIZED INTERACTING ELECTRON GAS

Assuming spatial homogeneity of this system, we will operate in the momentum representation. Then the equations determining the behavior of the spin-polarized interacting electrons are

$$G^{-1}(p)=\omega-\varepsilon_{\mathbf{p}}-\Sigma(p), \tag{13}$$

$$\Sigma(p)=i\int\frac{d^4k}{(2\pi)^4}G(p+k)W(k)\Gamma(k), \tag{14}$$

$$W(k)=v(k)/\varepsilon(k), \tag{15}$$

$$\varepsilon(k)=1+v(k)\Pi_0(k)\Gamma(k), \tag{16}$$

$$\Pi_0(k)=i\int\frac{d^4p}{(2\pi)^4}G(p+k)G(p), \tag{17}$$

$$\Gamma(q)=1-\frac{\Gamma(q)}{\Pi_0(q)}\int\frac{d^4p\,d^4k}{(2\pi)^8}G(p)G(p+q)G(p+k)\times G(p+k+q)W(k)\Gamma(k). \tag{18}$$

Here $p\equiv(\mathbf{p},\omega)$; $v(\mathbf{k})=4\pi e^2/\mathbf{k}^2$ is the regular Coulomb potential; and $\Pi_0(k)$ is the polarization operator determined by means of the exact Green's functions. We then as usual, introduce the local field correction $F(q,\omega)$ using the following representation for the permittivity function:

$$\varepsilon(\mathbf{q},\omega)=1+\frac{v(q)\Pi_0(\mathbf{q},\omega)}{1-F(\mathbf{q},\omega)v(\mathbf{q})\Pi_0(\mathbf{q},\omega)}. \tag{19}$$

Comparing this equation to Eq. (16) we obtain directly

$$\Gamma^{-1}(q)=1-F(q)v(q)\Pi_0(q), \tag{20}$$

which confirms the claim above that the local field correction is related to the vertex function, which depends solely on the transferred momentum. Then, using Eq. (20) we find an equation for $F(q)$:

$$F(q)=-\frac{1}{v(q)\Pi_0^2(q)}\int\frac{d^4p\,d^4k}{(2\pi)^8}G(p)G(p+q)G(p+k)\times G(p+k+q)\tilde{W}(k). \tag{21}$$

This system of equations is completely closed. An exact solution of this system cannot be obtained even numerically. As a first iteration in place of the exact self-consistent equation

$$\tilde{W}(k)=\frac{4\pi e^2}{\mathbf{k}^2+[1-F(k)]\Pi_0(k)} \tag{22}$$

we utilize an equation that is valid for this system in the long-wavelength static limit

$$\tilde{W}(q)=\frac{4\pi e^2}{\mathbf{q}^2+k_F^2\lambda^2}, \tag{23}$$

where λ^2 is a dimensionless screening parameter which must be found by requiring self-consistency. Here the self-energy part $\Sigma(p)$ is given by

$$\Sigma(p)=\int\frac{d^3k}{(2\pi)^3}n_{\mathbf{k}}\frac{4\pi e^2}{|\mathbf{p}-\mathbf{k}|^2+k_F^2\lambda^2}, \tag{24}$$

while the one-particle excitation spectrum takes the form

$$E_{\mathbf{p}}=\varepsilon_{\mathbf{p}}+\Sigma(p). \tag{25}$$

One advantage of using this equation for $\tilde{W}(q)$ is that all subsequent calculations can be carried out completely. The fundamentally important screening effect can thus be accounted for, albeit only approximately.

Then evaluating for Eq. (17) the long-wavelength limit

$$\lim_{k\to 0}\Pi_0(k)=\frac{1}{2\pi^2}k_F^2\left(\frac{\partial E_{\mathbf{p}}}{\partial p}\right)^{-1}_{p=p_F} \tag{26}$$

and noting that for small momenta, as we easily see from Eq.

(22), $F(q)$ is proportional to q^2, we obtain a self-consistent equation determining λ^2:

$$\lambda^2=\frac{2\alpha}{\pi}r_s\left\{1-\frac{\alpha}{\pi}r_s\left[1-\left(\frac{1}{2}+\frac{\lambda^2}{4}\right)\ln\frac{4+\lambda^2}{\lambda^2}\right]\right\}^{-1}, \tag{27}$$

where $\alpha=(2/9\pi)^{1/3}$.

We can easily show that $\lambda^2=(2\alpha/\pi)r_s$ holds in the limiting cases of large and small densities. In the intermediate range it turns out that λ^2 is also, with good accuracy (better than 10%), close to the value

$$\lambda^2=\lambda_{RPA}^2=\frac{2\alpha}{\pi}r_s. \tag{28}$$

This result was obtained independently by the present authors in a previous study[17] and in Ref. 18. The screening effect clearly results in a significant weakening of the potential $\tilde{W}(k)$. We go over to the dimensionless form of the Coulomb potential to prove this statement, by relating the Coulomb potential to the characteristic energy:

$$\frac{4\pi e^2}{\Omega_0 k_F^2}\frac{1}{\varepsilon_F}\frac{1}{k^2}=6\alpha^4 r_s\frac{1}{k^2}\approx\frac{0{,}18r_s}{k^2}, \tag{29}$$

where $k=q/k_F$ and Ω_0 is the volume per electron. As a result the function $\tilde{W}(k)$ can be given in dimensionless form as

$$\tilde{W}(k)\approx\frac{0{,}18r_s}{k^2+0{,}26r_s}. \tag{30}$$

For comparison purposes we note that the unscreened Coulomb interaction (29) continues to be proportional to r_s which keeps it from being regarded as small for $r_s>5$.

It is worth recalling, however, that some care should be taken in using approximate Eq. (30) in place of the exact Eq. (22) for $\tilde{W}(k)$. The problem here is that the function Π_0 is dependent on the wave vector, and for $q\leqslant 2k_F$, for example, the Lindhard equation yields $\Pi_0(2k_F)=\Pi_0(0)/2$. This imposes a constraint on the range of the effective smallness of $\tilde{W}$. Indeed, $\tilde{W}(k)$ for $k=2k_F$ will no longer be determined by Eq. (30) but rather by

$$W(2k_F)\approx\frac{0{,}18r_s}{4+0{,}13r_s}.$$

Here the requirement $\tilde{W}<1$ establishes the possible range of these results for $r_s<100$. The auxiliary factor $1-F(q)$ narrows this range even further, although, as demonstrated by the calculations given below, $F(q)$ decays rapidly with increasing r_s and at large values of this parameter is proportional to rs^{-1} for $q\leqslant 2k_F$. A rough upper estimate of $F(q)$ for $q\leqslant 2k_F$ and large r_s can be obtained directly from Eq. (21) by replacing $\tilde{W}$ with a constant of order unity. Then $F(q)\approx 2r_s^{-1}q^2/k_F^2$, which yields a constraint of $(r_s)_{\rm cr}\approx 60$. This estimate is in good agreement with Monte-Carlo calculations of the phase states of electron gas.[19] A rise in r_s above such values will cause the effective potentials $\tilde{W}$ to grow. This in turn will result in a fundamental rearrangement of the one-particle spectrum and will significantly alter the character of the screening. Ultimately a transition to the Wigner crystal state is possible. Thus the approximation for $\tilde{W}$ used above will be valid if $r_s<(r_s)_{\rm cr}\approx 60$. Using Eqs. (25) and (21) we obtain the equation for the local field correction

$$F(q,\omega)=\frac{1}{v(q)\Pi_0^2(q,\omega)}\int\frac{d^3p\,d^3k}{(2\pi)^6}\cdot\frac{(\theta_{\mathbf{p}}-\theta_{\mathbf{p+q}})(\theta_{\mathbf{k}}-\theta_{\mathbf{k+q}})}{(\omega+E_{\mathbf{p}}-E_{\mathbf{p+q}}+i\delta)(\omega+E_{\mathbf{k}}-E_{\mathbf{k+q}}+i\delta)}\frac{4\pi e^2}{|\mathbf{p}-\mathbf{k}|^2+\lambda^2k_F^2}, \tag{31}$$

where θ_p is the Heaviside unit function. We analyze this equation in the most interesting static case, $\omega=0$. Then a result for $F(q,0)$ is obtained in closed form in the limit of small and large wave vectors.

We note that many studies (see survey[3]) that account for exchange-correlation effects introduced the permittivity in a somewhat different manner. Specifically,

$$\varepsilon(\mathbf{q},\omega)=1-\frac{v(\mathbf{q})\chi_0(\mathbf{q},\omega)}{1+G(\mathbf{q},\omega)v(\mathbf{q})\chi_0(\mathbf{q},\omega)}, \tag{32}$$

where $\chi_0(\mathbf{q},\omega)$ is the Lindhard function, while $G(\mathbf{q},\omega)$ (not to be confused with the Green's function) is also called the correction to the local field. This function is related to $F(\mathbf{q},\omega)$ as follows:

$$G(\mathbf{q},\omega)=F(\mathbf{q},\omega)-\frac{1}{v(\mathbf{q})}[\Pi_0^{-1}(\mathbf{q},\omega)+\chi_0^{-1}(\mathbf{q},\omega)]. \tag{33}$$

In the long-wavelength limit the quantity $G(q,0)$ for the spin-polarized electron gas takes the form

$$\lim_{q\to 0}G(q,0)=\frac{1}{2}\left(\frac{q}{k_F}\right)^2\left(1-\frac{\lambda^2}{4}\ln\frac{4+\lambda^2}{\lambda^2}\right), \tag{34}$$

and this result coincides exactly with the linear approximation with respect to $\tilde{W}$ for $\Pi_0^{-1}(q)$. Reference 20 derived a similar equation, although with a different value for the screening parameter λ^2. For large wave vectors the equation for $G(q,0)$ is more involved:

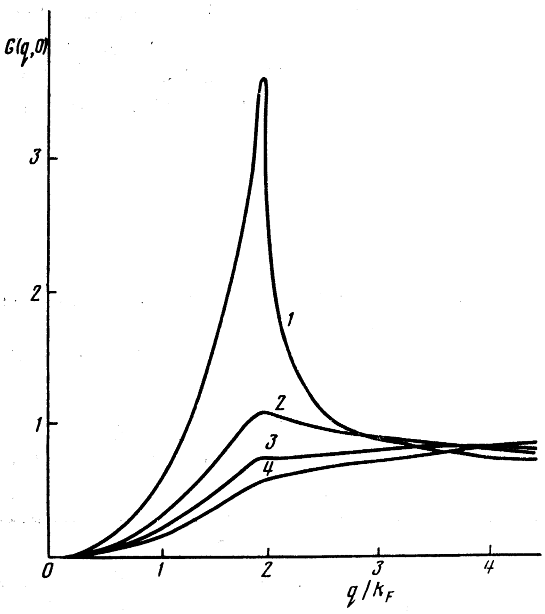


FIG. 1.—Plot of the function $G(q,0)$ for various values of the parameter r_s: 1—$r_s=0.01$; 2—$r_s=4.5$; 3—$r_s=10.0$; 4—$r_s=15.0$.

$$\lim_{q\to\infty} G(q) = \frac{2}{3} + \frac{3}{4}\lambda^2 - \lambda^3 \operatorname{arctg}\frac{2}{\lambda} - \frac{1}{8}\lambda^4 + \left(\frac{3}{8}\lambda^4 + \frac{\lambda^6}{32}\right)\ln\frac{4+\lambda^2}{\lambda^2} + \frac{2\alpha}{\pi} r_s (I_1^2 - I_2). \tag{35}$$

Here

$$I_1(\lambda) = \frac{2}{3}\int \frac{d^3k\, d^3p}{(4\pi)^2}\theta_p\theta_k \frac{1}{|\mathbf{p}-\mathbf{k}|^2+\lambda^2},$$
$$I_2(\lambda) = \frac{2}{9}\int \frac{d^3k\, d^3p\, d^3q}{(4\pi)^3}\theta_p\theta_k\theta_q \frac{1}{|\mathbf{p}-\mathbf{k}|^2+\lambda^2}\,\frac{1}{|\mathbf{k}-\mathbf{q}|^2+\lambda^2}. \tag{36}$$

Here

$$\lim_{\lambda\to 0} G(q\to\infty; 0) = {}^2/_3, \quad \text{and} \quad \lim_{\lambda\to\infty} G(q\to\infty, 0) = 1,$$

i.e., the limiting cases of large and small densities are also determined by an approximation linear in $\widetilde{W}$ for the function $\Pi_0^{-1}(q)$ given by (31), (33). The agreement of the limiting values from Eqs. (34) and (35) with the results from the linear approximation with respect to $\widetilde{W}$ in Eqs. (31), (33) provides some hope that the linear approximation will be entirely suitable for use across the entire range of wave vectors. We again emphasize that the validity of this statement is essentially based on the effective smallness of the interparticle potential $\widetilde{W}(k)$.

Numerical results for the correction $G(q,0)$ to the local field for different r_s in the approximation linear in $\widetilde{W}$ are provided in the figure.

One distinguishing characteristic of the resulting correction to the local field is its strong dependence on the electron density, which is a new result in the microscopic approach. Note that the function $G(q,\omega)$ for the case where the effective interelectron potential $\widetilde{W}(q)$ is replaced by the unscreened Coulomb potential $v(q)$ becomes the exact corresponding expression for the correction to the local field obtained by a wide variety of different techniques and has become the most "popular" function among those defined within the framework of the microscopic approach.[3,8] However it will become clear from this analysis that the unscreened Coulomb potential in Eq. (25), accounting only for the approximation that is linear in the potential, is valid for the spin-polarized electron gas only for $r_s \leqslant 5$ [see estimate (30)].

As we see from the figure the sharp peak at $q \approx 2k_F$, which is characteristic of virtually all typical corrections to the local field,[3] appears in $G(q,0)$ only for r_s small; the peak almost vanishes entirely in the range $r_s \sim 10$.

An analysis of the behavior of the permittivity function in the limit of small wave vectors demonstrates that in this approach the screening radius and the compressibility of interacting electron gas determined from the equation

$$\varepsilon(q\to 0, 0) = 1 + \left(\frac{\lambda_{TF}}{q}\right)^2 \frac{\varkappa}{\varkappa_f}, \tag{37}$$

remain positive over a broad range of intermediate values.

In the same approach we examine the behavior of the one-electron energy which provides the possibility in principle for, first, using these results in band calculations and, second, directly estimating the value of r_s^* at which the system makes the transition to the spin-polarized state. This energy can be written (see Ref. 3) as

$$\varepsilon(r_s) = \frac{3}{5\alpha^2 r_s^2} - \frac{2}{\pi\alpha r_s^2}\int_0^{r_s} dr_s \int_0^{\infty} dx [1 - S(x)], \tag{38}$$

where $S(x)$ is the structure factor and $x = q/k_F$. The structure factor is calculated through the permittivity by means of the fluctuation-dissipation theorem. Equation (38) is valid for both the spin-polarized and unpolarized electronic states.

Numerical calculations with Eq. (38) were carried out using the static local field correction derived above. The results are given in the table.

Analysis of the resulting one-electron energy values demonstrates the possibility of a transition to the spin-polarized state for $r_s \sim 25$–30, when its energy drops below the unpolarized electron gas energy. This estimate for the transition point is in good agreement with Monte-Carlo calculations.[19] Nonetheless our results should be treated with some care, since more accurate calculations require knowledge of the correction to the local field across the entire range of q, ω and r_s. Moreover, partial cancellation of higher-order diagrams (12) will occur only in the unpolarized state.

The possible transition point can also be estimated from the conditions which define the region within which the dimensionless interpartical potential analogous to Eqs. (28)–(30), is effectively small in the unpolarized state. In this case

TABLE I. The exchange-correlation energy per electron in Ry for the spin-polarized ($\varepsilon_{xc}^{\uparrow\uparrow}$) and unpolarized ($\varepsilon_{xc}^{\uparrow\uparrow}$) electron states.

r_s	1	2	3	5	10
$\varepsilon_{xc}^{\downarrow\uparrow}$	−1,04	−0,553	−0,384	−0,189	−0,132
$\varepsilon_{xc}^{\uparrow\uparrow}$	−1,24	−0,681	−0,455	−0,273	−0,135
r_s	15	20	25	30	50
$\varepsilon_{xc}^{\downarrow\uparrow}$	−0,088	−0,068	−0,059	−0,046	−0,028
$\varepsilon_{xc}^{\uparrow\uparrow}$	−0,089	−0,069	−0,059	−0,047	−0,03

we obtain $r_s^* \approx 28$, which is also in agreement with the values reported above.

4. CONCLUSION

The analysis of the features of screening of interelectron interaction carried in the present paper is based on an exact closed equation for the vertex function. The fundamental advantage of this equation, aside from its consistent derivation, lies in the precise procedure for deriving a series in a certain new parameter $\widetilde{W}$ which automatically arises in the problem. Physically the quantity $\widetilde{W}$ is equivalent to the effective interparticle interaction potential, where the screened Coulomb potential and the renormalized vertex enter into the equations self-consistently. The primary contribution to the vertex in this approach for spin-polarized electrons is found to first order in $\widetilde{W}$, since cancellation of the diagrams occurs in the higher-order terms.

We therefore obtain an explicit expression for the correction to the local field that rather fully accounts for the exchange-correlation effects and is valid over a broad electron-density range. This correction turns out to be strongly dependent on the electron density and will not alter the compressibility sign in the range of r_s analyzed here.

The authors express their sincere gratitude to D. E. Khmel'nikskii for critical commentary.

[1] *High-Temperature Superconductivity*, Consultants, New York, 1982.

[2] O. V. Dolgov and E. G. Maksimov, Usp. Fiz. Nauk. **135**, 441 (1981) [Sov. Phys. Usp. **24**, 170 (1981)].

[3] V. D. Gorobchenko and E. G. Maksimov, Usp. Fiz. Nauk. **130**, 65 (1980) [Sov. Phys. Usp. **23**, 35 (1980)].

[4] F. Toigo and T. O. Woodruff, Phys. Rev. B. **2**, 3958 (1970).

[5] P. Vashishta and K. S. Singvi, Phys. Rev. B. **6**, 875 (1972).

[6] V. D. Gorobchenko, Zh. Eksp. Teor. Fiz. **77**, 1197 (1979) [Sov. Phys. JETP **50**, 603 (1979)].

[7] V. D. Gorobchenko and V. G. Kon, Zh. Eksp. Teor. Fiz. **80**, 754 (1981) [Sov. Phys. JETP **53**, 381 (1981)].

[8] J. T. Devreese, F. Brosens, and L. F. Lemmens, Phys. Rev. B. **21**, 1349 (1980).

[9] J. T. Devreese, F. Brosens, and L. F. Lemmens, Phys. Rev. B. **21**, 1362 (1980).

[10] K. Utsumi and S. Ichimaru, Phys. Rev. B. **22**, 5203 (1980).

[11] K. Utsumi and S. Ichimaru, Phys. Rev. B. **23**, 3291 (1981).

[12] A. D. Margulis and Vl. A. Margulis, Zh. Eksp. Teor. Fiz. **93**, 1800 (1987) [Sov. Phys. JETP **66**, 1028 (1987)].

[13] V. A. Khodel' and V. R. Shaginyan, Yad. Fiz. **46**, 1638 (1987) [Sov. J. Nucl. Phys. **46**, 1638 (1987)].

[14] E. G. Maksimov, Zh. Eksp. Teor. Fiz. **69**, 2236 (1975) [Sov. Phys. JETP **42**, 1138 (1975)].

[15] D. C. Langreth, Phys. Rev. **181**, 753 (1969).

[16] A. K. Rajagopal and K. P. Jain, Phys. Rev. A. **5**, 1475 (1972).

[17] S. V. Ivliev and V. N. Sobakin, Preprint of the Moscow Engineering-Physics Institute 008-85. MEPI, Moscow, 1985.

[18] P. Streitenberger, Phys. Stat. Sol. **125**, 681 (1984).

[19] D. Ceperley, Phys. Rev. B. **18**, 3126 (1978).

[20] B. S. Shartry, S. S. Tha and A. K. Rajagopal, Phys. Rev. B. **9**, 2000 (1974).

Translated by Kevin S. Hendzel