

Single-particle spectrum of a rarefied electron gas

M. V. Zverev

Moscow Engineering-Physics Institute, 115409 Moscow, Russia

V. A. Khodel'

Kurchatov Institute, 123182, Moscow, Russia

V. R. Shaginyan

St. Petersburg Institute of Nuclear Physics, Russian Academy of Sciences, 188350 Gatchina, Russia

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The spectrum $\varepsilon(p)$ of single-particle excitations of a homogeneous 3D electron gas is calculated in the jellium model with consideration of correlation corrections. The value of the Coulomb parameter α at which the system becomes unstable against a phase transition with the formation of a fermion condensate is found. It is shown that the special points on the $\varepsilon(p)$ curve corresponding to this phase transition first appear when $\alpha \approx 3.6$ ($r_s \approx 21$) at $p \approx 0.6p_F$. © 1996 American Institute of Physics. [S1063-7761(96)02803-8]

1. INTRODUCTION

For a long time there has been a widely held opinion (see, for example, Ref. 1) that the Landau approach to the theory of homogeneous Fermi liquids, in which the ground-state energy is treated as the quasiparticle distribution functional $n(\mathbf{p})$, admits only a unique, Fermi type of solution with only two permissible values of $n(\mathbf{p})$ equal to 0 and 1. Such an assertion implies that the energy functional $E_0[n(\mathbf{p})]$ of the Fermi system always achieves a minimum at one of the boundary points of the functional space $[n]$, whose boundaries are specified by Pauli's principle. This notion is valid for an ideal Fermi gas or systems with a weak interaction, but it is arbitrary from the mathematical standpoint. Also, since the model functional $E_0[n(p)]$, which achieves a minimum in a certain distribution $0 < n(p) < 1$ with a finite derivative dn/dp in a definite region of phase space, was devised in Ref. 2, there have been several papers,³⁻⁶ in which new model functionals with a non-Fermi distribution $n(\mathbf{p})$ were devised. Mathematically, when the form of $E_0[n(\mathbf{p})]$ is assigned, the search for the minimum reduces to solving the variational equation

$$\varepsilon(\mathbf{p}, n(\mathbf{p})) = \frac{\delta E_0[n(\mathbf{p})]}{\delta n(\mathbf{p})} = \mu, \quad (1)$$

(where μ denotes the chemical potential) in a finite region of the phase space, whose boundaries themselves are determined by the form of the energy functional. The chemical potential appears, as always, because of constraints imposed on the variation by the conservation law for the number of particles.

In the Landau theory the variational derivative $\varepsilon(\mathbf{p}) = dE_0/dn(\mathbf{p})$ is nothing but the quasiparticle energy. Thus, if the energy functional does, in fact, achieve a minimum at some internal point in the functional space $[n]$, it means that the plot of the spectrum of single-particle excitations $\varepsilon(\mathbf{p})$ has a plateau lying on the Fermi surface. Therefore, the Fermi system divides into two subsystems, one of which is dispersionless, i.e., has an infinite effective mass,

and was called a fermion condensate in Ref. 2. At the temperature $T=0$ this phenomenon is observed for definite values of the input parameters, and the transition associated with the appearance of the plateau has features of a second-order phase transition with the condensate density as the order parameter. In Ref. 7 this phase transition was also studied from the standpoint of the topological structure of a single-particle Green's function.

The microscopic theory of this phenomenon has scarcely been developed, and many involved questions pertaining to fermion condensates as systems with multiple degeneracy have not been solved. The purpose of this paper is more modest. Staying within the traditional Landau approach, we wish to find the conditions under which a transition might be made to some real physical system.

Unfortunately, there is still no fully developed theory for the single-particle spectrum of normal Fermi systems with a fairly strong interparticle interaction. Practically all the methods for numerically calculating it suffer from shortcomings. In this paper we use a method proposed within the functional approach³ for this purpose. Being also approximate, it has several advantages, one of which is the fact that the approximations made in it are fairly straightforward, and, in addition, it employs basically the same amplitudes which appear in the ground-state energy problem. The functional approach, within which this method was developed, was described in detail in the review in Ref. 8. The basic equation of the approach is the functional equation for an effective interaction R , which specifies the difference between the linear response function χ of the system and the response function χ_0 of a system of noninteracting particles. The use of the local approximation makes it possible to reduce the functional equation to an integrodifferential equation,⁸ which is solved by standard numerical methods. The local approximation has proved itself for systems in which the distance between the particles is less than the radius of action of the forces, i.e., an electron gas and the dense neutron material in neutron stars. The main relations of the microscopic method for calculating the single-particle spectra of Fermi systems

within the functional approach were formulated in Ref. 3. In this paper we use these relations to study the single-particle spectra of a rarefied 3D electron gas, and we elucidate the behavior of these spectra with variation of the parameter $r_s = a_B/r_0$ (a_B is the Bohr radius, and r_0 is the distance between the particles). We also calculate the ratio M/M^* of the bare electron mass to the effective electron mass as a function of r_s and find the point where this ratio vanishes.

2. BASIC RELATIONS OF THE MICROSCOPIC THEORY OF THE SINGLE-PARTICLE SPECTRUM OF A FERMI SYSTEM

In this paper we investigate the stability of the normal state of a homogeneous Fermi liquid, in which quasiparticles fill the Fermi sphere, $n(p) = \theta(p_F - p)$, up to the Fermi momentum p_F . The restrictions of the Landau theory are usually related to Pomeranchuk's stability conditions,⁹ which contain second variational derivatives of the energy functional $E_0[n(\mathbf{p})]$. It was shown in Refs. 2 and 3 that apart from these conditions, which have the character of sufficient conditions, there is also a necessary condition containing first functional derivatives for stability of the ground state of a Landau Fermi liquid. We focus our attention on a violation of this stability condition, which is formulated as a condition stipulating that the variation of the ground-state energy E_0 is nonnegative under any permissible variations of the quasiparticle distribution function $n(\mathbf{p})$:

$$\delta E_0 = \int [\varepsilon(\mathbf{p}, n(\mathbf{p})) - \mu] \delta n(\mathbf{p}) \frac{d^3 p}{(2\pi)^3}. \quad (2)$$

Here μ is the chemical potential of the system, and $\varepsilon(\mathbf{p}, n(\mathbf{p}))$ is the quasiparticle energy, which, in turn, is also a functional of the quasiparticle distribution $n(\mathbf{p})$. For a Fermi distribution the variations of $n_F(p)$ allowed by the Pauli exclusion principle clearly have the same sign as the difference $p - p_F$. Therefore, starting from Eq. (2) and replacing the chemical potential μ for a homogeneous normal Fermi system in it by the quasiparticle energy $\varepsilon(p_F, n_F(p))$, we can easily reformulate the necessary condition for stability of the Fermi distribution in a somewhat different form, if we require that the quantity

$$s(p) = 2M \frac{\varepsilon(p, n(p)) - \varepsilon(p_F, n_F(p))}{p^2 - p_F^2} \quad (3)$$

be positive at all values of the momentum p . In the weak-coupling limit we clearly have $s(p) \approx 1$. If the sign of $s(p)$ changes with increasing coupling constant g , which determines the intensity of the pairwise vacuum potential $V(q)$, instability and restructuring of the Fermi distribution $n_F(p)$ occur as a result.

Thus, the investigation of the stability of a homogeneous Fermi liquid against restructuring of its quasiparticle distribution (which leaves the system homogenous) involves calculating the single-particle spectrum of the system. We do this, using Eq. (3) and the results in Ref. 3.

The calculation of the single-particle spectrum $\varepsilon(\mathbf{p})$ starts out with the formula for the ground-state energy E_0 , which relates it to the linear response function of the system $\chi(\mathbf{k}, \omega)$ (Ref. 10):

$$E_0 = \tau + W, \quad (4)$$

where τ is the kinetic energy of the system of noninteracting particles and the interaction energy is given by the expression

$$W = \frac{1}{2} \rho^2 V(0) - \frac{1}{2} \int \int \int_0^g V(\mathbf{q}) [\text{Im} \chi(\mathbf{q}, \omega) + 2\pi\rho \delta(\omega)] \frac{d\omega d^3 q dg}{(2\pi)^4 g}. \quad (5)$$

The function $\chi(\mathbf{q}, \omega)$, which depends on the momentum \mathbf{q} and the frequency ω , is related to the response function of a system of noninteracting particles $\chi_0(\mathbf{q}, \omega)$ by the expression⁸

$$\chi(q) = \chi_0(q) + \chi_0(q) R(q) \chi(q), \quad (6)$$

where $R(q)$ is an effective interaction, which is defined as the second variational derivative of the interaction energy with respect to the density:

$$R(q) = \frac{\delta^2 W}{\delta \rho(q) \delta \rho(-q)}. \quad (7)$$

A calculation of this derivative from (5) gives⁸

$$R(k) = V(\mathbf{k}) - \frac{1}{2} \frac{\delta^2}{\delta \rho(k) \delta \rho(-k)} \int \int \int_0^g V(\mathbf{q}) \times \text{Im} \chi(\mathbf{q}, \omega) \frac{d\omega d^3 q dg}{(2\pi)^4 g}. \quad (8)$$

The calculation of the effective interaction $R(k)$ is inseparable from the solution of the problem of determining the ground-state energy of the system. We assume that this problem has already been solved and that $R(k)$ is the function found for the 4-momentum k . Methods for solving it were described in the review in Ref. 8.

Varying the expressions (4) and (5) with respect to $n(\mathbf{p})$, we obtain

$$\varepsilon(\mathbf{p}) = \varepsilon_p^0 + \rho V(0) - \frac{1}{2} \int V(\mathbf{q}) \frac{d^3 q}{(2\pi)^3} - \frac{1}{2} \int \int \int_0^g V(\mathbf{q}) \text{Im} \frac{\delta \chi(\mathbf{q}, \omega)}{\delta n(\mathbf{p})} \frac{d\omega d^3 q dg}{(2\pi)^4 g}. \quad (9)$$

Calculating the variational derivative $\delta \chi(\mathbf{q}) / \delta n(\mathbf{p})$ with the aid of (6), for the single-particle spectrum we obtain

$$\varepsilon(\mathbf{p}) = \varepsilon_p^0 + \rho V(0) + \varepsilon_1(\mathbf{p}) + \varepsilon_v(\mathbf{p}), \quad (10)$$

where

$$\varepsilon_1(\mathbf{p}) = -\frac{1}{2} \int V(\mathbf{q}) \frac{d^3 q}{(2\pi)^3} - \frac{1}{2} \int \int \int_0^g V(\mathbf{q}) \text{Im} \left\{ \varphi(q) \frac{\delta \chi_0(q)}{\delta n(\mathbf{p})} \varphi(q) \right\} \times \frac{d\omega d^3 q dg}{(2\pi)^4 g}, \quad (11)$$

$$\varepsilon_v(\mathbf{p}) = -\frac{1}{2} \int \int \int_0^g V(\mathbf{q}) \text{Im} \left\{ \chi(q) \frac{\delta R(\mathbf{q})}{\delta n(\mathbf{p})} \chi(q) \right\}$$

$$\frac{d\omega d^3q dg}{(2\pi)^4 g}, \quad (12)$$

$$\varphi(q) = \frac{1}{1 - R(\mathbf{q})\chi_0(q)}. \quad (13)$$

Substitution of the explicit form of the variational derivative

$$\begin{aligned} \frac{\delta\chi_0(\mathbf{q}, \omega)}{\delta n(\mathbf{p})} &= \frac{n(\mathbf{p}-\mathbf{q})}{\varepsilon_{\mathbf{p}}^0 - \omega - \varepsilon_{\mathbf{p}-\mathbf{q}}^0 - i\delta} + \frac{1 - n(\mathbf{p}-\mathbf{q})}{\varepsilon_{\mathbf{p}}^0 - \omega - \varepsilon_{\mathbf{p}-\mathbf{q}}^0 + i\delta} \\ &+ \frac{n(\mathbf{p}-\mathbf{q})}{\varepsilon_{\mathbf{p}}^0 + \omega - \varepsilon_{\mathbf{p}-\mathbf{q}}^0 - i\delta} + \frac{1 - n(\mathbf{p}-\mathbf{q})}{\varepsilon_{\mathbf{p}}^0 + \omega - \varepsilon_{\mathbf{p}-\mathbf{q}}^0 + i\delta} \end{aligned} \quad (14)$$

into (11) gives the following expression for the term $\varepsilon_1(\mathbf{p})$ in Eq. (10) for the single-particle spectrum:^{2,3}

$$\varepsilon_1(\mathbf{p}) = \varepsilon_1^{(1)}(\mathbf{p}) + \varepsilon_1^{(2)}(\mathbf{p}) + \varepsilon_1^{(3)}(\mathbf{p}), \quad (15)$$

where

$$\varepsilon_1^{(1)}(\mathbf{p}) = - \int_{q < p} V(\mathbf{p}-\mathbf{q}) \frac{d^3q}{(2\pi)^3}, \quad (16)$$

$$\begin{aligned} \varepsilon_1^{(2)}(\mathbf{p}) &= \int_{q < p} \int_0^g V(\mathbf{p}-\mathbf{q})(1 - n_F(q)) \varphi^2(\mathbf{p}-\mathbf{q}, \varepsilon_{\mathbf{p}}^0 \\ &- \varepsilon_{\mathbf{q}}^0) \frac{d^3q dg}{(2\pi)^3 g} - \int_{q > p} \int_0^g V(\mathbf{p}-\mathbf{q}) n_F(q) \varphi^2 \\ &\times (\mathbf{p}-\mathbf{q}, \varepsilon_{\mathbf{p}}^0 - \varepsilon_{\mathbf{q}}^0) \frac{d^3q dg}{(2\pi)^3 g}, \end{aligned} \quad (17)$$

$$\begin{aligned} \varepsilon_1^{(3)}(\mathbf{p}) &= \int_{-\infty}^{\infty} \int_0^g V(\mathbf{q})(\varphi^2(q) - 1) \\ &\times \frac{\varepsilon_{\mathbf{p}}^0 - \varepsilon_{\mathbf{q}-\mathbf{q}}^0}{(\varepsilon_{\mathbf{p}}^0 - \varepsilon_{\mathbf{q}-\mathbf{q}}^0)^2 + \omega^2} \frac{d\omega d^3q dg}{(2\pi)^4 g}. \end{aligned} \quad (18)$$

We see that the term $\varepsilon_1(\mathbf{p})$ is calculated for a "frozen" effective interaction $R(k)$, and if it is known, $\varepsilon_1(\mathbf{p})$ is found by direct integration.

We now turn to the contribution $\varepsilon_v(\mathbf{p})$ to the single-particle spectrum, which depends on the variation of the effective interaction $R(k)$ upon variation of the quasiparticle distribution $n_F(p)$ (hereinafter, for the sake of brevity we shall call it the variational contribution). The variational contribution is a part of the total correlation contribution to the single-particle spectrum, which is equal to the variational derivative of the correlation energy of the system E_c with respect to $n(\mathbf{p})$. The correlation contribution includes not only $\varepsilon_v(\mathbf{p})$, but also the term $\varepsilon_1^{(3)}(\mathbf{p})$ and part of the term $\varepsilon_1^{(2)}(\mathbf{p})$ obtained by replacing φ^2 in (17) by $\varphi^2 - 1$. To calculate the function $\delta R(k)/\delta n(\mathbf{p})$, we calculate the variational derivatives of both sides of Eq. (8) with respect to the quasiparticle distribution $n(\mathbf{p})$, thereby obtaining

$$\begin{aligned} \frac{\delta R(k)}{\delta n(\mathbf{p})} &= - \frac{1}{2} \frac{\delta^2}{\delta\rho(k)\delta\rho(-k)} \int \int \int_0^g V(\mathbf{q}) \\ &\times \text{Im} \left\{ \varphi(q) \frac{\delta\chi_0(q)}{\delta n(\mathbf{p})} \varphi(q) \right\} \frac{d\omega d^3q dg}{(2\pi)^4 g} \end{aligned}$$

$$\begin{aligned} &- \frac{1}{2} \frac{\delta^2}{\delta\rho(k)\delta\rho(-k)} \int \int \int_0^g V(\mathbf{q}) \\ &\times \text{Im} \left\{ \chi(q) \frac{\delta R(q)}{\delta n(\mathbf{p})} \chi(q) \right\} \frac{d\omega d^3q dg}{(2\pi)^4 g}. \end{aligned} \quad (19)$$

which is the functional equation for $\delta R(k)/\delta n(\mathbf{p})$.

To solve Eq. (19) we can use the same approximate method which was used in Ref. 8 to solve Eq. (8). The method calls for the use of a local approximation for the second variational derivative of the functional, say $Y(q, \rho)$, in the form

$$\frac{\delta^2 Y(q, \rho)}{\delta\rho(k)\delta\rho(-k)} = \frac{d^2 Y(q-k, \rho)}{d\rho^2}. \quad (20)$$

This relation becomes exact in the limit $k \rightarrow 0$. In the language of the coordinate representation this means that the local approximation takes into account the value of ρ at the point under consideration and treats all the terms containing density gradients approximately. Such an approximation holds best when the radius of action of the forces exceeds the distance between the particles. An electron gas satisfies this condition exactly. This is also confirmed by calculations of the correlation contribution to the ground-state energy (the difference between the total energy and the Hartree-Fock energy) of an unpolarized electron gas in the "jellium" model,⁸ which exhibit excellent agreement (to within 1%) with the results of Monte Carlo calculations¹¹ for values of r_s ranging from 1 to 50.

Use of the local approximation in the functional equations (8) and (19) transforms them into integrodifferential equations:

$$\begin{aligned} R(\mathbf{k}) &= V(\mathbf{k}) - \frac{1}{2} \frac{d^2}{d\rho^2} \int \int \int_0^g V(\mathbf{q}-\mathbf{k}) \\ &\times \text{Im} \chi(\mathbf{q}, \omega) \frac{d\omega d^3q dg}{(2\pi)^4 g}, \end{aligned} \quad (21)$$

$$\begin{aligned} \frac{\delta R(\mathbf{k})}{\delta n(\mathbf{p})} &= - \frac{1}{2} \frac{d^2}{d\rho^2} \int \int \int_0^g V(\mathbf{q}-\mathbf{k}) \text{Im} \left\{ \varphi(q) \frac{\delta\chi_0(q)}{\delta n(\mathbf{p})} \varphi(q) \right\} \\ &\times \frac{d\omega d^3q dg}{(2\pi)^4 g} - \frac{1}{2} \frac{d^2}{d\rho^2} \int \int \int_0^g V(\mathbf{q}-\mathbf{k}) \\ &\times \text{Im} \left\{ \chi(q) \frac{\delta R(q)}{\delta n(\mathbf{p})} \chi(q) \right\} \frac{d\omega d^3q dg}{(2\pi)^4 g}. \end{aligned} \quad (22)$$

In Eq. (21) it is convenient to switch to a calculation of the integral over ω along the imaginary axis,⁸ as is usually done when the interaction energy is calculated from Eq. (5).¹⁰ Owing to the real character of the function χ on the imaginary axis,¹⁰ Eq. (21) is brought into the form

$$\begin{aligned} R(\mathbf{k}) &= V(\mathbf{k}) - \frac{1}{2} \frac{d^2}{d\rho^2} \int_{-\infty}^{\infty} \int \int_0^g V \\ &\times (\mathbf{q}-\mathbf{k}) \chi(\mathbf{q}, i\omega) \frac{d\omega d^3q dg}{(2\pi)^4 g}. \end{aligned} \quad (23)$$

The integrals over ω in the formulas (11) and (12) and in Eq. (22) can be calculated by the same technique, but variation

with respect to the occupation numbers alters the analytic properties of the integrand, and these changes should be taken into account when the path unfolds onto the imaginary axis.

3. SPECTRUM OF THE SINGLE-PARTICLE EXCITATIONS OF A HOMOGENEOUS 3D ELECTRON GAS IN THE LOCAL APPROXIMATION

Using equations from the preceding section, we calculate the single-particle spectrum of a homogenous 3D electron gas in the jellium model. In this model it is assumed that $V(0)=0$, and in this case the expression for the spectrum has the form

$$\varepsilon(p) = \varepsilon_p^0 + \varepsilon_1(p) + \varepsilon_v(p). \quad (24)$$

We begin by calculating the contribution $\varepsilon_1(p)$. Substituting

$$V(\mathbf{q}) = \frac{4\pi e^2}{q^2} \quad (25)$$

into (16), for the first term in Eq. (15) we have

$$\varepsilon_1^{(1)}(p) = -\frac{e^2 p}{\pi} = -\alpha \frac{p p_F}{M}, \quad (26)$$

where $\alpha = M e^2 / \pi p_F$ is the Coulomb parameter.

To calculate the term $\varepsilon_1^{(2)}(p)$, we rewrite (17) in the form

$$\begin{aligned} \varepsilon_1^{(2)}(\mathbf{p}) = & - \int_{-\infty}^{\infty} \int \int_0^g V(\mathbf{q}) H(\mathbf{q}, \omega, \mathbf{p}) \varphi^2(\mathbf{q}, \omega) \\ & \times \frac{d\omega d^3q dg}{(2\pi)^4 g}, \end{aligned} \quad (27)$$

where

$$\begin{aligned} H(\mathbf{q}, \omega, \mathbf{p}) = & -2\pi(1 - n_F(\mathbf{p} - \mathbf{q})) \delta(\varepsilon_{\mathbf{p}}^0 - \varepsilon_{\mathbf{p}-\mathbf{q}}^0 - \omega) \theta(\omega) \\ & + 2\pi n_F(\mathbf{p}) \delta(\varepsilon_{\mathbf{p}}^0 - \varepsilon_{\mathbf{p}-\mathbf{q}}^0 - \omega) \theta(-\omega). \end{aligned} \quad (28)$$

Averaging the expression (27) over the directions of the vector \mathbf{p} , integrating over the frequency ω , and going over to the variables

$$t = \frac{q}{2p_F}, \quad u = \frac{p}{p_F}, \quad (29)$$

we obtain (for the details of the calculation, see the Appendix)

$$\varepsilon_1^{(2)}(p) = -\frac{\alpha p_F^3}{p 2M} \int \int_0^g \frac{sdtdg}{t g} \varphi^2(t, 0) \eta(t, u), \quad (30)$$

where the function $\eta(t, u)$ is given by Eqs. (A4)–(A7).

An analysis of Eq. (23)⁸ shows that the effective interaction R in a homogeneous 3D electron gas is reproduced well already by the first iteration R_0 of Eq. (23), i.e., by substitution of the function χ_0 instead of the exact linear response function χ under the integral sign on the right-hand side of that equation. Since R_0 is linear with respect to g , the integral over the coupling constant in Eq. (23) is easily calculated, and we ultimately obtain the following expression for the contribution under consideration in the single-particle spectrum:

$$\varepsilon_1^{(2)}(p) = -\frac{\alpha p_F^3}{p 2M} \int \frac{dt}{t} \varphi(t, 0) \eta(t, u). \quad (31)$$

Calculating the contribution $\varepsilon_1^{(3)}$ to the spectrum, we again employ the first iteration R_0 of Eq. (23) as the effective interaction R in (18). In this case the calculation of the integral over the coupling constant on the right-hand side of (18) is elementary. Then, calculating the integral over the angles and switching to the variables t and u introduced by Eq. (29) and the variable

$$z = \frac{\omega M}{p_F q}, \quad (32)$$

we obtain

$$\begin{aligned} \varepsilon_1^{(3)}(p) = & -\frac{\alpha p_F^3}{\pi p M} \int \int_0^{\infty} dt dz (\varphi(t, z) - 1) \\ & \times \ln \frac{z^2 + (u-t)^2}{z^2 + (u+t)^2}. \end{aligned} \quad (33)$$

Calculating the contribution of $\varepsilon_1(p)$ to the ratio M/M^* at small α , we can easily prove that $\varepsilon_1^{(2)}(p)$ makes the contribution

$$\frac{M^{(2)}}{M^*} = \frac{1}{2} \alpha \ln \frac{1}{\alpha} \quad (34)$$

and that $\varepsilon_1^{(3)}(p)$ makes the contribution $(M/M^*)^{(3)} \sim \alpha^2$. Since, as follows from (26), $(M/M^*)^{(1)} = \alpha$, at small α we obtain exactly the Gell-Mann–Galitskiĭ formula¹²

$$\frac{M}{M^*} = 1 + \frac{1}{2} \alpha \left(\ln \frac{1}{\alpha} - 2 \right). \quad (35)$$

We turn now to the calculation of the variational contribution $\varepsilon_v(p)$ defined by Eq. (12). The variational derivative $\delta R(q)/\delta n(p)$ in this expression is determined from Eq. (22). The solution of this equation will be the subject of a separate report. A preliminary analysis shows that for a Coulomb gas the iterations of Eq. (22) for $\delta R(q)/\delta n(p)$, like those of Eq. (23) for the effective interaction $R(q)$, rapidly converge, and to calculate the variational contribution $\varepsilon_v(p)$ it is sufficient to take the first iteration $\delta R_0(q)/\delta n(p)$ of Eq. (22) as $\delta R(q)/\delta n(p)$, i.e., to substitute χ_0 instead of χ on the right-hand side and to set $\varphi(q) = 1$. The function $\delta R_0(q)/\delta n(p)$ is calculated in the Appendix. In the dimensionless variables (29) it has the form

$$\frac{\delta R_0(2p_F t)}{\delta n(p_F u)} = \frac{\pi^3 e^2}{2p_F^5} Y(t, u), \quad (36)$$

where $Y(t, u)$ is given by Eq. (A21).

Now substituting the expression (36) into (12) as the variational derivative $\delta R(q)/\delta n(p)$ and switching from integration over q , w , and g to integration over t , z , and α , we obtain

$$\varepsilon_v(p) = -\frac{2 p_F^2}{\pi M} \int_0^{\infty} \int dz dt \chi_0^2(t, z) Y(t, u) \Lambda(t, z, \alpha), \quad (37)$$

where

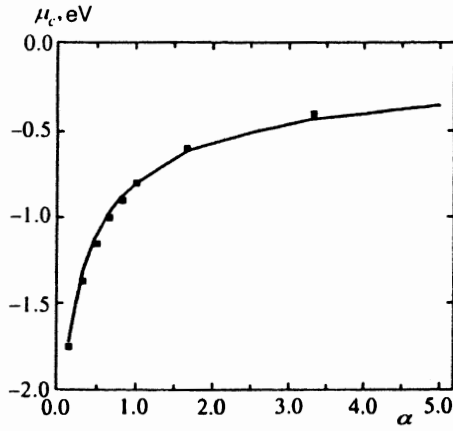


FIG. 1. Correlation contribution to the chemical potential μ_c as a function of α . Solid line—calculation in the present work; filled squares—Monte Carlo calculation.¹¹

$$\Lambda(t, z, \alpha) = \int_0^\alpha \frac{\alpha_1 d\alpha_1}{(1 - \alpha_1 \hat{R}_0 \hat{\chi}_0)^2}, \quad (38)$$

$$\hat{\chi}_0 = \frac{\pi^2}{M p_F} \chi_0, \quad (39)$$

$$\hat{R}_0 = \frac{p_F^2}{\pi e^2} R_0 = \frac{M p_F}{\pi^2 \alpha} R_0. \quad (40)$$

Performing the elementary integration over α in Eq. (38), we obtain

$$\Lambda(t, z, \alpha) = \frac{1}{(\hat{R}_0 \hat{\chi}_0)^2} \ln |1 - \alpha \hat{R}_0 \hat{\chi}_0| + \frac{\alpha}{\hat{R}_0 \hat{\chi}_0 (1 - \alpha \hat{R}_0 \hat{\chi}_0)}. \quad (41)$$

4. DISCUSSION

We used the equations in the preceding section to calculate the single-particle spectra of a homogeneous unpolarized electron gas in the jellium model. The accuracy of the calculation of the complete correlation contribution to the spec-

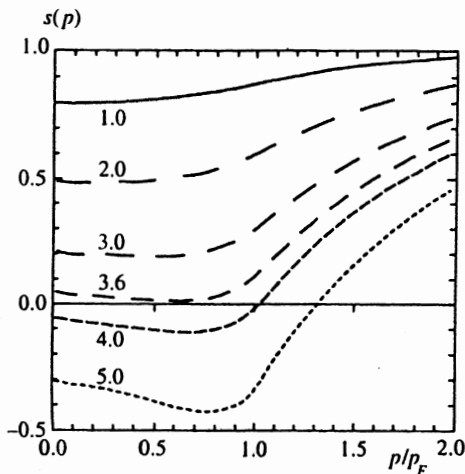


FIG. 2. Plots of $s(p)$ for various values of the Coulomb parameter. The numbers near the curves are the values of α .

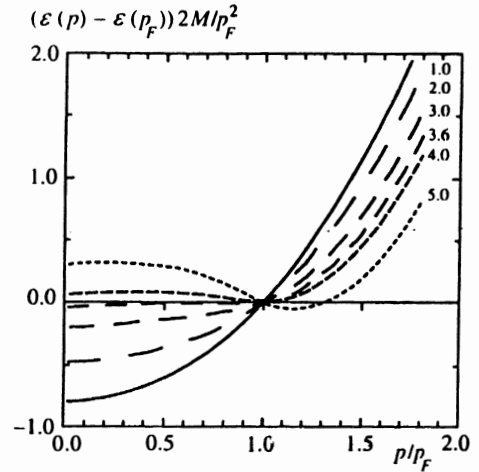


FIG. 3. The dimensionless single-particle spectra $\varepsilon(p) - \mu$ for various values of the Coulomb parameter. The numbers near the curves are the values of α .

trum can be evaluated by comparing the correlation contribution to the chemical potential $\mu_c = \varepsilon_1^{(2)}(p_F) + \varepsilon_1^{(3)} \times (p_F) + \varepsilon_v(p_F)$ with the analogous quantity μ_c^{MC} , which is obtained using the formula

$$\mu_c^{MC} = \mathcal{E}_c^{MC} - \frac{r_s}{3} \frac{d\mathcal{E}_c^{MC}}{dr_s} \quad (42)$$

from the results of Monte Carlo calculations of the correlation energy \mathcal{E}_c^{MC} per particle of a homogeneous unpolarized electron gas.¹¹ The correlation contributions μ_c calculated in the present work are depicted in Fig. 1 together with the Monte Carlo contributions μ_c^{MC} . A comparison shows that the difference between μ_c and μ_c^{MC} is at most 8% in the range of α from 0.166 to 3.32, which corresponds to a variation of r_s from 1 to 20.

Figure 2 shows the function $s(p)$ calculated for various values of the Coulomb parameter α ranging from 1 to 5. The dimensionless difference $(\varepsilon(p) - \mu)2M/p_F^2$ for the same values of α is depicted in Fig. 3. The function $s(p)$ first vanishes at $\alpha \approx 3.6$ at the point $p_c \approx 0.6p_F$. The appearance

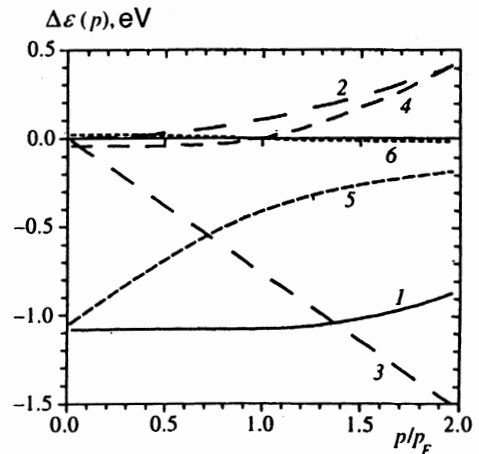


FIG. 4. The contribution $\Delta\varepsilon(p)$ to the single-particle spectrum for $\alpha = 3.6$: 1) $\varepsilon(p)$; 2) ε_p^0 ; 3) $\varepsilon_1^{(1)}(p)$; 4) $\varepsilon_1^{(2)}(p)$; 5) $\varepsilon_1^{(3)}(p)$; 6) $\varepsilon_v(p)$.

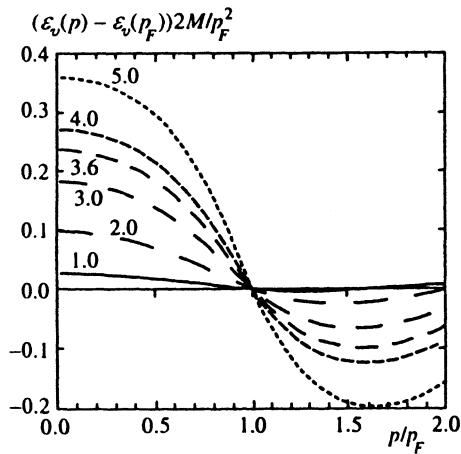


FIG. 5. The dimensionless variational contributions $\varepsilon_v(p) - \varepsilon_v(p_F)$ for various values of the Coulomb parameter. The numbers near the curves are the values of α .

of negative values of $s(p)$ means that the Fermi distribution of the quasiparticles with respect to the momentum $n_F(p)$ has become unstable against small variations, and this results in restructuring of the ground state of the system, i.e., fermion condensation. The appearance of a momentum range $p < p_F$, where $s(p)$ takes negative values, at $\alpha > 3.6$ fits the fact that $\varepsilon(p)$ exceeds $\varepsilon(p_F)$ in this region of the spectrum $\varepsilon(p)$.

The absolute values of the contributions of the individual terms to the spectrum $\varepsilon(p)$ for $\alpha = 3.6$ are given in Fig. 4 in electron volts. The role of the variational contribution in the phenomenon under study merits a separate discussion. It is clearly seen in Fig. 4 that the absolute values of the variational term in the spectra are small in comparison with the remaining terms. However, since the spectrum flattens out when $\alpha \sim 3$, the slope of the variational term as a function of p begins to play a more important role. Figure 5 presents the dimensionless differences $(\varepsilon_v(p) - \varepsilon_v(p_F))2M/p_F^2$ for various values of α . This difference is greater than zero when $p < p_F$ and less than zero when $p > p_F$; therefore, the variational contribution to $s(p)$ is clearly negative over the entire momentum range studied. The importance of taking into account this contribution for the vanishing of $s(p)$ is demon-

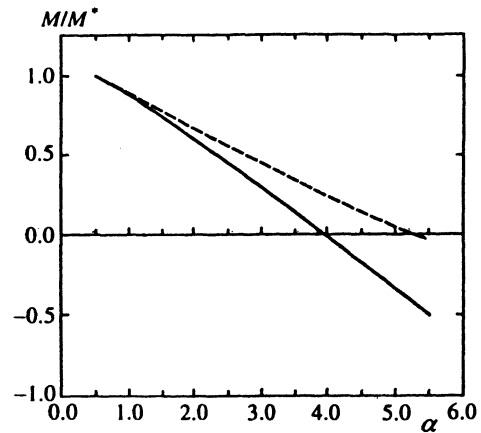


FIG. 7. Plots of M/M^* as a function of α calculated with (solid line) and without (dashed line) consideration of the variational contribution.

strated by Fig. 6. While $s(p)$ first has a vanishing point for $\alpha \approx 3.6$ when the variational contribution is taken into account (Fig. 6a), $s(p)$ first has a vanishing point only for $\alpha \approx 5$ when it is not taken into account (Fig. 6b). Thus, when $\alpha \approx 3.6$, another Fermi surface appears in the system under consideration at $p = 0.6p_F$, and the effective mass on this Fermi surface goes to infinity. From a rigorous standpoint, an investigation of the system beyond the point $\alpha \approx 3.6$ without consideration of the new phase appearing is not correct. Nevertheless, it is interesting to evaluate how rapidly the region occupied by the new phase, i.e., the fermion condensate, expands as α increases and at what values of α the entire $0.6p_F - p_F$ region will be occupied by the condensate. It follows from the calculations that the function $s(p)$ intersects the horizontal axis at the point $p = p_F$ when the Coulomb parameter $\alpha \approx 4$. In this case the right-hand boundary of the momentum range where $\varepsilon(p) > \varepsilon(p_F)$ reaches p_F . When α increases further, the right-hand boundary of the region for negative values of $s(p)$ shifts further to the right and embraces an area with $p > p_F$, in which we now have $\varepsilon(p) < \varepsilon(p_F)$. It is convenient to characterize this picture by the value of M/M^* calculated for $p = p_F$. Figure 7 presents the value of M/M^* as a function of the Coulomb parameter α . As is seen from the figure, when $\alpha = 3.6$, M/M^* equals

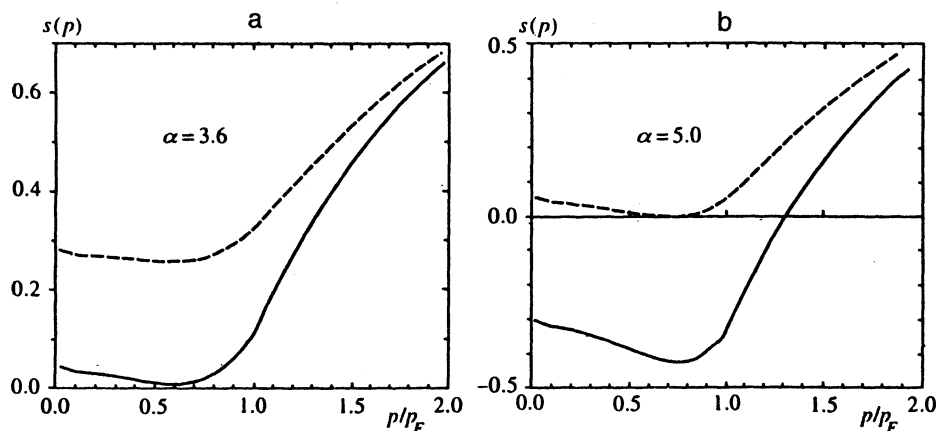


FIG. 6. Plots of $s(p)$ calculated for $\alpha = 3.6$ (a) and $\alpha = 5$ (b) with (solid line) and without (dashed line) consideration of the variational contribution.

≈ 0.08 . When $\alpha \approx 4$, this ratio vanishes. Neglect of the variational correction appreciably alters the slope of this function, displacing the sign change of M/M^* to $\alpha \approx 5.2$ (see Fig. 7).

The instability which we analyzed occurs at a relatively large value of α , which corresponds to a strongly correlated Fermi liquid. This raises the question of what other instabilities (phase transitions) might occur at comparable or smaller values of α . We shall restrict ourselves to consideration of the possibility of the appearance of the three known instabilities in an electron gas: superconductivity, a ferromagnetic (antiferromagnetic) phase transition, and the appearance of charge-density waves (a Wigner crystal). The possibility of superconductivity (superfluidity) in systems with a repulsive interaction has been discussed in the literature.¹³ However, such a phase transition does not occur in an electron gas when $\alpha < 5$ (Ref. 14). Nevertheless, had such a phase transition occurred, it would not have prevented fermion condensation.^{2,8} According to Monte Carlo calculations, a ferromagnetic phase transition occurs in an electron gas when $\alpha \approx 12.4$ (Ref. 11). Also, no antiferromagnetic phase transition could be detected in calculations with $\alpha < 6$ (Ref. 14). We note that these phase transitions likewise do not preclude the development of fermion condensation. We propose to address in another paper both this question and the instability associated with the appearance of charge-density waves.

Crystallization (a Wigner crystal) appears in an electron gas at $\alpha \approx 16$ (Ref. 11); therefore, charge-density waves could hardly be expected to appear at significantly smaller values of α . According to our calculations, this instability is manifested at $\alpha \approx 12$ (Ref. 15). Thus, we can conclude that fermion condensation is very likely the first instability appearing in a strongly interacting electron liquid.

5. CONCLUSIONS

The single-particle spectrum $\varepsilon(p)$ of a rarefied 3D electron gas has been studied in this work in the jellium model. To calculate $\varepsilon(p)$ we used the approximate method proposed in Ref. 3 within a functional approach to the theory of strongly correlated Fermi systems. The purpose of the study

was to ascertain the stability of the Fermi distribution of the quasiparticles with respect to the momentum $n_F(p) = \theta(p_F - p)$ as the Coulomb parameter α increases, i.e., to determine the value of α at which a necessary condition for the stability of $n_F(p)$ is violated. Mathematically, this condition is formulated as a requirement that the function $s(p)$ assigned by Eq. (3) be negative.

The value of α at which the system becomes unstable against a phase transition with the formation of a fermion condensate has been found. The function $s(p)$ first vanishes when $\alpha \approx 3.6$ ($r_s \approx 21$) at the point $p_c \approx 0.6p_F$. As α increases, the right-hand boundary of the region for negative values of $s(p)$ shifts toward higher values of p , and when $\alpha \approx 4$ it reaches p_F .

We have studied the role of the variational correction in the appearance of negative values of $s(p)$ due to modification of the effective interaction in response to the quasiparticle distribution, and the behavior of its boundaries as α increases. Neglect of this correction postpones the vanishing of $s(p)$ for the first time to $\alpha \approx 5$.

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APPENDIX A

We average over the directions of the vector \mathbf{p} and integrate over ω in Eq. (27). In the integrand the dependence on \mathbf{p} is confined to the function $H(\mathbf{q}, \omega, \mathbf{p})$. Integrating over angles, we obtain

$$\varepsilon_1^{(2)}(p) = - \int_{-\infty}^{\infty} \int \int_0^g V(q) \Theta(q, \omega, p) \varphi^2(\mathbf{q}, \omega) \frac{d\omega d^3q dg}{(2\pi)^4 g}, \quad (A1)$$

where

$$\Theta(q, \omega, p) = \int H(\mathbf{q}, \omega, \mathbf{p}) \frac{dO_{\mathbf{p}}}{4\pi} = \begin{cases} -\frac{\pi M}{pq} & \text{in the range } p > p_F, \quad 0 < \omega < \frac{p^2}{2M} - \frac{p_F^2}{2M}, \\ & p - \sqrt{p^2 - 2M\omega} < q < p + \sqrt{p^2 - 2M\omega}; \\ \frac{\pi M}{pq} & \text{in the range } p < p_F, \quad \frac{p^2}{2M} - \frac{p_F^2}{2M} < \omega < 0, \\ & -p + \sqrt{p^2 - 2M\omega} < q < p + \sqrt{p^2 - 2M\omega}; \\ 0 & \text{in other ranges.} \end{cases} \quad (A2)$$

To calculate $\varepsilon(p)$ at values of the momentum p not too far from p_F , it is sufficient to take the function $\varphi(\mathbf{q}, \omega)$ at $\omega = 0$, and the dependence on ω then remains only in the function $\Theta(q, \omega, p)$. The calculation of the integral

$$\eta(q, p) = \int \Theta(q, \omega, p) \frac{d\omega}{2\pi} \quad (A3)$$

of the function (A2) is elementary. In the variables t and u

(29) it has the form

$$\eta(t,u) = \begin{cases} \eta^{(1)}(t,u), & u \geq 1; \\ \eta^{(2)}(t,u), & \frac{1}{3} \leq u \leq 1; \\ \eta^{(3)}(t,u), & 0 \leq u \leq \frac{1}{3}, \end{cases} \quad (A4)$$

$$\eta^{(1)}(t,u) = \begin{cases} \frac{t-u}{2u}, & 0 \leq t \leq \frac{u-1}{2}; \\ \frac{1-u^2}{8ut}, & \frac{u-1}{2} \leq t \leq \frac{u+1}{2}; \\ \frac{t-u}{2u}, & \frac{u+1}{2} \leq t \leq u, \end{cases} \quad (A5)$$

$$\eta^{(2)}(t,u) = \begin{cases} \frac{u+t}{2u}, & 0 \leq t \leq \frac{1-u}{2}; \\ \frac{1-u^2}{8ut}, & \frac{1-u}{2} \leq t \leq u; \\ \frac{1-(2t-u)^2}{8ut}, & u \leq t \leq \frac{u+1}{2}, \end{cases} \quad (A6)$$

$$\eta^{(3)}(t,u) = \begin{cases} \frac{u+t}{2u}, & 0 \leq t \leq u; \\ 1, & u \leq t \leq \frac{1-u}{2}; \\ \frac{1-(2t-u)^2}{8ut}, & \frac{1-u}{2} \leq t \leq \frac{1+u}{2}. \end{cases} \quad (A7)$$

Now substituting the calculated function $\eta(t,u)$ into Eq. (A1) as the integral of $\Theta(q,\omega,p)$ over ω , we obtain Eq. (30).

We now calculate the variational derivative

$$\frac{\delta R(k)}{\delta n(p)} = -\frac{1}{2} \frac{\delta}{\delta n(p)} \frac{d^2}{d\rho^2} \int \frac{d^3 q}{(2\pi)^3} V \times (\mathbf{q}-\mathbf{k}) \int_0^\infty \frac{1}{\pi} \text{Im} \chi_0(\mathbf{q},\omega) d\omega. \quad (A8)$$

We represent (A8) in the form

$$\frac{\delta R(k)}{\delta n(p)} = -\frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} V(\mathbf{q}-\mathbf{k}) D(q,p), \quad (A9)$$

and we first calculate

$$D(q,p) = \int_0^\infty \frac{1}{\pi} \text{Im} \int \frac{dO_{\mathbf{p}}}{4\pi} \frac{\delta}{\delta n(\mathbf{p})} \frac{d^2 \chi_0(\mathbf{q},\omega)}{d\rho^2} d\omega. \quad (A10)$$

For this purpose we represent $\chi_0(\mathbf{q},\omega)$ in the form

$$\chi_0(\mathbf{q},\omega) = \text{Tr} \int G_0(\mathbf{p}',\varepsilon) G_0(\mathbf{p}'-\mathbf{q},\varepsilon-\omega) \frac{d\mathbf{p}' d\varepsilon}{(2\pi)^4 i}, \quad (A11)$$

where

$$G_0(\mathbf{p}',\varepsilon) = \frac{n(\mathbf{p}')}{\varepsilon - \varepsilon_{\mathbf{p}'}^0 - i\delta} + \frac{1-n(\mathbf{p}')}{\varepsilon - \varepsilon_{\mathbf{p}'}^0 - i\delta}, \quad (A12)$$

and the trace is calculated over the spin indices.

The variational derivative of the Green's function (A12) has the form

$$\frac{\delta G_0(\mathbf{p}',\varepsilon)}{\delta n(\mathbf{p})} = (2\pi)^4 i \delta(\varepsilon - \varepsilon_{\mathbf{p}'}^0) \delta(\mathbf{p}' - \mathbf{p}). \quad (A13)$$

Formulating the action integral of the second derivative $d^2/d\rho^2$ in terms of $\delta/\delta n(\mathbf{p})$:

$$\frac{d^2}{d\rho^2} = \int \frac{dO_{\mathbf{p}_1} dO_{\mathbf{p}_2}}{(4\pi)^2} dp_1 dp_2 \delta(p_2 - p_F) \times \left\{ \frac{\pi^2}{p_F^2} \delta'(p_1 - p_F) \frac{\delta}{\delta n(\mathbf{p}_1)} + \delta(p_1 - p_F) \frac{\delta^2}{\delta n(\mathbf{p}_1) \delta n(\mathbf{p}_2)} \right\}, \quad (A14)$$

we can easily obtain the following expression for the variational derivative:

$$\frac{\delta}{\delta n(\mathbf{p})} \frac{d^2 \chi_0(\mathbf{k},\omega)}{d\rho^2} = -\frac{i\pi^4}{2p_F^2} \int dO_{\mathbf{p}_1} dO_{\mathbf{p}_2} dp_1 \delta'(p_1 - p_F) \delta'(\mathbf{p}_1 - \mathbf{k} - \mathbf{p}) \times [\delta(\varepsilon_{\mathbf{p}_1}^0 - \varepsilon_{\mathbf{p}_1 - \mathbf{k} - \mathbf{p}}^0 - \omega) + \delta(\varepsilon_{\mathbf{p}_1}^0 - \varepsilon_{\mathbf{p}_1 - \mathbf{k} + \mathbf{p}}^0 + \omega)]. \quad (A15)$$

Calculating the integral and substituting it into Eq. (A10), for $D(k,p)$ we obtain the expression

$$D(k,p) = -\frac{\pi^4}{p_F^2 p k} [\tilde{\Theta}(k,p,p_F) - p_F \tilde{\delta}(k,p,p_F)], \quad (A16)$$

where

$$\tilde{\Theta}(k,p,p_F) = \begin{cases} \theta(p_F + p - k) - \theta(p_F - p - k) & p < p_F, \\ \theta(p_F + p - k) - \theta(p - p_F - k) & p > p_F, \end{cases} \quad (A17)$$

$$\tilde{\delta}(k,p,p_F) = \begin{cases} \delta(k - p_F - p) - \delta(k - p_F + p) & p < p_F, \\ \delta(k - p_F - p) + \delta(k + p_F - p) & p > p_F. \end{cases} \quad (A18)$$

We now calculate the integral over the angle in Eq. (A9), and as a result we have

$$\frac{\delta R_0(k)}{\delta n(p)} = -\frac{e^2}{2\pi k} \int \ln \left| \frac{q+k}{q-k} \right| D(q,p) q dq. \quad (A19)$$

Substituting (A16) into (A19) and integrating over q , we obtain the final expression for $\delta R_0(k)/\delta n(p)$. In the dimensionless variables $t = k/2p_F$ and $u = p/p_F$ it has the form

$$\frac{\delta R_0(2p_F T)}{\delta n(p_F u)} = \frac{\pi^3 e^2}{2p_F^5} Y(t,u), \quad (A20)$$

where

$$Y(t, u) = \frac{1}{u} \left\{ \left(t + \frac{u}{2} \right) \ln \left| \frac{t + \frac{u+1}{2}}{t + \frac{u-1}{2}} \right| + \left(t - \frac{u}{2} \right) \ln \left| \frac{t - \frac{u+1}{2}}{t - \frac{u-1}{2}} \right| \right\}. \quad (\text{A21})$$

We also present the explicit form of the first iteration of Eq. (23) for an effective interaction

$$\hat{R}_0(t) = \frac{1}{t^2} - \frac{1}{3} \left[t^2 \ln \left| 1 - \frac{1}{t^2} \right| + \frac{1}{t} \ln \left| \frac{t+1}{t-1} \right| + 1 \right]. \quad (\text{A22})$$

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