Method of effective-potential expansion for the many-body problem: Two-dimensional electron gas in two-body approximation

Yasutami Takada
Department of Physics, Purdue University, West Lafayette, Indiana 47907
*and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106**
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Following previous work in which a variational method for the many-body problem was proposed wherein an effective potential $\tilde{V}$ was introduced as a variational parameter to construct a trial wave function, we apply the method to the two-dimensional electron gas. In the method, every physical quantity is expanded in powers of $\tilde{V}$ instead of the bare potential as in the usual perturbation-theoretic approach. Because of this choice of expansion parameter, the expansion series converges rapidly even in the strong-coupling region. The result for the correlation energy in the two-dimensional electron gas agrees very well with that given by the variational Monte Carlo method even in the lowest-order calculation (i.e., to second order in $\tilde{V}$). The difference is within several percent for $1 < r_s < 100$.

I. INTRODUCTION

Thanks to the rapid progress of computational techniques in the last decade, we can perform an exact stochastic simulation of the Schrödinger equation for a large (but finite) number of particles. The result extrapolated to an infinite number of particles is considered to give exact data on the ground-state properties of a many-body system. This numerical method, usually called the Green's-function Monte Carlo (GFMC),[1] has been applied successfully to several systems including the electron gas.[2]

The appearance of GFMC seems to have modified the role of analytic approaches to the many-body problem. We expect an analytic method to reproduce the ground-state properties obtained by the GFMC preferably without introducing any adjustable parameters. What is more important is that the method should be as simple as possible so that we cannot only clarify the essential physics unambiguously but also extend it without much difficulty to the study of excited states in connection with the response theory to external fields and finite-temperature problems.

Since the homogeneous electron gas embedded in a neutralizing positive background provides an excellent testing ground, all the many-body techniques thus far proposed have treated this problem.[3] Among them, the perturbation-theoretic approach succeeded in deriving the exact result in the high-density limit for the first time by taking a partial infinite sum of divergent terms in the perturbation series.[4] There have been many attempts to treat the metallic density region along this line.[5–7] Because the expansion parameter is the bare potential $V(q)$ in this approach, a main problem is that the expansion itself is meaningless in the strong-coupling region unless an infinite sum is made very carefully and all the remaining terms are found to be small.

The variational approach of a Bijl-Dingle-Jastrow trial function[8] has produced fruitful results in the strong-coupling region,[9] though it cannot reproduce the rigorous result in the high-density limit. In this approach, a cluster expansion is obtained with the expansion parameter $f(r)^2-1$, where $f(r)$ is the so-called correlation function in the definition of Jastrow-type trial functions. As usually performed by the Fermi hypernetted-chain (FHNC) method,[10] it is necessary to make a partial infinite sum of this expansion series, partly because the convergence is slow (particularly when there is a long-range correlation in the system), and partly because the Pauli principle does not hold order by order in the expansion.

In other approaches such as the equation-of-motion[11,12] and the coupled-cluster[13,14] methods, an infinite sum is also performed by solving some integral equation. Generally speaking, if such an infinite sum is always necessary in order to obtain physically meaningful results, terms which do not fit well in the sum should be either neglected, or estimated roughly, even if they should be treated more seriously. In a sense, the perturbation-theoretic method is composed of a series of such approximations. We can also find an example in the coupled-cluster theory. The "mean spherical approximation" was introduced to ignore dependence other than the momentum transfer in the evaluation of the energy denominator.[14] The same treatment was discussed in the recent development of the correlated-basis-function (CBF) method.[15]

Since there is an infinite number of degrees of freedom in a many-body system, one might think it inevitable to perform an infinite sum. But if we examine actual calculations more carefully, we find that none of those methods allow us to sum all terms. Only some partial part is considered to infinite order and so an infinite number of terms is neglected. This observation suggests that if we can expand with an expansion parameter which includes all the important physical processes that are taken into account by some infinite sum in other methods, we may obtain an excellent result with only a finite number of terms. If we can find such an expansion parameter, we moderate the complications associated with some infinite summation.

Motivated by the above consideration, the present au-

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thor has proposed a new cluster-expansion theory in a previous paper[16] hereafter referred to as I. The first essential idea is to expand with respect to an effective potential $\tilde{V}$ in order to include physically important processes without making any explicit infinite sum. Owing to the choice of $\tilde{V}$, no divergence appears in any term of the expansion. In addition, even in the strong-coupling region, $\tilde{V}$ is expected to remain small to bring about a rapid convergence. The second essential idea is to determine $\tilde{V}$ by a variational procedure. This is very important in order to make the theory not phenomenological but rather a first-principle and self-contained calculation. Another idea is to treat the direct and exchange terms in a manifestly antisymmetric way so as to make the Pauli principle hold order by order.

Although the expansion was formulated for the first time in I, the idea to employ the effective potential as an expansion parameter is not new. Macke[17] was probably the first to introduce the idea. Its usefulness has been emphasized in the CBF. Furthermore, there is some conceptual relation with the local-field correction[3] and the polarization potential of Pines,[18] though the effective potential in these approaches is a little different from ours and may be regarded as the sum of our $\tilde{V}$ and an approximate exchange contribution. There were also a few discussions on finite-order calculations. Talman[19] showed that if $\ln f(r)$ instead of $f(r)^2-1$ was chosen as an expansion parameter in the Jastrow-type approach, lowest-order calculations were not unsatisfactory. A similar discussion was given by Horsch and Fulde.[20] They started from a Gutzwiller-type trial function[21] and argued the usefulness of calculations up to second order of an expansion parameter which was essentially the same as that of Talman. The present author believes, however, that the choice of $\tilde{V}$ for an expansion parameter is more fruitful and informative than any other choice.

In this paper we neglect all terms higher than second order in $\tilde{V}$. As suggested in I, the physical picture of this treatment is very clear. The many-body problem is reduced to a two-body one. The effective interaction between the two particles, $\tilde{V}$, takes account of the effect of other particles and is determined variationally. Every process in the two-body problem will be evaluated rigorously term by term. Thus, the relative importance of each process can be seen unambiguously. Hereafter, we will denote as the two-body approximation the cutoff of our cluster expansion at this level. In the high-density three-dimensional (3D) electron gas, the $\ln r_s$ term, the leading term in the r_s expansion of the correlation energy ϵ_c, is correctly derived in this approximation, as shown in I. At finite but small r_s, the result for ϵ_c gives a very good upper bound to the rigorous value.[4] For example, the error is about 6% at $r_s=0.1$. Thus, the purpose of this paper is to examine to what extent the two-body approximation is useful in the strong-coupling region.

The actual calculation is done for the two-dimensional (2D) electron gas, rather than 3D one, in order to make numerical computations a little easier. Electrons trapped on the surface of liquid helium or those in the inversion layer of a metal-oxide-semiconductor (MOS) interface are considered to be 2D.[22] Qualitatively, there is no difference between 2D and 3D systems. Therefore, once our method is confirmed to work well in a 2D system, the same will hopefully be true in a 3D one. Concerning the quantitative difference, Ceperley's work[23] is quite informative. He estimated the r_s value for the ferromagnetic transition in both 2D and 3D electron-gas systems by employing the variational Monte Carlo (VMC) method.[24] The result was that $r_s \sim 13$ for a 2D system, while it was about 26 in a 3D one. He also made a similar calculation for the Wigner-lattice transition to find that $r_s \sim 33$ and 67 for 2D and 3D systems, respectively. Therefore, we may conclude that the situation of $r_s=3$, for example, in a 2D system corresponds to that of $r_s=6$ in a 3D one.

A disadvantage in the choice of the 2D electron gas is that the GFMC result is not available now. However, this is not so serious, because, in addition to several results obtained by various methods,[25–29] there is a result of VMC.[23] This is known to give an ϵ_c only a few percent higher than that of GFMC over a very wide range of r_s in the 3D electron gas. Thus, we can check our result by comparing with that of VMC.

In Sec. II we review our method and give equations to evaluate physical quantities such as ϵ_c and the pair distribution function in the two-body approximation. These equations hold as well in any spin-$\frac{1}{2}$ system and dimension. We present the calculated results for the 2D electron gas in Sec. III. After describing how to evaluate each term numerically, we treat the high-density limit first. The two leading terms (constant and $r_s \ln r_s$ terms) are reproduced rigorously in the present approximation. Then, we find that ϵ_c in the Singwi-Tosi-Land-Sjölander (STLS) method[11] calculated by Jonson[26] is reproduced by the use of the spin-independent effective potential. We can improve our result by introducing the spin-dependent effective interaction $\tilde{V}_{\sigma\sigma'}(q)$ in such a way as $\tilde{V}_{\uparrow\uparrow}(q) < \tilde{V}_{\uparrow\downarrow}(q)$ for $q \lesssim 2k_F$, while $\tilde{V}_{\uparrow\uparrow}(q) > \tilde{V}_{\uparrow\downarrow}(q)$ for $q \gtrsim 2k_F$, where k_F is the Fermi wave vector. The final result for ϵ_c is in good agreement with that of the VMC. The difference is within 4% for $2 < r_s < 50$. As for the spin-dependent pair distribution function $g_{\sigma\sigma'}(r)$, $g_{\uparrow\uparrow}(r)$ always behaves reasonably. In accordance with the Pauli principle, $g_{\uparrow\uparrow}(r)$ is zero at $r=0$ and always positive elsewhere. However, $g_{\uparrow\downarrow}(r)$ becomes slightly negative near $r \approx 0$ for $r_s \gtrsim 2.5$. In Sec. IV we summarize our results and discuss problems, particularly that of the negative $g_{\uparrow\downarrow}(r)$.

II. EFFECTIVE-POTENTIAL EXPANSION

A. Cluster expansion for the ground-state energy

We consider the normal ground state of a quantum Fermi liquid by employing the variational method developed in I. Since the description in I was a little too general, we give here a rather detailed account of the formulation. We restrict ourselves to the system in which only two-particle correlations are important.

The Hamiltonian of an N-particle system is written as

$$H = H_0 + V . \tag{1}$$

In second quantization, the noninteracting part H_0 is

given by

$$H_0=\sum_{\vec{k},\sigma}\epsilon_{\vec{k}}C^{\dagger}_{\vec{k}\sigma}C_{\vec{k}\sigma}\ , \tag{2}$$

and the two-body potential part V is described with the use of Fourier transform of the bare potential $V(q)$ as

$$V=\tfrac{1}{2}\sum_{\vec{q}}\sum_{\vec{k},\sigma}\sum_{\vec{k}'\sigma'}V(q)C^{\dagger}_{\vec{k}+\vec{q},\sigma}C^{\dagger}_{\vec{k}'-\vec{q},\sigma'}C_{\vec{k}',\sigma'}C_{\vec{k},\sigma}\ , \tag{3}$$

where $C_{\vec{k}\sigma}$ is the destruction operator of a particle specified by wave vector $\vec{k}$ and spin σ, and $\epsilon_{\vec{k}}$ is the kinetic energy of the particle. For the ground-state wave function, we consider the following trial function:

$$|\Phi_0\rangle=|0\rangle+\frac{(-1)^1}{1!}\sum_{l_1(\neq 0)}\frac{|l_1\rangle\langle l_1|\tilde{V}|0\rangle}{E_{l_1}-E_0}+\frac{(-1)^2}{2!}\sum_{l_1(\neq 0)}\sum_{l_2(\neq 0)}\frac{|l_1,l_2\rangle\langle l_1|\tilde{V}|0\rangle\langle l_2|\tilde{V}|0\rangle}{(E_{l_1}-E_0)(E_{l_2}-E_0)}+\cdots\ . \tag{4}$$

The first term of Eq. (4), $|0\rangle$, is the ground state of H_0 (i.e., the state described by a plane-wave Slater determinant). The second term is constructed by a (2p-2h) state in which two particles below the Fermi surface are excited above it and leave two holes. Thus, $|l_1\rangle$ is defined by

$$|l_1\rangle=C^{\dagger}_{\vec{p}_1+\vec{q},\sigma_1}C^{\dagger}_{\vec{p}\,'_1-\vec{q},\sigma'_1}C_{\vec{p}\,'_1,\tau'_1}C_{\vec{p}_1,\tau_1}|0\rangle\ , \tag{5}$$

with $|\vec{p}_1+\vec{q}|>k_F$, $|\vec{p}\,'_1-\vec{q}|>k_F$, $|\vec{p}_1|<k_F$, and $|\vec{p}\,'_1|<k_F$. The spin indices satisfy the relation of either $\sigma_1=\tau_1$ and $\sigma'_1=\tau'_1$, or $\sigma_1=\tau'_1$ and $\sigma'_1=\tau_1$. The energy denominator $E_{l_1}-E_0$ is given by

$$E_{l_1}-E_0=\epsilon_{\vec{p}_1+\vec{q}}+\epsilon_{\vec{p}\,'_1-\vec{q}}-\epsilon_{\vec{p}_1}-\epsilon_{\vec{p}\,'_1}\ . \tag{6}$$

In general, the nth-order term in Eq. (4) is composed of n such $(2p-2h)$ states, denoted by $|l_1,l_2,\ldots,l_n\rangle$. These n $(2p-2h)$ states are taken to be uncorrelated to each other. Thus, only two-particle correlations are included in $|\Phi_0\rangle$.

The effective potential $\tilde{V}$ in the definition of Eq. (4) is a variational parameter. In the present paper we assume that $\tilde{V}$ depends only on the magnitude of momentum transfer and the relative spin orientation. Therefore, we may write $\tilde{V}$ as

$$\tilde{V}=\tfrac{1}{2}\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{k},\sigma}\sum_{\vec{k}'\sigma'}\tilde{V}_{\sigma\sigma'}(q)C^{\dagger}_{\vec{k}+\vec{q},\sigma}C^{\dagger}_{\vec{k}'-\vec{q},\sigma'}\times C_{\vec{k}',\sigma'}C_{\vec{k},\sigma}\ . \tag{7}$$

We have excluded the case of $\vec{q}=\vec{0}$ in Eq. (7), because the state created by the $\vec{q}=\vec{0}$ excitation is nothing but $|0\rangle$.

Physically, $\tilde{V}$ determines the scattering amplitude of two particles. Let us consider the scattering event to create the state $|l_1\rangle$ in Eq. (5) from the Fermi sphere $|0\rangle$. For particles with antiparallel spins, the scattering amplitude is proportional to $\tilde{V}_{\uparrow\downarrow}(q)$, while for those with parallel spins, it is proportional to $\tilde{V}_{\uparrow\uparrow}(q)-\tilde{V}_{\uparrow\uparrow}(|\vec{p}\,'_1-\vec{p}_1-\vec{q}|)$. In our expansion, therefore, the direct and exchange terms are incorporated in a manifestly antisymmetric way which guarantees that the Pauli exclusion principle is satisfied order by order.

The expectation value of the Hamiltonian with respect to the trial function (4) has been derived in I. The result is a cluster expansion of the ground-state energy with the expansion parameter $\tilde{V}$ and is given by

$$\langle H\rangle=\langle\Phi_0|H|\Phi_0\rangle/\langle\Phi_0|\Phi_0\rangle=\sum_{n=0}^{\infty}E^{(n)}\ , \tag{8}$$

with

$$E^{(0)}=C_{0,0}(H_0)+C_{0,0}(V)\ , \tag{9a}$$

and for $n\geq 1$,

$$E^{(n)}=C_{n,n-1}(V)+C_{n-1,n}(V)+C_{n,n}(H_0)+C_{n,n}(V)\ . \tag{9b}$$

The correlation function $C_{n,n'}(A)$ is defined by

$$C_{n,n'}(A)=\sum_{l_1}\cdots\sum_{l_n}\sum_{l'_1}\cdots\sum_{l'_{n'}}(-1)^{m+m'}\prod_{m=1}^{n}\frac{\langle 0|V|l_m\rangle}{E_{l_m}-E_0}\prod_{m'=1}^{h'}\frac{\langle l'_{m'}|\tilde{V}|0\rangle}{E_{l'_{m'}}-E_0}\frac{\langle l_1,\ldots,l_n|A|l'_1,\ldots,l'_{n'}\rangle_C}{n!n'!}\ , \tag{10}$$

where A is either H_0 or V, and the subscript C denotes the instruction to take only connected diagrams. This function can be calculated with the use of Feynman diagrams, as prescribed in I. But when $\tilde{V}$ does not depend on the frequency ω as in the present case, $C_{n,n'}(A)$ can also be obtained by Goldstone diagrams.

B. Correlation functions in two-body approximation

The zeroth-order term $E^{(0)}$ in Eq. (8) is the energy in the Hartree-Fock approximation. Namely, we obtain

$$E^{(0)}=\langle 0|H|0\rangle\ . \tag{11}$$

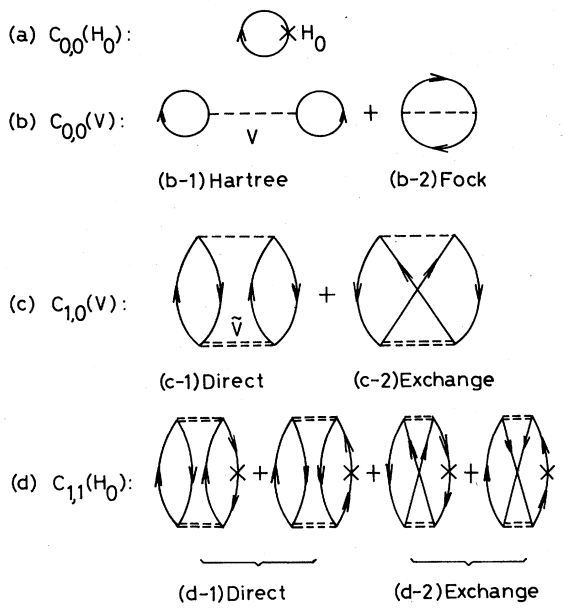

FIG. 1. Goldstone diagrams for $C_{0,0}(H_0)$, $C_{0,0}(V)$, $C_{1,0}(V)$, and $C_{1,1}(H_0)$.

The diagrammatic expression for this term is given in Figs. 1(a) and 1(b). The first-order term $E^{(1)}$ can be rewritten as

$$E^{(1)}=\langle\Phi_0^{(1)}\,|\,H\,|\,\Phi_0^{(1)}\rangle_C-E^{(0)}\,, \tag{12}$$

where $|\Phi_0^{(1)}\rangle$ is defined by the first two terms in Eq. (4). Since only two particles are involved in $|\Phi_0^{(1)}\rangle$, as can be seen in Eq. (5), $E^{(1)}$ is composed of all the processes that the two-body problem can produce. In this sense, the N-body problem is reduced to a two-body one at this level.

There are four correlation functions in $E^{(1)}$: $C_{1,0}(V)$, $C_{0,1}(V)$, $C_{1,1}(H_0)$, and $C_{1,1}(V)$. The first and the second give just the same result. There are two contributions to $C_{1,0}(V)$. One is the direct one $C_{1,0}^{(d)}$, and the other is the exchange one $C_{1,0}^{(e)}$. These two are shown in Fig. 1(c) in terms of Goldstone diagrams. They are expressed, respectively, as

$$C_{1,0}^{(d)}(V)=-\tfrac{1}{2}\sum_{\vec{q}(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}V(q)\tilde{V}_{\sigma\sigma'}(q)\times W_1(q;\vec{p}\sigma;\vec{p}\,'\sigma')\,, \tag{13a}$$

and

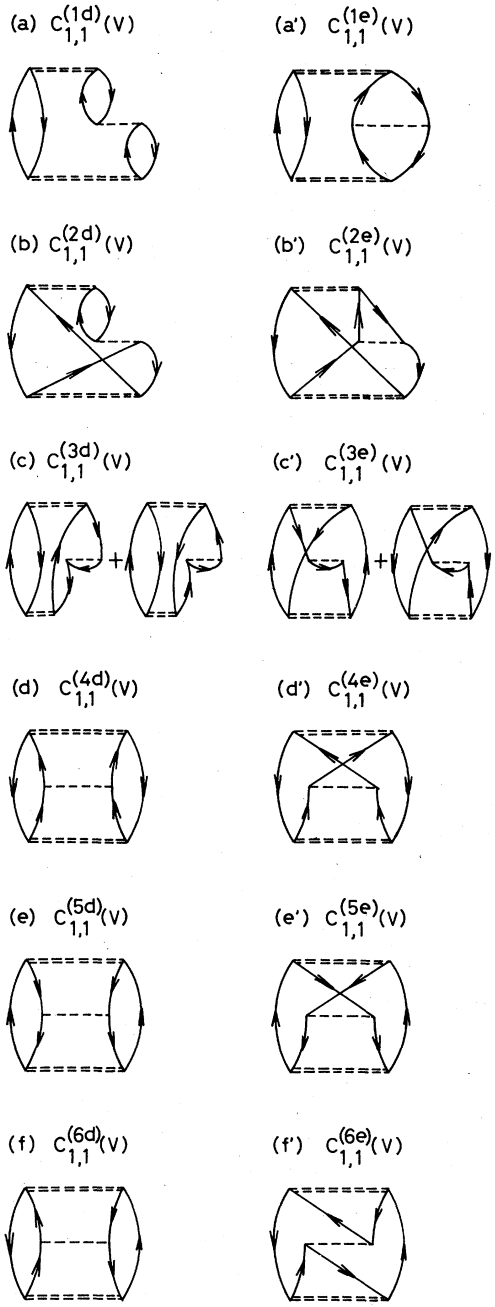

FIG. 2. Goldstone diagrams for $C_{1,1}(V)$.

$$C_{1,0}^{(e)}(V)=\tfrac{1}{2}\sum_{\vec{q}\,(\neq\vec{p}\,'-\vec{p})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\delta_{\sigma\sigma'}V(q)\tilde{V}_{\sigma\sigma'}(\,|\,\vec{p}\,'-\vec{p}-\vec{q}\,|\,)W_1(q;\vec{p},\sigma;\vec{p}\,',\sigma')\,, \tag{13b}$$

where

$$W_1(q;\vec{p},\sigma;\vec{p}\,',\sigma')=\frac{n_{\vec{p},\sigma}(1-n_{\vec{p}+\vec{q},\sigma})n_{\vec{p}\,',\sigma'}(1-n_{\vec{p}\,'-\vec{q},\sigma'})}{\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}\,'-\vec{q}}-\epsilon_{\vec{p}\,'}} \tag{14}$$

with the Fermi distribution function $n_{\vec{p},\sigma}$ at $T=0$ and the Kronecker's δ function $\delta_{\sigma\sigma'}$.

The diagrammatic expression for $C_{1,1}(H_0)$ is given in Fig. 1(d). Combining two contributions for the direct term

$C_{1,1}^{(d)}(H_0)$, we obtain

$$C_{1,1}^{(d)}(H_0)=\frac{1}{2}\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\tilde{V}_{\sigma\sigma'}(q)^2 W_1(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma')\ . \tag{15a}$$

Similarly, the exchange contribution is given by

$$C_{1,1}^{(e)}(H_0)=-\frac{1}{2}\sum_{\vec{q}\,(\neq\vec{p}\,'-\vec{p})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\delta_{\sigma\sigma'}\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(|\vec{p}\,'-\vec{p}-\vec{q}\,|)W_1(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma')\ . \tag{15b}$$

Calculation of $C_{1,1}(V)$ is rather difficult. There are six sets for $C_{1,1}(V)$, each of which is composed of direct and exchange terms. Thus, we may write

$$C_{1,1}(V)=\sum_{n=1}^{6}[C_{1,1}^{(nd)}(V)+C_{1,1}^{(ne)}(V)]\ . \tag{16}$$

The expression in the Goldstone diagrams for these terms is given in Fig. 2. The first term is the contribution of the ring diagram, obtained as

$$C_{1,1}^{(1d)}(V)=\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\sum_{\vec{p}\,'',\sigma''}V(q)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma''}(q)W_{2a}(\vec{q};p,\sigma;p',\sigma';p'',\sigma'')\ , \tag{17a}$$

and the exchange partner is given by

$$C_{1,1}^{(1e)}(V)=-\sum_{\vec{q}\,(\neq 0)}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\sum_{\vec{p}\,'',\sigma''}\delta_{\sigma'\sigma''}V(|\vec{p}\,'-\vec{p}\,''|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma''}(q)W_{2a}(\vec{q};p,\sigma;p;\sigma';p'',\sigma'')\ , \tag{17b}$$

where

$$W_{2a}(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma';\vec{p}\,'',\sigma'')=\frac{n_{\vec{p},\sigma}(1-n_{\vec{p}+\vec{q},\sigma})n_{\vec{p}\,',\sigma'}(1-n_{\vec{p}\,'-\vec{q},\sigma'})n_{\vec{p}\,'',\sigma''}(1-n_{\vec{p}\,''-\vec{q},\sigma''})}{(\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}\,'-q}-\epsilon_{\vec{p}\,'})(\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}\,''-\vec{q}}-\epsilon_{\vec{p}\,''})}\ . \tag{18}$$

Another exchange contribution to $C_{1,1}^{(1d)}$ is given by $C_{1,1}^{(2d)}$ which is written as

$$C_{1,1}^{(2d)}(V)=-2\sum_{\substack{\vec{q}\,(\neq\vec{0})\\ \vec{q}\neq\vec{p}\,'-\vec{p}}}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\sum_{\vec{p}\,'',\sigma''}\delta_{\sigma\sigma'}V(q)\tilde{V}_{\sigma\sigma}(|\vec{p}\,'-\vec{p}-\vec{q}\,|)\tilde{V}_{\sigma\sigma''}(q)W_{2a}(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma';\vec{p}\,'',\sigma'')\ , \tag{19a}$$

while its exchange partner is obtained as

$$C_{1,1}^{(2e)}(V)=2\sum_{\substack{\vec{q}\,(\neq\vec{0})\\ \vec{q}\neq\vec{p}\,'-\vec{p}}}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\sum_{\vec{p}\,'',\sigma''}\delta_{\sigma\sigma'}\delta_{\sigma'\sigma''}V(|\vec{p}\,'-\vec{p}\,''|)\tilde{V}_{\sigma\sigma''}(q)\tilde{V}_{\sigma\sigma}(|\vec{p}\,'-\vec{p}-\vec{q}\,|)W_{2a}(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma';\vec{p}\,'',\sigma'')\ . \tag{19b}$$

Terms $C_{1,1}^{(3d)}$ and $C_{1,1}^{(3e)}$ are the contribution of the self-energy correction and are given, respectively, by

$$C_{1,1}^{(3d)}(V)=\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\sum_{\vec{p}\,'',\sigma''}\delta_{\sigma'\sigma''}V(|\vec{p}\,'-\vec{p}\,''|)[\tilde{V}_{\sigma\sigma'}(q)]^2 W_{2b}(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma';\vec{p}\,'',\sigma'')\ , \tag{20a}$$

and

$$C_{1,1}^{(3e)}(V)=-\sum_{\substack{\vec{q}\,(\neq\vec{0})\\ \vec{q}\neq\vec{p}\,'-\vec{p}}}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\sum_{\vec{p}\,'',\sigma''}\delta_{\sigma\sigma'}\delta_{\sigma'\sigma''}V(|\vec{p}\,'-\vec{p}\,''|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma}(|\vec{p}\,'-\vec{p}-\vec{q}\,|)W_{2b}(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma';\vec{p}\,'',\sigma'')\ , \tag{20b}$$

with

$$W_{2b}(\vec{q};\vec{p},\sigma;\vec{p}\,',\sigma';\vec{p}\,'',\sigma'')=\frac{n_{\vec{p},\sigma}(1-n_{\vec{p}+\vec{q},\sigma})n_{\vec{p}\,',\sigma'}(1-n_{\vec{p}\,'-\vec{q},\sigma})(n_{\vec{p}\,'',\sigma''}-n_{\vec{p}\,''-\vec{q},\sigma''})}{(\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}\,'-\vec{q}}-\epsilon_{\vec{p}\,'})^2}\ . \tag{21}$$

Next is the particle-particle ladder term $C_{1,1}^{(4d)}$ and its exchange partner $C_{1,1}^{(4e)}$ given by

$$C_{1,1}^{(4d)}(V)=\frac{1}{2}\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{q}\,'(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}V(|\vec{q}\,'-\vec{q}\,|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(q')W_{2c}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')\ , \tag{22a}$$

and

$$C_{1,1}^{(4e)}(V)=-\frac{1}{2}\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{q}\,'(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\delta_{\sigma\sigma'}V(|\vec{p}\,'-\vec{p}-\vec{q}-\vec{q}\,'|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(q')W_{2c}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,'\sigma')\,, \tag{22b}$$

where

$$W_{2c}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')=\frac{n_{\vec{p},\sigma}(1-n_{\vec{p}+\vec{q},\sigma})(1-n_{\vec{p}+\vec{q}\,',\sigma})n_{\vec{p}\,',\sigma'}(1-n_{\vec{p}\,'-\vec{q},\sigma'})(1-n_{\vec{p}\,'-\vec{q}\,',\sigma'})}{(\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}\,'-\vec{q}}-\epsilon_{\vec{p}\,'})(\epsilon_{\vec{p}+\vec{q}\,'}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}\,'-\vec{q}\,'}-\epsilon_{\vec{p}\,'})}\,. \tag{23}$$

Similarly, the hole-hole ladder terms are obtained as

$$C_{1,1}^{(5d)}(V)=\frac{1}{2}\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{q}\,'(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}V(|\vec{q}\,'-\vec{q}\,|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(q')W_{2d}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')\,, \tag{24a}$$

and

$$C_{1,1}^{(5e)}(V)=-\frac{1}{2}\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{q}\,'(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\delta_{\sigma\sigma'}V(|\vec{p}\,'-\vec{p}-\vec{q}-\vec{q}\,'|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(q')W_{2d}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')\,, \tag{24b}$$

with

$$W_{2d}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')=\frac{(1-n_{\vec{p},\sigma})n_{\vec{p}+\vec{q},\sigma}n_{\vec{p}+\vec{q}\,',\sigma}(1-n_{\vec{p}\,',\sigma'})n_{\vec{p}\,'-\vec{q},\sigma'}n_{\vec{p}\,'-\vec{q}\,',\sigma'}}{(\epsilon_{\vec{p}}-\epsilon_{\vec{p}+\vec{q}}+\epsilon_{\vec{p}\,'}-\epsilon_{\vec{p}\,'-\vec{q}})(\epsilon_{\vec{p}}-\epsilon_{\vec{p}+\vec{q}\,'}+\epsilon_{\vec{p}\,'}-\epsilon_{\vec{p}\,'-\vec{q}\,'})}\,. \tag{25}$$

Finally, the particle-hole ladder terms are written by

$$C_{1,1}^{(6d)}(V)=-\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{q}\,'(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}V(|\vec{q}\,'-\vec{q}\,|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(q')W_{2e}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')\,, \tag{26a}$$

and

$$C_{1,1}^{(6e)}(V)=\sum_{\vec{q}\,(\neq\vec{0})}\sum_{\vec{q}\,'(\neq\vec{0})}\sum_{\vec{p},\sigma}\sum_{\vec{p}\,',\sigma'}\delta_{\sigma\sigma'}V(|\vec{p}\,'-\vec{p}\,|)\tilde{V}_{\sigma\sigma'}(q)\tilde{V}_{\sigma\sigma'}(q')W_{2e}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')\,, \tag{26b}$$

where

$$W_{2e}(\vec{q},\vec{q}\,';\vec{p},\sigma;\vec{p}\,',\sigma')=\frac{(1-n_{\vec{p},\sigma})n_{\vec{p}+\vec{q},\sigma}n_{\vec{p}+\vec{q}\,',\sigma}n_{\vec{p}\,',\sigma'}(1-n_{\vec{p}\,'+\vec{q},\sigma'})(1-n_{\vec{p}\,'+\vec{q}\,',\sigma'})}{(\epsilon_{\vec{p}}-\epsilon_{\vec{p}+\vec{q}}+\epsilon_{\vec{p}\,'+\vec{q}}-\epsilon_{\vec{p}\,'})(\epsilon_{\vec{p}}-\epsilon_{\vec{p}+\vec{q}\,'}+\epsilon_{\vec{p}\,'+\vec{q}\,'}-\epsilon_{\vec{p}\,'})}\,. \tag{27}$$

In the two-body approximation, we neglect all terms in $E^{(n)}$ for $n\geq 2$. The best effective potential in this approximation may be given by the functional derivative of $E^{(1)}(\tilde{V})$:

$$\frac{\delta E^{(1)}(\tilde{V})}{\delta\tilde{V}_{\sigma\sigma'}(q)}=0\,. \tag{28}$$

When we set Eqs. (13)—(26) in $E^{(1)}$ and take the derivative, we obtain a linear integral equation to determine $\tilde{V}_{\sigma\sigma'}(q)$. In this paper, however, we will not try to solve Eq. (28) explicitly. We will use it only to obtain the asymptotic behavior of $\tilde{V}_{\sigma\sigma'}(q)$. One reason is that the integral equation is rather complicated to solve numerically. But the real reason is that it is more instructive to show that, even if we do not know the precise $\tilde{V}_{\sigma\sigma'}(q)$, we can obtain a very good value for the ground-state energy. In fact, calculated energies are rather insensitive to the choice of $\tilde{V}$. This may be related to the general statement that in a variational approach the error of calculated energy is of order δ^2 for a trial function having an error of order δ.

C. Pair distribution function

Since the energy will not provide a good measure to estimate the error of our treatment, we also calculate the pair distribution function to evaluate the method. This function itself is also interesting and informative for the study of the system.

The spin-dependent pair distribution function is defined by

$$g_{\sigma\sigma'}(\vec{r})=\frac{1}{(N/2)(N/2-\delta_{\sigma\sigma'})}\times\sum_{\vec{q}}\sum_{\vec{p},\vec{p}\,'}e^{i\vec{q}\cdot\vec{r}}\times\langle C_{\vec{p},\sigma}^{\dagger}C_{\vec{p}\,',\sigma'}^{\dagger}C_{\vec{p}\,'-\vec{q},\sigma'}C_{\vec{p}+\vec{q},\sigma}\rangle\,. \tag{29}$$

When we compare this definition with that of $\langle V\rangle$, we can see easily that $g_{\sigma\sigma'}(\vec{r})$ is obtained by changing $\frac{1}{2}V(q)$ into $e^{i\vec{q}\cdot\vec{r}}$ in, for example, Eq. (13a). Thus, we will not give here explicit equations for $g_{\uparrow\uparrow}(\vec{r})$ equivalent to those for $\langle H\rangle$. However, it will be an easily task to see that at $\vec{r}=\vec{0}$, each direct term is just cancelled by its exchange partner. Thus, $g_{\uparrow\uparrow}(0)$ is always zero, as it should be from the Pauli principle.

In the two-body approximation, $g_{\uparrow\downarrow}(\vec{r})$ has seven terms and can be rewritten as

$$g_{\uparrow\downarrow}(\vec{r})=\left[\frac{2}{N}\right]^2\sum_{\vec{p},\vec{p}'}n_{\vec{p},\uparrow}n_{\vec{p}',\downarrow}\left|1-\sum_{\vec{q}}e^{i\vec{q}\cdot\vec{r}}\tilde{V}_{\uparrow\downarrow}(q)\frac{(1-n_{\vec{p}+\vec{q},\uparrow})(1-n_{\vec{p}'-\vec{q},\downarrow})}{\epsilon_{\vec{p}+\vec{q}}-\epsilon_{\vec{p}}+\epsilon_{\vec{p}'-\vec{q}}-\epsilon_{\vec{p}'}}\right|^2+g^{(r)}_{\uparrow\downarrow}(\vec{r})+g^{(h)}_{\uparrow\downarrow}(\vec{r})\ . \tag{30}$$

The first term is composed of the Hartree term [Fig. 1(b-1)], the direct one in Fig. 1(c-1), and the particle-particle ladder term [Fig. 2(d)]. This contribution is manifestly positive. The second term $g^{(r)}_{\uparrow\downarrow}(\vec{r})$ is the contribution of the ring-type diagrams [Figs. 2(a) and 2(b)]. Since these two terms almost cancel each other, $g^{(r)}_{\uparrow\downarrow}$ is always very small. Unlike other terms, $g^{(h)}_{\uparrow\downarrow}(\vec{r})$ is always negative and is not always small, because the negative contribution of the particle-hole ladder [Fig. 2(f)] is larger than the positive one of the hole-hole ladder [Fig. 2(e)] by about a factor of 2. This can be explained simply as follows: In Fig. 2(f) there are two channels, i.e., one in which a hole line is constructed by an up-spin particle, while a particle line is that of a down-spin one, and for the other channel the opposite is the case. In Fig. 2(e), however, there is only one channel. Thus, if $g_{\uparrow\downarrow}(\vec{r})$ happens to become negative in our approximation, it is entirely due to the particle-hole ladder diagram.

III. TWO-DIMENSIONAL ELECTRON GAS

A. Preliminaries

We consider an idealized 2D system in which electrons are confined in an infinitely thin layer with a uniform neutralizing background and interact with each other through a Coulomb potential. This system is characterized by

$$\epsilon_{\vec{k}}=\hbar^2\vec{k}^{\,2}/2m\ , \tag{31}$$

and

$$V(\vec{q})=\begin{cases}2\pi e^2/q & \text{for } \vec{q}\neq\vec{0}\ ,\\ 0 & \text{for } \vec{q}=\vec{0}\ ,\end{cases} \tag{32}$$

where $\vec{k}$ and $\vec{q}$ are 2D wave vectors. In the following, we measure momenta and energies in units of $\hbar k_F$ and $Nme^4/2\hbar^2$, respectively. Then this system can be described by one parameter r_s defined by $r_s=me^2/\alpha k_F\hbar^2$ with $\alpha=1/\sqrt{2}$. For example, the Hartree-Fock energy $\langle 0\,|\,H\,|\,0\rangle$ is obtained as

$$\langle 0\,|\,H\,|\,0\rangle=\frac{1}{r_s^2}-\frac{1.2004}{r_s}\ , \tag{33}$$

and the correlation energy ϵ_c is given by $E^{(1)}$ in the two-body approximation.

B. Weight function

In order to show how to evaluate each term in $E^{(1)}$ numerically, let us consider $C^{(e)}_{1,0}(V)$ first. We can rewrite Eq. (13b) as

$$C^{(e)}_{1,0}(V)=\frac{1}{8\pi^3}\sum_{\sigma}\int d^2q\int d^2q'\int d^2p\frac{1}{q}\phi_{\sigma\sigma}(q')\times\frac{1}{-\vec{q}\cdot\vec{q}'}\ , \tag{34}$$

where $\phi_{\sigma\sigma'}(q)$ is defined by

$$\phi_{\sigma\sigma'}(q)=\frac{k_F}{2\pi e^2}\tilde{V}_{\sigma\sigma'}(k_Fq)\ , \tag{35}$$

and the integral should be done under the condition

$$|\vec{p}\,|<1,\quad |\vec{p}+\vec{q}+\vec{q}\,'|<1\ ,$$
$$|\vec{p}+\vec{q}\,|>1,\ \text{and}\ |\vec{p}+\vec{q}\,'|>1\ . \tag{36}$$

When we introduce polar coordinates and take account of the fact that only the relative spin orientation is important in the paramagnetic state, Eq. (34) can be transformed further as

$$C^{(e)}_{1,0}(V)=\int_0^\infty dq\int_0^\infty dq'\frac{1}{q}\phi_{\uparrow\uparrow}(q')w_1(q,q')\ , \tag{37}$$

with the "weight function" $w_1(q,q')$ defined by

$$w_1(q,q')=\frac{1}{2\pi^2}\int_{-\pi}^{\pi}d\theta\int d^2p\frac{1}{-\cos\theta}\ , \tag{38}$$

where θ is the angle between $\vec{q}$ and $\vec{q}\,'$. We can calculate $w_1(q,q')$ by the Gauss quadrature procedure, although the condition (36) makes the three-dimensional integral in Eq. (38) a little complicated. This function is non-negative (which is the reason why it is called the weight function) and vanishes unless

$$|q-q'|\leq 2\ , \tag{39}$$

because of the Fermi statistics, or the condition (36).

Once we obtain $w_1(q,q')$ in the form of a numerical table, we cannot only evaluate $C^{(e)}_{1,0}(V)$ by Eq. (37) but also $C^{(d)}_{1,0}(V)$, $C^{(d)}_{1,1}(H_0)$, and $C^{(e)}_{1,1}(H_0)$. For example, $C^{(d)}_{1,0}(V)$ is given by

$$C^{(d)}_{1,0}(V)=-\int_0^\infty dq\int_0^\infty dq'\,w_1(q,q')\frac{1}{q}[\phi_{\uparrow\uparrow}(q)+\phi_{\uparrow\downarrow}(q)]\ . \tag{40}$$

In order to check the accuracy of our procedure, let us set $1/q'$ for $\phi_{\uparrow\uparrow}(q')$ in Eq. (37). Then $C^{(e)}_{1,0}(V)$ is just the second-order exchange term in the usual perturbation theory. This has been evaluated analytically to be 0.228 714.[28] In our numerical calculation, it is found to be 0.228 742.

We can evaluate other terms in $E^{(1)}$ by introducing appropriate weight functions. For example, the particle-particle ladder terms are given by

$$C_{1,1}^{(4d)}(V)=\alpha r_s \int_0^\infty dq \int_0^\infty dq' w_{2c}^{(d)}(q,q') \times[\phi_{\uparrow\uparrow}(q)\phi_{\uparrow\uparrow}(q') +\phi_{\uparrow\downarrow}(q)\phi_{\uparrow\downarrow}(q')] , \quad (41a)$$

and

$$C_{1,1}^{(4e)}(V)=-\alpha r_s \int_0^\infty dq \int_0^\infty dq' w_{2c}^{(e)}(q,q')\phi_{\uparrow\uparrow}(q)\phi_{\uparrow\uparrow}(q') , \quad (41b)$$

with the suitable definition of $w_{2c}^{(d)}(q,q')$ and $w_{2c}^{(e)}(q,q')$, each of which has a five-dimensional integral. All the weight functions except $w_{2c}^{(d)}$ and $w_{2c}^{(e)}$ satisfy the condition (39). Unlike other terms, both $C_{1,1}^{(4d)}(V)$ and $C_{1,1}^{(4e)}(V)$ have four electron lines and only two hole lines. Thus, the restriction coming from the Fermi statistics is not so severe that $w_{2c}^{(d)}$ and $w_{2c}^{(e)}$ are not zero over the entire (q,q') plane. Because of this property, the particle-particle ladder terms become predominantly important in the high-q processes.

Terms in $g_{\sigma\sigma'}(r)$ are also evaluated by the introduction of weight functions. In fact, the same weight functions can be applied to the study of any 2D fermion system. In 3D systems, we have to obtain weight functions having a multiple integral up to seven dimensions, compared to five in 2D ones. This is the main reason why the 2D, instead of the 3D, electron gas is studied first.

C. High-density limit

In the high-density limit ($r_s \ll 1$), only a long-range part of the effective interaction is important. Diagrammatically, the ring diagrams, given by $C_{1,0}^{(d)}(V)$, $C_{1,1}^{(d)}(H_0)$, and $C_{1,1}^{(1d)}(V)$, are responsible for such parts of the interaction. When we set these terms into $E^{(1)}(\tilde{V})$ in Eq. (28) and take derivatives, we obtain the following solution in the small-q limit:

$$\phi_{\uparrow\uparrow}(q)=\phi_{\uparrow\downarrow}(q)=\frac{1}{q+\lambda q_{\mathrm{TF}}} , \quad (42)$$

where q_{TF} is the Thomas-Fermi screening length in the 2D electron gas, given by $2\alpha r_s$ in units of k_F. The factor λ is 0.447, which should be compared with 0.434 in the 3D electron gas.[16]

Substituting Eq. (42) into $E^{(1)}$ and leaving terms up to order $r_s \ln r_s$, we obtain the correlation energy ϵ_c as

$$\epsilon_c=-A-Br_s \ln r_s+O(r_s) , \quad (43)$$

with

$$A=\int_0^\infty dq \frac{1}{q} \int_0^\infty dq'[2w_1(q,q')/q -w_1(q,q')/q']=0.385 , \quad (44)$$

and

$$B=\alpha\frac{4}{3\pi}(10-3\pi)=0.173 . \quad (45)$$

This reproduces the exact result which has been obtained by the perturbation-theoretic approach.[27]

When we neglect terms of order r_s and higher, the pair distribution functions are reduced to those in the Hartree-Fock approximations, given by

$$g_{\uparrow\uparrow}^{(\mathrm{HF})}(\vec{r})=1-\left[\frac{2}{k_F r}J_1(k_F r)\right]^2 , \quad (46)$$

and

$$g_{\uparrow\downarrow}^{(\mathrm{HF})}(\vec{r})=1 , \quad (47)$$

where $J_1(z)$ is the Bessel function of first order.

D. Numerical results I: spin-independent effective interaction

The effective electron-electron interaction is usually described by the use of the dielectric function. When such a dielectric-function formalism is employed, the problem is how to incorporate the so-called local-field correction. Quite a number of papers have treated this problem,[3] but we will include this correction in an average way by making the parameter λ in Eq. (42) a variational one.

Although the local-field correction takes account of the electron-hole scattering processes in the calculation of the dielectric function, it cannot treat the effect of electron-electron ladder processes properly. Since the main role of this ladder term is to keep each electron away from the other ones, the effective interaction with this term will be weaker than without it. This is particularly true for large q. We will treat this reduction of the effective interaction by introducing another variational parameter μ in the numerator of Eq. (42), that is,

$$\phi_{\uparrow\uparrow}(q)=\phi_{\uparrow\downarrow}(q)=\frac{\mu}{q+\lambda q_{\mathrm{TF}}} . \quad (48)$$

The spin-dependence is neglected altogether here.

Substituting Eq. (48) into $E^{(1)}$ and using a variational procedure to determine λ and μ, we obtain ϵ_c as a function of r_s. The result is shown by the solid curve in Fig. 3, in which those of STLS (Ref. 26) and VMC (Ref. 23)

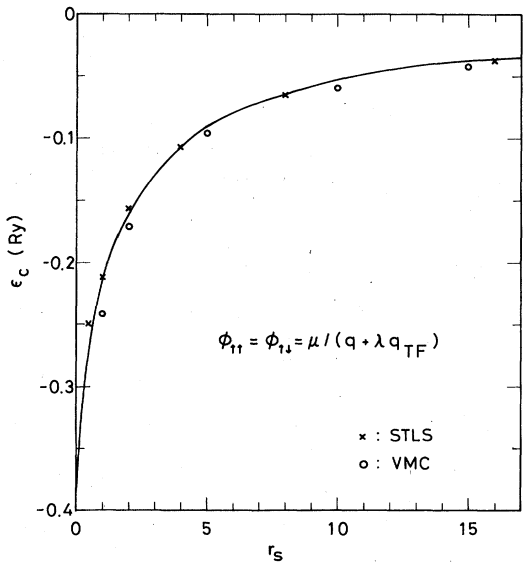

FIG. 3. Correlation energy per particle in Ry. A spin-independent form (48) for the effective potential is used. The results of STLS method, given by Jonson, and VMC by Ceperley are also shown.

methods are also shown for comparison. The present result is essentially the same as that of STLS. Compared to VMC, $|\epsilon_c|$ is smaller by about 10% in this range of r_s. As r_s becomes larger, the difference increases (up to 25% at $r_s=100$). Optimized values of λ and μ decrease monotonically with the increase of r_s, as shown in Fig. 4. Thanks to this rapid decrease of μ, the series (8) converges very rapidly even in the strong-coupling region.

In Fig. 5, $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$ are given for $r_s=0.5$, 4, and 16. The average of these two, defined by

$$g(r)=\tfrac{1}{2}[g_{\uparrow\uparrow}(r)+g_{\uparrow\downarrow}(r)]\ , \tag{49}$$

is also shown by a dashed curve in order to compare our result with that of the STLS method. The result of $g_{\uparrow\uparrow}(r)$ is always reasonable. It starts from zero at $r=0$ and increases gradually. At small r (i.e., $k_F r \lesssim 2.5$), $g_{\uparrow\uparrow}(r)$ is smaller than $g_{\uparrow\uparrow}^{(\mathrm{HF})}(r)$ by a very small amount. This indicates that, although the correlation effect between two parallel-spin electrons exists, it is very small compared to the exchange effect. For r_s less than 2.2, there appears to be no problem in $g_{\uparrow\downarrow}(r)$. However, when r_s exceeds this value, $g_{\uparrow\downarrow}(r)$ becomes negative near $r\approx 0$. With a further increase of r_s, $g_{\uparrow\downarrow}(0)$ becomes positive, but $g'_{\uparrow\downarrow}(0)$ is negative and brings about a negative region, as shown in Fig. 5(c).

The adequacy of an approximation in the electron-gas problem is usually checked by investigating whether $g(0)$ is positive or not, but $g'(0)$ is seldom discussed. This is probably due to Kimball's general statement[30] that $g'(0)$ is related to $g(0)$ through

$$\left.\frac{dg(r)}{d(k_F r)}\right|_{r=0} = 2\alpha r_s g(0)\ , \tag{50}$$

in the 2D electron gas.[27] Thus, the negative $g'(0)$ is just as unphysical as that of $g(0)$. However, the problem of negative $g'(0)$ seems to be more serious than that of negative $g(0)$, when we try to obtain physical information for the behavior of two electrons at small r from the calculated curve of $g(r)$. Once $g'(0)$ is negative, it implies that two electrons are attracted rather than repelled at a very short distance.

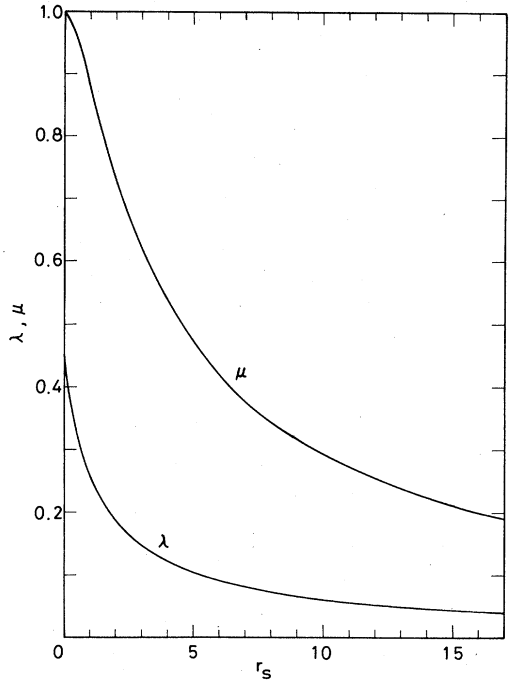

FIG. 4. Variationally determined λ and μ, which are defined in Eq. (48).

E. Asymptotic behavior of the effective interaction

As far as the energy is concerned, our simplest choice [Eq. (48)] was not unsatisfactory. But when r_s is larger than 4, $g'_{\uparrow\downarrow}(0)$ in addition to $g_{\uparrow\downarrow}(0)$ becomes negative. In order to correct this unphysical behavior, let us consider the large-q limit of the effective interaction more seriously. The electron-electron ladder diagrams, given by $C_{1,0}^{(d)}(V)$, $C_{1,0}^{(e)}(V)$, $C_{1,1}^{(d)}(H_0)$, $C_{1,1}^{(e)}(H_0)$, $C_{1,1}^{(4d)}(V)$, and $C_{1,1}^{(4e)}(V)$, are important in this limit. When we include only these terms in $E^{(1)}$ and take derivatives as indicated by Eq. (28), we obtain the following equations for $\phi_{\sigma\sigma'}(q)$:

$$\phi_{\uparrow\uparrow}(q)\int_0^\infty dq' w_1(q,q') = \frac{1}{q}\int_0^\infty dq' w_1(q,q') - \int_0^\infty dq' w_1(q,q')\left[\frac{1}{q'}-\phi_{\uparrow\uparrow}(q')\right]$$
$$-\alpha r_s \int_0^\infty dq'[w_{2c}^{(d)}(q,q')-w_{2c}^{(e)}(q,q')]\phi_{\uparrow\uparrow}(q')\ , \tag{51}$$

and

$$\phi_{\uparrow\downarrow}(q)\int_0^\infty dq' w_1(q,q') = \frac{1}{q}\int_0^\infty dq' w_1(q,q') - \alpha r_s \int_0^\infty dq' w_{2c}^{(d)}(q,q')\phi_{\uparrow\downarrow}(q')\ . \tag{52}$$

When q and q' are large, the weight functions in these equations have the following form:

$$\int_0^\infty dq' w_1(q,q') \sim \frac{1}{2q}\ , \tag{53}$$

and

$$w_{2c}^{(d)}(q,q') \sim w_{2c}^{(e)}(q,q') \sim \begin{cases} 1/2q^2 q', & q \gg q' \\ 1/2qq'^2, & q \ll q'\ . \end{cases} \tag{54}$$

Substituting Eq. (54) into Eq. (51), we find easily that for large q, $\phi_{\uparrow\uparrow}(q)$ approaches the bare potential, i.e.,

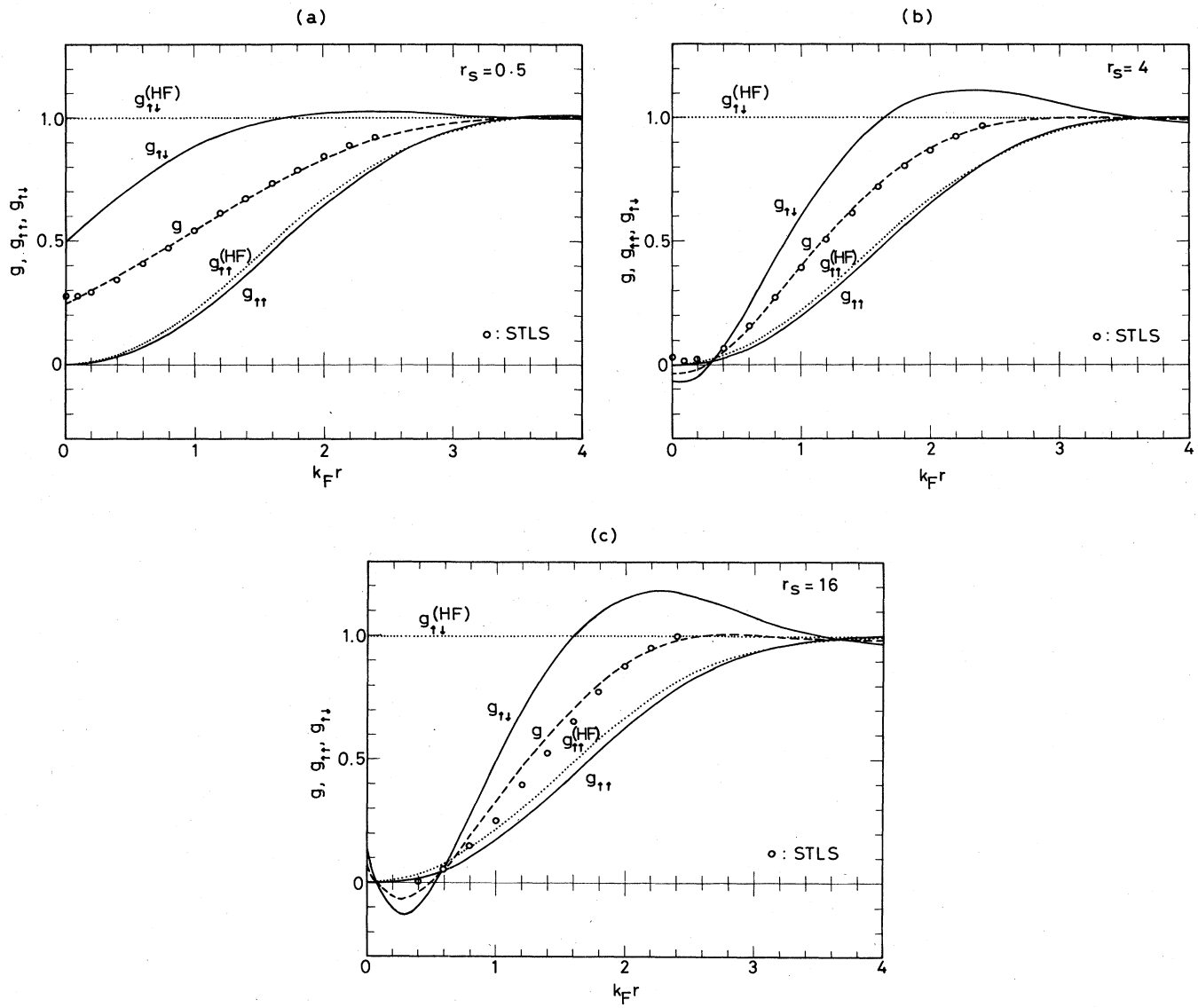

FIG. 5. Pair distribution functions, $g(r)$, $g_{\uparrow\uparrow}(r)$, and $g_{\uparrow\downarrow}(r)$, calculated with the effective potential (48). Open circles are the result for $g(r)$ in STLS method, given by Jonson. The Hartree-Fock values, $g^{(HF)}_{\uparrow\uparrow}$ and $g^{(HF)}_{\uparrow\downarrow}$, are also shown by dotted curves. (a), (b), and (c) treat, respectively, the case of $r_s = 0.5$, 4, and 16.

$$\phi_{\uparrow\uparrow}(q) \sim 1/q \ . \tag{55}$$

On the other hand, Eq. (52) is just the Bethe-Salpeter equation for the electron-electron ladder vertex in the usual perturbation theoretic approach. This equation has been treated by several workers in the 3D electron gas.[6,7] The method of Yasuhara[7] provides the simplest way to obtain the solution of Eq. (52) in the large-q limit. Let us make an approximation for $w^{(d)}_{2c}$ as

$$w^{(d)}_{2c}(q,q') = \frac{\Theta(q-q_0)\Theta(q'-q_0)}{2qq'} \times \left[\frac{\Theta(q-q')}{q} + \frac{\Theta(q'-q)}{q'} \right] , \tag{56}$$

where $\Theta(x)$ is the Heaviside function and q_0 is introduced to cutoff the low-q region. With the use of the modified Bessel functions $I_0(z)$ and $I_1(z)$, Eq. (52) can be solved and the result is

$$\phi_{\uparrow\downarrow}(q) = \frac{1}{I_0[2(\alpha r_s/q_0)^{1/2}]} \left[\frac{q}{\alpha r_s} \right]^{1/2} I_1[2(\alpha r_s/q)^{1/2}]/q \ , \tag{57}$$

which has the following form in the large-q limit:

$$\phi_{\uparrow\downarrow}(q) \approx \mu/q \ , \tag{58}$$

with

$$\mu = 1/I_0[2(\alpha r_s/q_0)^{1/2}] \tag{59}$$

Because μ in Eq. (59) depends on the cutoff q_0, the actual value of μ is not determined until we know $\phi_{\uparrow\downarrow}(q)$ for $q \lesssim 1$. However, it is clear that $|\mu|$ becomes exponentially small for large r_s. Thus the behavior of $\phi_{\uparrow\downarrow}(q)$ is very different from that of $\phi_{\uparrow\uparrow}(q)$. Physically, this can be ex-

plained as follows. At very short distance, two electrons avoid each other and thus the actual potential between the two is reduced in effectiveness. However, the nature of the repulsion is different for parallel- and antiparallel-spin pairs. In the former case, the Pauli principle is the major source and the bare potential $V(q)$ works in each elementary process. Thus, the actual potential for the scattering process $(\vec{p}\uparrow,\vec{p}\,'\uparrow)\rightarrow(\vec{p}+\vec{q}\uparrow,\vec{p}\,'-\vec{q}\uparrow)$ is given by $V(q)-V(|\vec{p}\,'-\vec{p}-\vec{q}|)$, which is very small for large q. For the antiparallel-spin case, the Coulomb correlation is the only effect which moderates the actual potential. Thus the effective potential $\tilde{V}_{\uparrow\downarrow}(q)$ becomes small for large q, as shown in Eq. (58).

F. Numerical results II: spin-dependent effective interaction

According to Eqs. (55) and (58), the effective interaction should be spin dependent. The simplest choice for $\phi_{\sigma\sigma'}(q)$ which satisfies these equations as well as the small-q behavior [Eq. (42)] is given by

$$\phi_{\uparrow\uparrow}(q)=\frac{1}{q+\lambda q_{\mathrm{TF}}}\ , \tag{60}$$

and

$$\phi_{\uparrow\downarrow}(q)=\frac{\mu}{q+\lambda\mu q_{\mathrm{TF}}}\ , \tag{61}$$

with two variational parameters λ and μ. However, we have found that this choice gives almost the same results for both energy and pair distribution function as the previous choice of Eq. (48). The reason is simple. The correlation energy in the paramagnetic state is mostly due to antiparallel-spin pairs. Thus $\phi_{\uparrow\downarrow}(q)$ is much more important than $\phi_{\uparrow\uparrow}(q)$. The choice of Eq. (61) gives essentially the same $\phi_{\uparrow\downarrow}(q)$ as that of Eq. (48).

In order to gain more insight into $\phi_{\sigma\sigma'}(q)$, let us consider the effective interaction between an up-spin electron at the origin and another electron at a distance r. When r is very large, it does not matter how the second electron's spin is oriented. However, when r becomes as small as $1/k_F$, there appears a difference. According to Fig. 5, $g_{\uparrow\downarrow}(r)$ is much larger than $g_{\uparrow\uparrow}(r)$ in this region. This means that the screening cloud for the first electron is mainly composed of down-spin electrons. Thus, if the second electron has an up-spin, the screening cloud is disturbed only by the Coulomb repulsion. However, if it has a down-spin, they are disturbed by both the Coulomb repulsion and Pauli principle. Therefore, the down-spin electron has a weaker screening effect. Namely, $\tilde{V}_{\uparrow\downarrow}$ is stronger than $\tilde{V}_{\uparrow\uparrow}$ in this region. In momentum space, we have the following conclusion:

$$\phi_{\uparrow\downarrow}(q)>\phi_{\uparrow\uparrow}(q)\quad\text{for } q\sim 1\ . \tag{62}$$

Kukkonen and Overhauser have obtained the same result by using a different approach.[31]

Combining this result with Eqs. (55) and (58), we find that there is a crossover effect between $\phi_{\uparrow\uparrow}(q)$ and $\phi_{\uparrow\downarrow}(q)$. They are the same at $q=0$, but the latter becomes larger near $q\sim 1$. With a further increase of q, the former becomes much larger. The choice of Eqs. (60) and (61) can not produce this behavior.

There are several possibilities for including this crossover effect in a choice of $\phi_{\sigma\sigma'}(q)$. For example, we can extend the local-field-correction formalism to the spin-dependent form.[18,31] After several trials, however, we found that we could obtain a substantial improvement simply by choosing $\phi_{\uparrow\uparrow}(q)$ as in Eq. (60) and $\phi_{\uparrow\downarrow}(q)$ as

$$\phi_{\uparrow\downarrow}(q)=\frac{\mu}{q+\lambda q_{\mathrm{TF}}}+\frac{1-\mu}{\lambda q_{\mathrm{TF}}}F(q)\ , \tag{63}$$

where $F(0)$ is taken to be unity in order to satisfy the relation $\phi_{\uparrow\uparrow}(0)=\phi_{\uparrow\downarrow}(0)$. The final result for the energy is very insensitive to the choice of $F(q)$, provided that $F(q)$ decreases quite rapidly for $q>2$. A possible guess is

$$F(q)=\exp(-q^2/\xi^2)\ , \tag{64}$$

with another variational parameter ξ. This parameter is found to increase monotonically from 1.50 at $r_s=1$ to 2.81 at $r_s=100$.

The resulting correlation energy is given in the row II of Table I for several values of r_s. (Units are in Ry.) Results of VMC and those in Sec. III D are also shown in the rows indicated by VMC and I, respectively. The difference between II and VMC is always less than 4% for $2\le r_s\le 40$.

Figure 6 gives the radial distribution function of the antiparallel-spin pair $g_{\uparrow\downarrow}(r)$ for several values of r_s. Although $g'_{\uparrow\downarrow}(0)$ is improved and positive for $r_s<20$, $g_{\uparrow\downarrow}(0)$ is still negative for $r_s>2.5$. Unlike the ground-state energy, the value $g_{\uparrow\downarrow}(0)$ depends rather strongly on the choice of $F(q)$ in Eq. (63). For example, $g_{\uparrow\downarrow}(0)$ varies from -0.05 to -0.1 at $r_s=4$.

The variationally determined effective potential is shown in Fig. 7. Instead of $\phi_{\sigma\sigma'}(q)$, we have shown $\alpha r_s\phi_{\sigma\sigma'}(q)$, because this is just the expansion parameter of the series (8). Even if r_s becomes larger by 20 times, the change of $\alpha r_s\phi_{\sigma\sigma'}(q)$ is very moderate. The interesting point in Fig. 7 is that μ, and thus $\phi_{\uparrow\downarrow}(q)$, becomes negative

TABLE I. Correlation energy of the 2D electron gas in Ry units. Row I represents the results with the effective potential given by Eq. (48). Row II gives the result with the choice of Eq. (60) for $\tilde{V}_{\uparrow\uparrow}$ and Eq. (63) for $\tilde{V}_{\uparrow\downarrow}$. Row III is obtained with the use of Eqs. (65) and (66). The row indicated by VMC is the result obtained by Ceperley (Ref. 23).

r_s	1	2	5	10	15	20	30	40	50	100
I	−0.215	−0.158	−0.0903	−0.0528	−0.0374	−0.0289	−0.0199	−0.0152	−0.0123	−0.0063
II	−0.217	−0.165	−0.0998	−0.0617	−0.0449	−0.0353	−0.0245	−0.0186	−0.0149	−0.0073
III	−0.218	−0.165	−0.0998	−0.0618	−0.0450	−0.0354	−0.0245	−0.0187	−0.0151	−0.0078
VMC	−0.242	−0.172	−0.0957	−0.05915	−0.04323	−0.03429	−0.02441	−0.01909	−0.01571	−0.00838

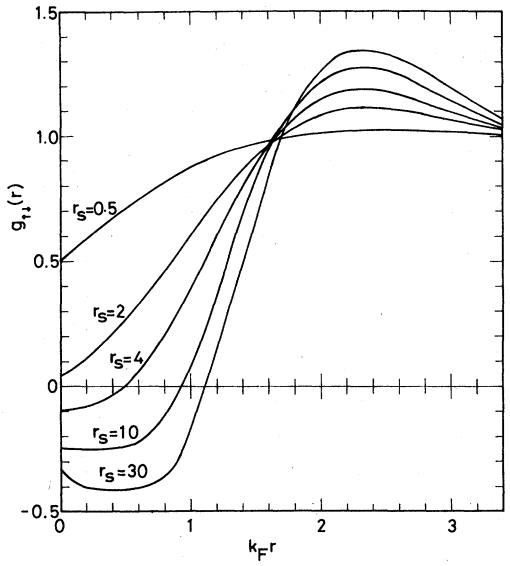

FIG. 6. Radial distribution function for the antiparallel-spin pair $g_{\uparrow\downarrow}(r)$ for $r_s=0.5$, 2, 4, 10, and 30 with the effective potentials $\phi_{\uparrow\uparrow}(q)$ in Eq. (60) and $\phi_{\uparrow\downarrow}(q)$ in Eq. (63).

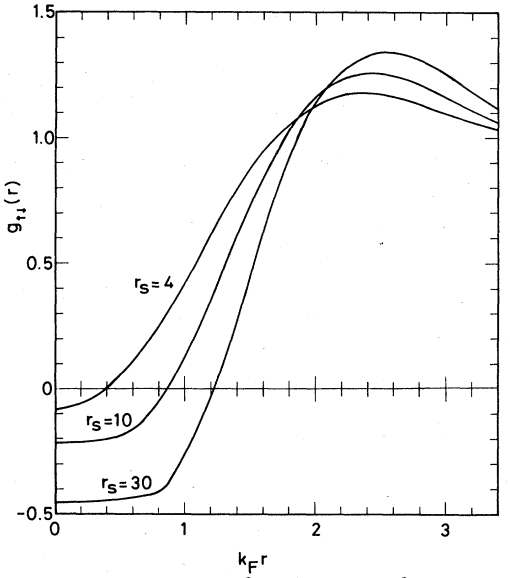

FIG. 8. Radial distribution function $g_{\uparrow\downarrow}(r)$ for $r_s=4$, 10, and 30 with the choice of $\phi_{\uparrow\uparrow}(q)$ in Eq. (65) and $\phi_{\uparrow\downarrow}(q)$ in Eq. (66).

for $r_s \gtrsim 5$. The value 5 depends on the choice of $F(q)$, but whatever choice we may make, $\phi_{\uparrow\downarrow}(q)$ becomes negative for $q \gtrsim 2$ when r_s becomes sufficiently large. The discussion in Sec. III E has already predicted the smallness of $|\mu|$ for large r_s. However, it could not tell the possibility of negative μ. This is due to the insufficient treatment of the correlation effects for $q \lesssim 1$. If we do not introduce the cutoff q_0 but treat $\phi_{\uparrow\downarrow}(q)$ more accurately for $q \lesssim 1$ in Eq. (52), it is not difficult to see that Eq. (52) can produce a solution of $\phi_{\uparrow\downarrow}(q)$ which becomes negative for large q. The negative $\phi_{\uparrow\downarrow}(q)$ is probably related to the spin-density-wave instability.[32]

Physically, $F(q)$ was included in Eq. (63) in order to take a better account of the correlation effect between antiparallel-spin electrons. The same procedure will be appropriate for the parallel-spin pair to improve the results for $r_s \gtrsim 20$, because in such low densities parallel-spin pairs will also need a better treatment of their correlation. Thus we try another choice for $\phi_{\sigma\sigma'}(q)$ as

$$\phi_{\uparrow\uparrow}(q)=\frac{1}{q+\lambda q_{\mathrm{TF}}}+\frac{\eta}{\lambda q_{\mathrm{TF}}}F(q)\ , \tag{65}$$

and

$$\phi_{\uparrow\downarrow}(q)=\frac{\mu}{q+\lambda q_{\mathrm{TF}}}+\frac{1-\mu+\eta}{\lambda q_{\mathrm{TF}}}F(q)\ , \tag{66}$$

with a further variational parameter η. $F(q)$ is chosen to have the form (64). The result for ϵ_c is shown in the row III of Table I. Figure 8 shows the result for $g_{\uparrow\downarrow}(r)$. The value $g'_{\uparrow\downarrow}(0)$ remains positive for $r_s<50$. In this way, $g'_{\uparrow\downarrow}(0)$ is seen to be a good criterion in the search for a better effective interaction. Compared to $\phi_{\uparrow\uparrow}(q)$ in Fig. 7, the main effect of $F(q)$ in Eq. (65) is found to decrease $\phi_{\uparrow\uparrow}(q)$ near $q\sim 1$, which leads to the larger difference between $\phi_{\uparrow\uparrow}(q)$ and $\phi_{\uparrow\downarrow}(q)$ in this region of q.

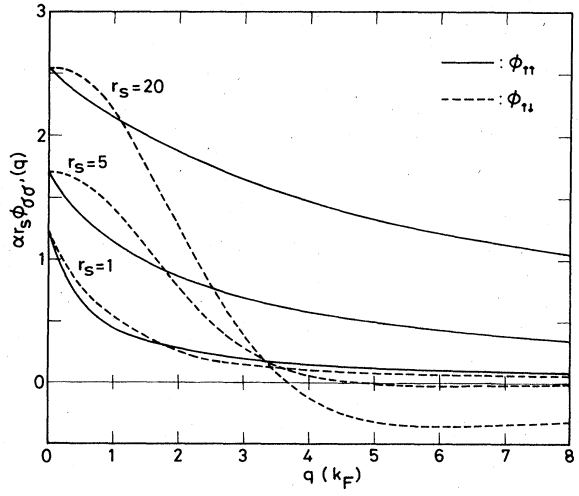

FIG. 7. Effective potential $\phi_{\uparrow\uparrow}(q)$ and $\phi_{\uparrow\downarrow}(q)$ determined variationally. The forms of Eqs. (60) and (63) with the function $F(q)$ in Eq. (64) are assumed.

IV. SUMMARY AND DISCUSSION

In this paper we have applied the method of effective-potential expansion proposed in I to the strongly-coupled many-body problem and have investigated how the lowest-order calculation works in the paramagnetic phase of the 2D electron gas. The result for the correlation energy ϵ_c agrees very well with that of the VMC for $1<r_s<100$. It is not known rigorously whether the value obtained for ϵ_c is an upper bound to the true value. However, when we combine the results in Table I with the fact that in the 3D electron gas, the VMC gives a higher value for ϵ_c than the GFMC by a few percent for $2<r_s<20$, we may conclude that our ϵ_c is very close to the true value, if not an upper bound. In addition to providing a very good result, the present method is simple from both the physical and computational points of view, because only a fi-

nite number of terms is considered. Thus, we think it highly promising for finding quantitative as well as qualitative information on such systems which are too complicated to be studied by the GFMC and other sophisticated many-body techniques.

Although we can reproduce the rigorous value of ϵ_c in the high-density limit, ϵ_c near $r_s \approx 1$ has a rather large discrepancy when compared to that of VMC. We ascribe this to both VMC and our method. Since the VMC produces so large an error as to have ϵ_c even lower than that of the GFMC at $r_s = 1$ in the 3D electron gas, ϵ_c obtained by the VMC is not as reliable in this density region as in the low-density region. In our treatment, the two-body approximation is not supposed to work well in the high-density region where the screening length is much longer than the interparticle spacing. When the long-range part of the effective interaction becomes really important, we also have to include higher-order terms such as the process of Fig. 9(a) and its exchange partners Fig. 9(a'), 9(b), and 9(b') in the third order of $\tilde{V}$. This can be understood by the fact that $\tilde{V}$ in the small-q region is relatively large and makes the convergence of our cluster expansion slow. This is also exemplified by the observation that any choice of $\tilde{V}_{\sigma\sigma'}(q)$ does not give a substantial improvement at $r_s = 1$ in the two-body approximation, as shown in Table I.

When r_s becomes large, $g_{\uparrow\downarrow}(r)$ becomes negative near $r \approx 0$ in the two-body approximation. As explained in Sec. II C this is caused by the electron-hole ladder process. If we neglect both electron-hole and hole-hole ladder processes, as has been done in several works[6,7] in which it is claimed that the radial distribution function is shown analytically to be always positive, we can also obtain a positive definite $g_{\uparrow\downarrow}(r)$. However, there seems to be no reason why such ladder processes can be neglected. It is true that these processes produce much smaller values than the electron-electron ladder term, as has been explained,[6,7] but the point is that when the electron-electron ladder term [Fig. 2(d)] is combined with both the Hartree

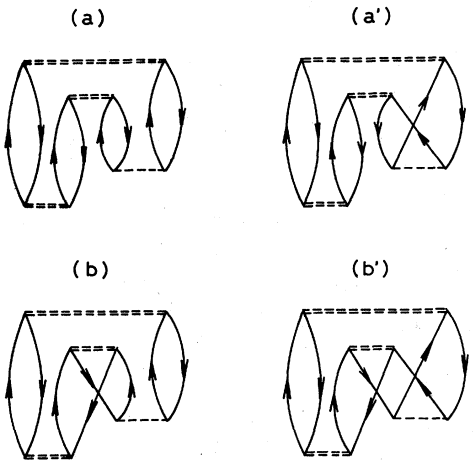

FIG. 9. Goldstone diagrams for an example of the ring diagrams in the third order and its exchange partners.

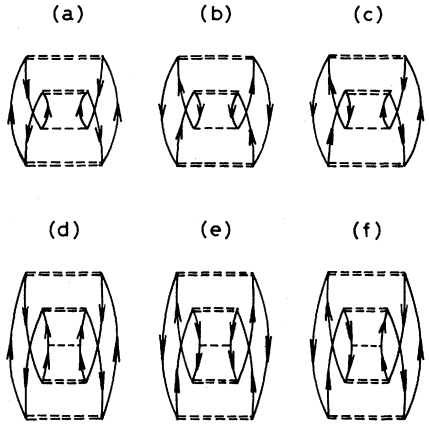

FIG. 10. Goldstone diagrams for the ladder-type terms in the third and fourth orders of the effective potential.

one [Fig. 1(b-1)] and the second-order direct one [Fig. 1(c-1)], the resulting contribution is just the same order of magnitude as the electron-hole or hole-hole ladder contribution.

In order to obtain a positive $g_{\uparrow\downarrow}(r)$, therefore, we have to consider higher-order terms. In third order, there is a contribution for $g_{\uparrow\downarrow}(r)$ from the ring-type diagrams [Figs. 9(a) and 9(b)], but these two are cancelled by each other. There are ladder-type terms as shown in Figs. 10(a)—10(c), but the sum of these terms are also negligibly small, because each of these terms has just the same number of particle lines as that of hole ones. The same argument can be applied to all $(2n+1)$th-order terms. In fourth order, however, the ladder terms, shown in Figs. 10(d)—10(f), give a positive contribution to $g_{\uparrow\downarrow}(r)$. This can be seen easily that the positive contribution of the diagram [10(d)] dominates the other two diagrams because it has the largest number of particle lines. The same is true for all $2n$th-order terms. Thus, the negative $g_{\uparrow\downarrow}(r)$ in the two-body approximation will be cured gradually as we increase the order of approximation in the cluster expansion. From this consideration, the magnitude of $|g_{\uparrow\downarrow}(0)|$ in the two-body approximation is seen to give a measure of the error of the cutoff procedure in the cluster expansion. If we compare $|g_{\uparrow\downarrow}(0)|$ with the largest term in $g_{\uparrow\downarrow}(0)$, i.e., the contribution described by Fig. 2(d), the estimated errors are 6 and 19% at $r_s = 4$ and 20, respectively.

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*Present address.

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