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Linked-cluster expansion for Jastrow-type wave functions and its application to the electron-gas problem

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A linked-cluster expansion for the expectation values of operators between correlated wave functions of the Jastrow type is described. The expansion is based on the logarithm of the correlation function and leads to terms that are explicitly proportional to the particle number for infinite systems. The lowest-order terms for a weakly interacting system of spin-1/2 particles are calculated explicitly. From these, the Euler-Lagrange equations for the correlation functions have been calculated. The equation for the correlation function between particles of antiparallel spin can be solved by Fourier transform, and it is shown that for $r \to \infty$, the correlation function behaves like $1 + A/r^2$. In the case of a system of particles interacting by hard-core repulsions, the logarithm of the correlation function does not exist inside the hard-core radius. It is then necessary to sum over ladder diagrams as in the derivation of the reaction matrix in many-body perturbation theory. This is carried out to provide a low-density approximation to the ground-state energy of the system and the Euler-Lagrange equation for the correlation function. It is argued that the correlation function again behaves like $1 + A/r^2$ for large r. The expansion is applied to the problem of calculating the correlation energy of the electron gas. It is shown that a variational calculation based on the lowest-order terms in an expansion of the wave function leads to a divergent result (unbounded from below), but that a convergent result is obtained by summing over ring diagrams, which correspond to long-range polarization of the electron cloud. The result is similar to that of Gaskell obtained by a somewhat different method. It is shown analytically that at high densities the result behaves logarithmically, specifically as $0.0570 \ln r_s - 0.1324$ Ry. The lowest-order exchange contributions have also been calculated and found to contribute 0.040 Ry to the energy at densities of physical interest.

I. INTRODUCTION

The purpose of this article is to describe a new linked-cluster–type expansion for wave functions of the Jastrow type for fermion systems. The result resembles the familiar perturbation-theory cluster expansion of Brueckner and Goldstone much more than do previous expansions for Jastrow wave functions, and also permits a more systematic treatment of the exclusion principle. It may be that this expansion can be useful in further understanding the relation between the Brueckner and Jastrow theories.

The expansion is based on the logarithm $\phi(r)$ of the correlation function $f(r)$ of the Jastrow theory rather than on the function $f(r) - 1$ which it equals in first approximation. The use of $\phi(r)$ seems to correspond to a partial summation of terms in other expansions so that an expansion similar to the Goldstone expansion becomes valid.

The usual method of analyzing Jastrow-type wave functions is based on the method of Iwamoto and Yamada,[1] which is a rather complicated prescription dependent on the calculation of the derivative of the logarithm of the so-called generalized normalization integral. The expansion, and modifications of it, have been extensively discussed by Feenberg[2] and Clark and Westhaus[3] for generalized types of correlated wave functions.

The general expansion is described in Sec. II. It will be seen that the argument is similar to, but rather simpler than, the linked-cluster theorem of Goldstone. The argument given here is quite similar to one given in a different context by Da Providência and Shakin.[4]

In Sec. III the expansion will be applied to determining the variational equations for the correlation function of a weakly interacting system. These equations have apparently not been previously derived. The solution of the equations will be constructed explicitly, and it will be shown that the deviation of the correlation function from unity behaves like r^{-2} for large r.

The problem of carrying out the partial summations that are necessary for a system with strong repulsions is considered in Sec. IV. An expansion of the energy in powers of the density, based on the number of hole lines in a graph will be discussed. The contribution of graphs containing two hole lines will be summed explicitly for spin-$\frac{1}{2}$ particles and the variational equations for the correlation functions based on these terms will be obtained. The correlation functions in this case have the same asymptotic behavior as in the weakly interacting case. A general prescription for carrying out the partial summations necessary in the strongly interacting case has not so far been found.

The expansion formalism is applied in Sec. V to the electron-gas problem. In this case the lowest-energy correction term diverges because of the long range of the Coulomb force, and it is necessary to sum over terms that represent the polarization effect. The exchange correction terms and the results of the calculation are described in Sec. VI.

II. LINKED-CLUSTER EXPANSION FOR CORRELATED WAVE FUNCTIONS

The quantity of interest in the Jastrow-type variational calculation is the quotient

$$\langle H\rangle = \frac{\langle\Phi|F^\dagger HF|\Phi\rangle}{\langle\Phi|F^\dagger F|\Phi\rangle}, \tag{2.1}$$

where Φ is a Slater determinant, H is the Hamiltonian, and F is a correlation operator. For simplicity, only the case of two-particle spatial correlations will be considered; it will be evident that the argument applies to spatial correlation functions involving more than two particles. We will write F in the form

$$F = \exp\Big(\sum_{i<j}\phi(r_{ij})\Big), \tag{2.2}$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ and $\phi(r)$ is the logarithm of the two-particle correlation function. In this case $F^\dagger = F$.

It seems clear that an exact evaluation of Eq. (2.1) will never be made beyond the Hartree-Fock approximation $\phi(r) = 0$. In fact, we should recognize a difficulty involved in the calculation. The numerator and denominator of (2.1) may each vanish (or approach ∞) in the limit of large particle number, in analogy to the situation in perturbation theory in which the overlap of unperturbed and perturbed wave functions vanishes in the thermodynamic limit. A second difficulty related to this, is that if the numerator and denominator are separately expanded in powers of ϕ (or a parameter describing the strength of ϕ), the expansion contains arbitrarily large powers of the particle number. It is therefore necessary to achieve an exact division of the denominator into the numerator, and this is the object of a cluster expansion.

The numerator and denominator in $\langle H\rangle$ can be analyzed graphically by expanding

$$F = \sum_{p=0}^{\infty}\frac{1}{p!}\Big(\sum_{i<j}\phi(r_{ij})\Big)^p \tag{2.3}$$

and applying the operator

$$\Big(\sum_{i<j}\phi(r_{ij})\Big)^p$$

to Φ. The resulting matrix elements can then be represented graphically using Wick's theorem in a manner exactly the same as in the many-body perturbation theory in which matrix elements of the operator

$$\Big((E_0 - H_0)^{-1}(1-P)\sum_{i<j}V(r_{ij})\Big)^p$$

are represented graphically; we are here, however, dealing with the case $(E_0 - H_0)^{-1}(1-P) = 1$. For example, if $p = 5$, the graph shown in Fig. 1 may be generated. The only difference from a many-body perturbation-theory graph is that a factor of $(5!)^{-1}$ is to be included with the numerical contribution of the graph. The wavy vertices represent factors of the form

$$\tfrac{1}{2}\tilde{\phi}(ijkl) = \tfrac{1}{2}\langle\psi_i(r)\psi_j(r')|\,\phi(|\vec{r}-\vec{r}'|)\,|\,\psi_k(r)\psi_l(r')\rangle. \tag{2.4}$$

In calculating $\langle\Phi|F^\dagger HF|\Phi\rangle$, all graphs of the form shown in Fig. 2 must be considered. Vertices below the broken line belong to $F\Phi$, those above the broken line to $\Phi F^\dagger$, and the square box represents a vertex produced by H, which may have one or two entering and leaving lines depending on whether the term is a kinetic or a potential energy. The contribution in Fig. 2 is multiplied by $(2!5!)^{-1}$; the contribution of a general graph is multiplied by $(p!q!)^{-1}$ where p and q are the number of vertices above and below the broken line.

The general graph contributing to $\langle\Phi|F^\dagger HF|\Phi\rangle$ will consist of several, say r, disconnected pieces. The piece of the graph containing the H vertex will be called the main piece. Graphs which differ from one another only in the ordering of the vertices in one disconnected piece relative to the other disconnected pieces give the same contribution to the matrix element. There are

$$\frac{p!q!}{p_1!\cdots p_r!q_1!\cdots q_r!}$$

such permutations of vertices in disconnected pieces relative to one another, where p_i and q_i are the number of vertices in piece i above and below the broken line. (We are considering only permutations which keep the number of vertices above and below the broken line fixed.) It is there-

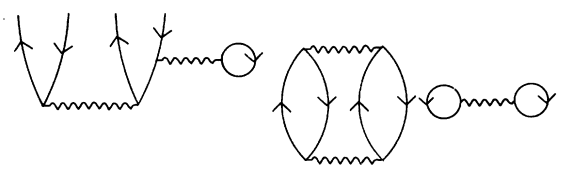

FIG. 1. Graph representing diagrammatically a possible contribution to $[\sum\phi(r_{ij})]^5\Phi$.

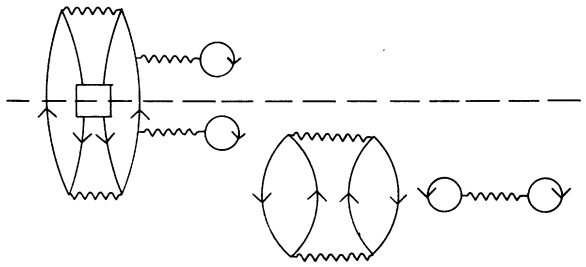

FIG. 2. Graph describing a contribution to the expansion of $\langle\Phi|F^\dagger AF|\Phi\rangle$. The square box represents a vertex corresponding to the operator A.

fore seen that the contribution of a graph such as that in Fig. 2 is just the product of the contributions of the various disconnected pieces, each taken with a factor $(p_i!q_i!)^{-1}$.

If there are several, say α, identical pieces, they should not be regarded as distinguishable so that in counting permutations of vertices in one piece relative to vertices in an identical piece, a problem in multiple counting occurs. If, however, a factor of $(\alpha!)^{-1}$ is included with each contribution, the identical pieces may be regarded as distinguishable, and the summation over permutations applied. The main piece is, of course, distinguishable from the other pieces.

It can be seen that $\langle\Phi|F^\dagger HF|\Phi\rangle$ can be factored into the product of the sum of the contribution of all linked graphs containing the H vertex, and the sum of the contribution of all graphs, linked or unlinked, containing only correlation-factor vertices.

The denominator $\langle\Phi|F^\dagger F|\Phi\rangle$ in $\langle H\rangle$ is given by the sum of the contributions of all graphs of the form shown in Fig. 2 except that in this case there is no piece with an H vertex. This sum is, however, the factor in $\langle\Phi|F^\dagger HF|\Phi\rangle$ given by the disconnected pieces containing only correlation-factor vertices. It is therefore seen that $\langle H\rangle$ is given by the sum of all linked graphs containing an H vertex, i.e., a graph such as that shown in Fig. 3. It should be noted that the contribution

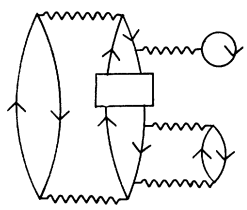

FIG. 3. Linked graph contributing to the expectation value of an operator in the correlated state $F\Phi$.

of this particular graph contains a factor $(2!3!)^{-1}$.

It is apparent that the above proof is exactly analogous to the proof[5] of the linked-cluster expansion in many-body perturbation theory except that it is much simpler in that there is no theorem on disentangling energy denominators to be proved. Therefore the rules for evaluating contributions in perturbation theory also apply in this situation, except that the factors $(p!q!)^{-1}$ must be included. For example, the so-called exclusion principle violating graphs in which two or more particles (or holes) in the same single-particle state are present in some intermediate state must be included. These arise, as was pointed out by Goldstone, because in the analysis by Wick's theorem, two terms contributing the same amount but with opposite signs exactly cancel; one of these terms contributes to a disconnected graph and so is eliminated when the unlinked pieces are divided out.

It is also clear that in the familiar case of a uniform system each term in the expansion for $\langle H\rangle$ is explicitly proportional to the particle number, as in the many-particle perturbation theory.

A further remark about the value of $\langle\Phi|F^\dagger F|\Phi\rangle$ may be in order. Let us consider a linked graph with p vertices containing only correlation-factor vertices, with r vertices below and $p-r$ vertices above the broken line. This contributes, in any term in which it occurs, a factor $[(p-r)!r!]^{-1}X$ where X is given by the structure of the graph. If we sum over graphs differing only in the number of vertices above and below the broken line we obtain

$$\sum_{r=0}^{p}\frac{1}{r!(p-r)!}X=\frac{2^p}{p!}X.$$

If a particular linked graph is repeated α times in a term in $\langle\Phi|F^\dagger F|\Phi\rangle$, it contributes a factor $X^\alpha/\alpha!$ to the term. It is now seen that

$$\langle\Phi|F^\dagger F|\Phi\rangle=\sum\frac{1}{\alpha_1!\cdots\alpha_s!}X_{i_1}^{\alpha_1}\cdots X_{i_s}^{\alpha_s},\qquad(2.5)$$

the sum being on $i_1,\ldots,i_s,\alpha_1,\ldots,\alpha_s$, where $s=0,1,\ldots$. Therefore

$$\langle\Phi|F^\dagger F|\Phi\rangle=e^{S'},\qquad(2.6)$$

where S' is the sum of all *linked* graphs in which each vertex factor is doubled, and a factor $(p!)^{-1}$ is included with the contribution of a graph with p vertices. This argument is essentially the same as one given previously by Da Providência.[6]

Since S' is known to be proportional to the particle number, it is seen that $\langle\Phi|F^\dagger F|\Phi\rangle$ approaches 0 or ∞ in the limit of large particle number.

It is possible to write

$$F^\dagger HF=F^\dagger TF^{-1}F^2+VF^2,$$

where T is the kinetic-energy operator. Since

$$F^2 = \exp\left(\sum_{ij} 2\phi(r_{ij})\right)$$

it can be seen that $\langle H\rangle$ is also given by the sum of all linked graphs in which each ϕ vertex factor is doubled and the *last* vertex is either V or FTF^{-1}. This may not be more useful, since FTF^{-1} is a complicated three-particle operator.

III. LOWEST-ORDER VARIATIONAL EQUATIONS

As an example, we consider a uniform infinite system of spin-$\frac{1}{2}$ particles in lowest order. That is, only terms in the kinetic energy that are second order in ϕ, and terms in the potential energy that are first order in ϕ will be considered. This is appropriate to a system of weakly interacting particles in which we anticipate that ϕ will be proportional to the coupling constant determining the strength of the potential.

The graphs shown in Fig. 4 indicate the contributions to be considered. In these graphs, a broken-line vertex represents a potential-energy factor and an X represents a kinetic-energy factor.

Since the system consists essentially of two different types of particles, spin-up and spin-down, there are two functions $\phi_p(r)$ and $\phi_a(r)$, corresponding to parallel and antiparallel spins, to be considered.

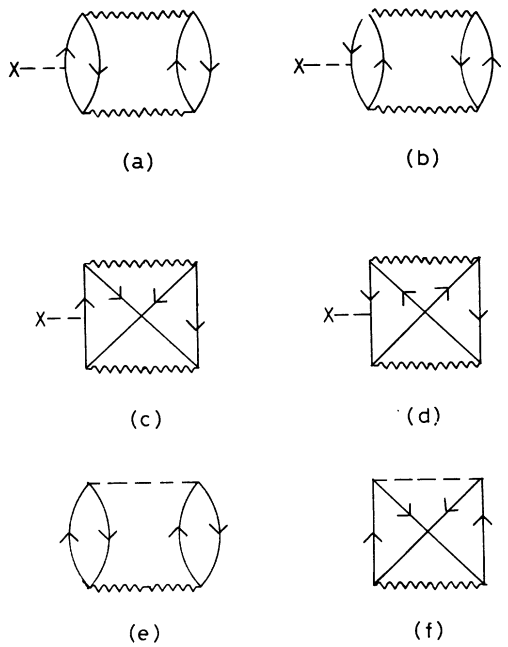

FIG. 4. Graphs contributing to the expectation value of the Hamiltonian in lowest order.

The contributions of the graphs in Figs. 4(a), 4(b), and 4(e) to the energy are

$$T_d = 2\sum (1/2m)(|\vec{k}_1+\vec{k}|^2 - k_1^2)\tilde{\phi}(k)^2 \tag{3.1}$$

and

$$V_d = 2\sum v(k)\tilde{\phi}(k). \tag{3.2}$$

The sums in (3.1) and (3.2) are to be taken over hole-line momenta $\vec{k}_1$ and $\vec{k}_2$ and particle-line momenta $\vec{k}_1+\vec{k}$ and $\vec{k}_2-\vec{k}$, where $\vec{k}$ is the momentum transfer at the ϕ and V vertices. It is therefore necessary to calculate the functions

$$h(k) = \frac{1}{(2\pi)^3}\int d^3k',$$

$$t(k) = \frac{1}{(2\pi)^3}\,\frac{1}{2m}\int d^3k'(k'^2 + 2\vec{k}\cdot\vec{k}'),$$

where the integrations are over $\vec{k}'$ values such that $|\vec{k}'|<k_F$, $|\vec{k}+\vec{k}'|>k_F$. These arise from the sums on $\vec{k}_1$ and $\vec{k}_2$.

Straightforward calculation shows that

$$h(k) = (1/8\pi^2)k_F^3\, y(1-\tfrac{1}{12}y^2), \quad k<2k_F$$
$$= (1/6\pi^2)k_F^3, \quad k>2k_F \tag{3.3}$$

where $y = k/k_F$ and

$$t(k) = (1/6\pi^2)k_F^3(k^2/2m). \tag{3.4}$$

The functions $\tilde{\phi}(k)$ and $v(k)$ in (3.1) and (3.2) are the Fourier transforms of the function $\phi(r)$ and $V(r)$, respectively. Equation (3.1) includes both the particle and hole kinetic-energy terms of Figs. 5(a) and 5(b) and factors of 2 from the two ways of connecting the graph, the fact that the kinetic-energy vertices can be on either particle or hole line, and the two spin states. Equation (3.2) contains a factor of 2 from the fact that the ϕ vertex may either precede or follow the V vertex.

It can now be seen that

$$T_d = \frac{2}{(2\pi)^3}\,\Omega\int d^3k\, t(k)h(k)\tilde{\phi}(k)^2, \tag{3.5}$$

$$V_d = \frac{2}{(2\pi)^3}\,\Omega\int d^3k\, v(k)\tilde{\phi}(k)h(k)^2, \tag{3.6}$$

where Ω is the system volume. There are two such contributions to the energy, given by ϕ_p and ϕ_a.

It is more useful for some purposes to express the contributions to the energy in configuration representation. Each contribution is then a multidimensional integral which is constructed by labeling the ends of vertex number i with integration variables $\vec{r}_i$ and $\vec{r}_i'$. The vertex contributes to the integrand a factor $\phi(|\vec{r}-\vec{r}'|)$ or $V(|\vec{r}_i-\vec{r}_i'|)$, and for

each hole or particle line joining vertex ends labeled $\vec{r}_i$ and $\vec{r}_j$ there is a factor $K_h(|\vec{r}_i-\vec{r}_j|)$ or $K_p(|\vec{r}_i-\vec{r}_j|)$ where

$$K_h(r)=\frac{1}{(2\pi)^3}\int_{p<k_F} e^{-i\vec{p}\cdot\vec{r}}d^3p = \frac{k_F^3}{2\pi^2}\frac{j_1(k_Fr)}{k_Fr}, \tag{3.7}$$

$$K_p(r)=\frac{1}{(2\pi)^3}\int_{p>k_F} e^{-i\vec{p}\cdot\vec{r}}d^3p = \delta(\vec{r})-K_h(r). \tag{3.8}$$

We will denote $K_h(r)$ by $K(r)$. We note that $K(0)=\frac{1}{2}\rho$ where ρ is the particle density. If a hole or particle line contains a kinetic-energy vertex, it contributes a factor

$$T_h(r)=-(\hbar^2/2m)\nabla^2K_h(r) \tag{3.9}$$

or

$$T_p(r)=-(\hbar^2/2m)\nabla^2K_p(r). \tag{3.10}$$

Since the various factors in the integrand depend only on coordinate differences, one integration can be done immediately and gives a factor Ω; one of the $\vec{r}_i$ is then replaced by 0.

When T_d and V_d are calculated in this way, it is found that

$$T_d=\tfrac{1}{4}\rho^2\Omega(\hbar^2/m)\int d\vec{r}\,|\nabla\phi(r)|^2-\tfrac{1}{2}\rho\Omega(\hbar^2/m)\int d\vec{r}_1\,d\vec{r}_2K(|\vec{r}_1-\vec{r}_2|)^2\nabla\phi(r_1)\cdot\nabla\phi(r_2), \tag{3.11}$$

$$V_d=\tfrac{1}{2}\rho^2\Omega\int d\vec{r}\,\phi(r)V(r)-2\rho\Omega\int d\vec{r}_1\,d\vec{r}_2\,\phi(r_1)K(|\vec{r}_1-\vec{r}_2|)^2V(r_2)+2\Omega\int d\vec{r}_1\,d\vec{r}_2\,d\vec{r}_2'\,\phi(r_1)K(|\vec{r}_1-\vec{r}_2|)^2V(|\vec{r}_2-\vec{r}_2'|)K(r_2')^2, \tag{3.12}$$

where ρ is the particle density. These results are essentially equivalent to (3.5) and (3.6) by a Fourier transformation of the factors involved.

A similar calculation for the exchange-energy–type terms of Figs. 5(c), 5(d), and 5(f) yields the results

$$T_e=-\Omega(\hbar^2/m)\int d\vec{r}\,|\nabla\phi(r)|^2K(r)^2+\Omega(\hbar^2/m)\int d\vec{r}\,d\vec{r}'\,\nabla\phi(|\vec{r}-\vec{r}'|)\cdot\nabla\phi(r)K(r)K(r')K(|\vec{r}-\vec{r}'|), \tag{3.13}$$

$$V_e=-2\Omega\int d\vec{r}\,K(r)^2\phi(r)V(r)+4\Omega\int d\vec{r}\,d\vec{r}'\,\phi(r)K(|\vec{r}-\vec{r}'|)K(r)K(r')V(r') - 2\Omega\int d\vec{r}\,d\vec{r}_1'\,d\vec{r}_2'\,\phi(r)K(|\vec{r}-\vec{r}'|)K(r_1')V(|\vec{r}_1'-\vec{r}_2'|)K(|\vec{r}-\vec{r}_2'|)K(r_2'). \tag{3.14}$$

Equations (3.13) and (3.14) contribute only for ϕ_p.

We consider now the Euler-Lagrange equations for ϕ_p and ϕ_a. The equation for ϕ_a is obtained from Eqs. (3.11) and (3.12) and is

$$-(\hbar^2/m)\nabla^2\phi_a+(2/\rho)\int d\vec{r}'\,(\hbar^2/m)\nabla^2K^2(|\vec{r}-\vec{r}'|)^2\phi_a(r')+V_{\rm eff}(r)=0, \tag{3.15a}$$

where

$$V_{\rm eff}(r)=V(r)-(4/\rho)\int d\vec{r}'\,K(|\vec{r}-\vec{r}'|)^2V(r')+(4/\rho^2)\int d\vec{r}'\,d\vec{r}''\,K(|\vec{r}-\vec{r}'|)^2\,V(|\vec{r}'-\vec{r}''|)K(r'')^2. \tag{3.15b}$$

The Euler-Lagrange equation for ϕ_p is similar to (3.15) but contains additional terms arising from the exchange energies. It is

$$-\frac{\hbar^2}{m}\nabla^2\phi_p+\frac{2}{\rho}\int d\vec{r}'\frac{\hbar^2}{m}[\nabla^2K^2](|\vec{r}-\vec{r}'|)\phi_p(r')+\frac{\hbar^2}{m}\frac{4}{\rho^2}\nabla\cdot[K(r)^2\nabla\phi_p] -\frac{\hbar^2}{m}\frac{4}{\rho^2}\nabla\cdot K(r)\int d\vec{r}'\,K(|\vec{r}-\vec{r}'|)K(r')\nabla\phi_p(|\vec{r}-\vec{r}'|)+V_{\rm eff}(r)-V'_{\rm eff}(r)=0, \tag{3.16a}$$

where

$$V'_{\rm eff}=(4/\rho^2)K(r)^2V(r)-(8/\rho^2)K(r)\int d\vec{r}'\,K(|\vec{r}-\vec{r}'|)K(r')V(r') +(4/\rho^2)\int d\vec{r}'\,d\vec{r}''\,K(|\vec{r}-\vec{r}'|)K(|\vec{r}-\vec{r}''|)K(r')K(r'')V(|\vec{r}'-\vec{r}''|). \tag{3.16b}$$

It is possible to obtain an explicit solution for Eqs. (3.15). This is most easily seen from the momentum-space representation of Eqs. (3.5) and (3.6). These lead to the variational equation

$$2t(k)h(k)\tilde{\phi}(k)+h(k)^2v(k)=0, \tag{3.17}$$

$$\tilde{\phi}(k)=-h(k)v(k)/2t(k). \tag{3.18}$$

This result for $\tilde{\phi}$ provides important information about the behavior of $\phi(r)$ for $r\to\infty$. This is governed by the nature of the singularity of $\tilde{\phi}(k)$ at $k=0$. It is seen from (3.3) and (3.4) that $\tilde{\phi}(k)=O(k^{-1})$ for $k\to 0$, and hence that

$$\phi(r)=O(r^{-2}) \tag{3.19}$$

for $r\to\infty$.

The common factor of $h(k)$ in Eq. (3.17) indicates that the corresponding Eq. (3.15) can be reduced. The equation

$$-(\hbar^2/m)\nabla^2\phi+V(r)-(2/\rho)\int d\vec{r}\,' K(|\vec{r}-\vec{r}\,'|)^2V(r')=0 \tag{3.20}$$

is in fact equivalent to (3.15) as can readily be seen by multiplying (3.20) by

$$K_p(|\vec{R}-\vec{r}|)K_h(|\vec{R}-\vec{r}|)=\tfrac{1}{2}\rho\delta(\vec{R}-\vec{r})-K(|\vec{R}-\vec{r}|)^2$$

and integrating over $\vec{r}$.

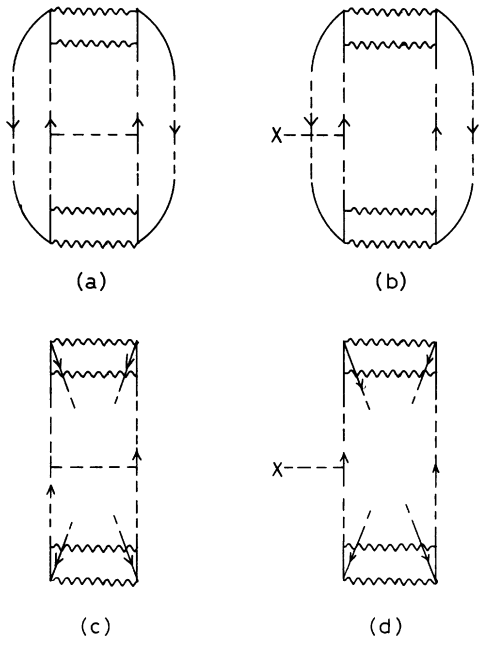

FIG. 5. Ladder diagrams containing two hole lines that are summed to give the ground-state energy to lowest order in the density. To obtain the results of Sec. IV, it is necessary to include also graphs in which the Hamiltonian vertices are on hole lines.

IV. SYSTEMS WITH STRONG REPULSIONS

The Jastrow-type wave function was originally introduced in an attempt to deal with systems in which the interparticle potentials have a hard core. In this case it is required that $\phi(r)=-\infty$ for $r<a$, the hard-core radius, and the series expansions that have been made fail. Therefore it is clearly necessary to sum over subsequences of terms in order to obtain a finite result, in the same way that ladder diagrams are summed in perturbation theory to lead to the reaction matrix. The problem of carrying out these partial summations to eliminate the singular function $\phi(r)$ has not been completely resolved. We will give here the results for lowest order in the density and the corresponding variational equations. These results are of considerable interest in themselves since the Jastrow-type wave function, involving only two-particle correlations, is essentially a low-density approximation.

The terms in the energy that are of lowest order in the density correspond to graphs with two hole lines as shown in Fig. 5. We recall also that $K_p(r)=\delta(\vec{r})-K_h(r)$; the second term is essentially equivalent to a hole line so that to lowest order we write $K_p(r)=\delta(\vec{r})$. This is the same as extending summations on particle momenta to the whole of momentum space, and will be called the closure approximation.

The graph of Fig. 5(a) calculated in configuration space can be seen to contribute

$$V_d=\Omega\frac{\rho^2}{4}\sum_{p,q}\frac{1}{p!q!}\int d\vec{r}\,\phi(r)^pV(r)\phi(r)^q$$

$$=\Omega\tfrac{1}{4}\rho^2\int d\vec{r}\,f(r)^2V(r), \tag{4.1}$$

in the closure approximation. The corresponding result from Fig. 5(b) for the kinetic energy is

$$T_d=\Omega(\hbar^2/m)(\rho^2/4)\int d\vec{r}\,|\nabla f(r)|^2. \tag{4.2}$$

The Euler-Lagrange equation for the correlation function f_a between particles with antiparallel spin can be derived from Eqs. (4.1) and (4.2) and is simply

$$-(\hbar^2/m)\nabla^2f_a+V(r)f_a=0. \tag{4.3}$$

This equation is to be solved with the boundary condition $f_a(\infty)=1$. These equations are not completely satisfactory, however, in that $f_a(r)-1=O(r^{-1})$ for $r\to\infty$ and this slow approach to zero gives rise to divergent integrals in higher-order correction terms. Also, the energy functional defined by (4.1) and (4.2) may be unbounded from below for sufficiently attractive potentials; this is known as the Emery difficulty.[7,8]

The results of Sec. III on the case of the weakly interacting system indicate that the difficulty with the asymptotic behavior of $f_a(r)$ stems from a failure to include terms in the energy that represent effects of the exclusion principle that are important at large r. The approximations that have been made in deriving Eqs. (4.1)–(4.3) correspond in the weakly interacting case to making the approximation $h(k)=\frac{1}{2}\rho$ in Eq. (3.17). It is seen from Eq. (3.3) that this is valid except for $k\to 0$. It is, however, the behavior of $\tilde{\phi}(k)$ at $k=0$ that determines the asymptotic behavior of $\phi(r)$. Equation (3.18) shows that approximating $h(k)$ by $\frac{1}{2}\rho$ changes the behavior of $\tilde{\phi}(k)$ from k^{-1} to k^{-2} at the origin, and hence changes the asymptotic behavior of $\phi(r)$ from $O(r^{-2})$ to $O(r^{-1})$.

This observation will be used as a guide for deriving more satisfactory results in the strongly interacting case. We again consider the graphs of Figs. 5(a) and 5(b), and make the closure approximation on the particle lines joining two ϕ vertices but retain the exact K_ρ for particle lines meeting a T or V vertex. It is also important to include the contribution of the diagram like Fig. 5(b) but with the kinetic-energy vertex on a hole line; in this approximation the diagrams with the potential-energy vertex on a hole line will be neglected, however. The reason for including the kinetic-energy vertex for a hole line is that although a graph containing such a vertex has an extra hole line, this does not give rise to an extra momentum sum over the Fermi sphere because of momentum conservation.

When these approximations are made, the sums over ladder diagrams can be carried out as in Eq. (4.1) and $\phi(r)$ replaced by $f(r)$. The kinetic-energy term is then the same as that given in Eq. (3.5) or (3.11) but with f replacing ϕ.

The potential-energy contribution can be written down in momentum representation as

$$V_d=\tfrac{1}{2}\rho^2\Omega v(0)+[2\Omega/(2\pi)^3]\int d\vec{k}\,h(k)^2v(k)\tilde{f}(k)$$
$$+[\Omega/(2\pi)^6]\int d\vec{k}\,d\vec{k}'\,F(\vec{k},\vec{k}')^2\tilde{f}(k)$$
$$\times v(|\vec{k}-\vec{k}'|)\tilde{f}(k'), \tag{4.4a}$$

$$F(\vec{k},\vec{k}')=[1/(2\pi)^3]\int d\vec{k}_1, \tag{4.4b}$$

where the integral defining $F(\vec{k},\vec{k}')$ is on $\vec{k}_1$ values such that $k_1<k_F$, $|\vec{k}_1+\vec{k}|>k_F$, and $|\vec{k}_1+\vec{k}'|>k_F$. In obtaining this result, it is necessary to isolate the graphs in which there is no ϕ vertex above (or below) the V vertex. The first term is from the graph in which there is no ϕ vertex, and the second term is from the graphs in which all the ϕ vertices are above or below the V vertex. The factor $\tilde{f}(k)$ is then the Fourier transform of $f(r)-1$.

The variational equation for f in momentum representation is now found to be

$$2h(k)t(k)\tilde{f}(k)+h(k)^2v(k)+[1/(2\pi)^3]$$
$$\times\int d\vec{k}'\,F(\vec{k},\vec{k}')^2v(|\vec{k}-\vec{k}'|)\tilde{f}(k')=0. \tag{4.5}$$

For $k'>2k_F$, it is seen that $F(\vec{k},\vec{k}')=h(k)$ as defined in Eq. (3.3). In the limit of low density, we can therefore approximate $F(\vec{k},\vec{k}')$ by $h(k)$ and Eq. (4.5) becomes

$$2t(k)\tilde{f}(k)+h(k)v(k)+[1/(2\pi)^3]h(k)$$
$$\times\int d\vec{k}'\,v(|\vec{k}-\vec{k}'|)\tilde{f}(k')=0. \tag{4.6}$$

In configuration space, Eq. (4.6) becomes

$$-(\hbar^2/m)\nabla^2 f+V(r)f(r)-(2/\rho)\int d\vec{r}'\,K(|\vec{r}-\vec{r}'|)^2$$
$$\times V(r')f(r')=0. \tag{4.7}$$

This equation is homogeneous, but should be solved with the inhomogeneous boundary conditions $|f(0)|<\infty$, $f(r)\to 1$ as $r\to\infty$. The integral over space of the second and third terms in Eq. (4.7) vanishes; this leads to the desired result, $f(r)-1=O(r^{-2})$.

Equation (4.4a) involves the quantities $v(k)$ which is meaningless for a potential with a hard core. On the other hand, Eq. (4.7) involves only the product $V(r)f(r)$ which is finite. In order to calculate the energy correction, it is necessary to express it in terms of the product $V(r)f(r)$; the result is given by Eqs. (3.11) and (3.12) with $f(r)$ substituted for $\phi(r)$ and $\frac{1}{2}V(r)f(r)$ substituted for $V(r)$. It can be noted that if Eq. (4.7) is multiplied by $f(R)[\frac{1}{2}\rho\delta(\vec{R}-\vec{r})-K(|\vec{R}-\vec{r}|)^2]$ and integrated over $\vec{R}$ and $\vec{r}$, it is possible, by using Green's theorem, to express the energy correction in terms of f' and the convolution of f and K^2, calculated at the core radius.

The contributions of the exchange diagrams of Fig. 6(c) and 6(d) can be treated in the same way. The approximation that has been made leads to replacing $\phi(r)$ by $f(r)$ and $V(r)$ by $\frac{1}{2}V(r)f(r)$ in the results for the exchange energies in the weakly interacting system given in Eqs. (3.13) and (3.14). The Euler-Lagrange equation for the correlation function between particles of parallel spin is obtained by substituting $f(r)$ for $\phi(r)$ and $V(r)f(r)$ for $V(r)$ in Eq. (3.16).

It can be seen without difficulty that the Fourier transform of the additional terms in (3.16) behaves like k^2 for $k\to 0$. This implies again that the Fourier transform of $f(r)-1$ behaves like k^{-1} and that $f(r)-1=O(r^{-2})$ for $r\to\infty$.

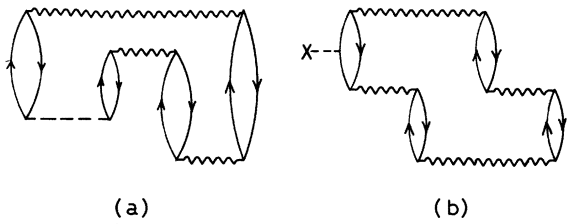

FIG. 6. Ring diagrams whose contributions to the potential and kinetic energies are summed to give Eq. (5.5).

V. APPLICATION TO THE ELECTRON-GAS PROBLEM

The formalism that has been developed can be applied to the electron-gas problem. This is a long-standing and extensively discussed problem, but the approach to be taken here does seem to be somewhat novel.

Previous calculations for the problem have been based on perturbation theory,[9] and modifications of perturbation theory that have come to be known as the dielectric formalism[10] and the random-phase approximation,[11] and on variational calculations.[12] Although these methods are superficially different, the important feature that must be taken into account in all of them is the effect of the polarization of the electron cloud or the screening at large distances. In the present calculation also, it is the correlations at large distances that are of primary importance.

The calculation reported here seems to be most similar to that of Gaskell[12] in that the results are similar. The method employed seems, however, to be much simpler, and the problem of computing the higher-order corrections seems to be more clearly defined in the present approach.

It is convenient to use units such that $m=\hbar=k_F=1$. In these units the natural density parameter is the Bohr radius a_0. Kinetic energies in Rydbergs are then given by $a_0^2k^2$ or $-a_0^2\nabla^2$, and $e^2=2a_0$ Ry. The density is the fixed number $(3\pi^2)^{-1}$ and the customary parameter r_s is $(9\pi/4)^{1/3}$. To transform to the usual units, in which $a_0=1$, we must put $a_0=(9\pi/4)^{1/3}/r_s$ in the results.

In this calculation, the effect of the exchange correction to the correlation function between electrons of parallel spin will be ignored, since these are of short range relative to the long-range Coulomb effects in which we are primarily interested.

The Coulomb interaction in momentum space is $v(k)=8\pi a_0k^{-2}$. At high density, the potential-energy terms are small compared with the kinetic-energy terms, and it is natural to attempt to apply the theory for the weakly interacting system. Equation (3.18) then gives

$$\begin{aligned}\tilde{\phi}(k)&=(3\pi/a_0)k^{-3}(1-\tfrac{1}{12}k^2), \quad k<2\\ &=(4\pi/a_0)k^{-4}. \quad k>2.\end{aligned} \tag{5.1}$$

This result is unsatisfactory because of the behavior of $\tilde{\phi}(k)$ for $k\to 0$. This leads to energy correction terms that are undefined.

This difficulty is apparently related to that observed by Gell-Mann and Brueckner which arises when the many-body perturbation theory is applied to the electron-gas problem. It arises in the present calculation from the failure to take into account sufficient terms in the energy to give a result that is bounded from below in the case of the Coulomb potential.

The direction indicated by Gell-Mann and Brueckner to avoid the low-momentum difficulty is to sum over the ring diagrams which produce the most divergent terms in the energy. A similar approach will be followed here, in which we will sum over diagrams of the form shown in Fig. 6.

The contribution of these graphs can be computed in momentum representation. We consider first the potential-energy term. The momentum transfer at each vertex is the same, so that the contribution of a graph with n vertices contains a factor $v(k)\tilde{\phi}(k)^n$. Each hole-particle line pair contributes a factor $h(k)$. The contribution of a ring diagram such as that in Fig. 6(a) is therefore seen to be

$$V_n=\frac{\Omega}{(2\pi)^3}A_n\int d\vec{k}\, v(k)\tilde{\phi}(k)^n h(k)^{n+1}, \tag{5.2}$$

where n is the number of vertices and A_n is a numerical factor determined as follows. There is a factor $(p!q!)^{-1}$ where p and q are the number of vertices preceding and following the V vertex. There are factors $1/2^{n+1}$ from the vertex factors and 2^n from the possibility of joining the hole-particle line pairs to either end of n vertices. There is a factor 2^{n+1} since each particle-hole pair can have spin-up or spin-down. There is also a factor $(p+q)!$ which is the number of ways of drawing the hole-particle pairs that keep the graph connected. Since

$$\sum\frac{(p+q)!}{p!q!}=2^n$$

we obtain $A_n=4^n$, $n=1,2,\ldots$.

The contribution of the kinetic-energy graphs as shown in Fig. 6(b) is

$$T_n=\frac{\Omega}{(2\pi)^3}B_n\int d\vec{k}\,\tilde{\phi}(k)^n h(k)^{n-1}t(k), \tag{5.3}$$

$$t(k)=(a_0^2/6\pi^2)k^2. \tag{5.4}$$

The numerical factor B_n contains factors 2^{-n} from the vertices, 2^n from the possibility of connecting

a hole-particle pair at either end of n vertices, a factor 2^n from the spins, and the factor $(p!q!)^{-1}$. There is also a factor $pq(p+q-2)!$ which arises since the kinetic-energy vertex can be connected to p vertices preceding it, q vertices following it, and the remaining hole-particle pairs can be placed in $(p+q-2)!$ ways that leave the graph connected overall. The sum on p and q for fixed n gives a factor 2^{n-2}. Therefore $B_n = 4^{n-1}$, $n = 2, 3, \ldots$.

It is seen that the sums on n for the ring diagrams are simply geometric, and that the energy term is given by

$$\frac{E}{N} = \frac{3}{8\pi}\int d\vec{k}\,\frac{4v(k)h^2(k)\tilde{\phi}(k) + 4h(k)t(k)\tilde{\phi}(k)^2}{1 - 4h(k)\tilde{\phi}(k)}\,. \tag{5.5}$$

The function $\tilde{\phi}$ that minimizes this integral is given by

$$\tilde{\phi}(k) = \frac{1}{4h(k)}\left[1 - \left(1 + \frac{4v(k)h(k)^2}{t(k)}\right)^{1/2}\right]. \tag{5.6}$$

The energy term corresponding to this choice of $\tilde{\phi}$ is

$$\begin{aligned}\frac{E}{N} &= \frac{3}{8\pi}\int d\vec{k}\,\frac{t(k)}{2h(k)}\left[\left(1 + \frac{4v(k)h(k)^2}{t(k)}\right)^{1/2} - 1 - \frac{2v(k)h(k)^2}{t(k)}\right] \\ &= a_0^2\int_0^2 k^3(1-\tfrac{1}{12}k^2)^{-1}\left[\left(1 + \frac{3}{\pi a_0}\frac{1}{k^2}(1-\tfrac{1}{12}k^2)^2\right)^{1/2} - 1 - \frac{3}{2\pi a_0}\frac{1}{k^2}(1-\tfrac{1}{12}k^2)^2\,dk\right] \\ &\quad + \tfrac{3}{4}a_0^2\int_2^\infty k^4\left[\left(1 + \frac{16}{3\pi a_0}\frac{1}{k^4}\right)^{1/2} - 1 - \frac{8}{3\pi a_0}\frac{1}{k^4}\right]dk.\end{aligned} \tag{5.7}$$

It is observed that the integrand behaves like k for small k. The singularity noticed in the lowest-order term is therefore completely removed by summing over the ring diagrams. It must be recognized, however, that $h(k)\tilde{\phi}(k) = O(k^{-1})$, so that the summation of the geometric series is purely formal.

The function $\phi(r)$ is given by

$$\phi(r) = \frac{1}{r}\int_0^2 \frac{\sin(kr)}{1-\frac{1}{12}k^2}\left[1 - \left(1 + \frac{3}{\pi a_0}\frac{1}{k^2}(1-\tfrac{1}{12}k^2)^2\right)^{1/2}\right]dk + \frac{3}{4}\frac{1}{r}\int_2^\infty k\sin(kr)\left[1 - \left(1 + \frac{16}{3\pi a_0}\frac{1}{k^4}\right)^{1/2}\right]dk. \tag{5.8}$$

The behavior of $\phi(r)$ for large r is governed by the singularity in $\tilde{\phi}(k)$ at $k=0$. It is seen that $\tilde{\phi}(k) = O(k^{-2})$ and hence that

$$\phi(r) \cong -\tfrac{1}{2}\pi(3/\pi a_0)^{1/2}(1/r) \tag{5.9}$$

for $r \to \infty$. This asymptotic behavior is not uniform, however; as a_0 becomes large, the range at which (5.9) becomes valid increases.

It will now be shown that the energy given by Eq. (5.7) behaves like $a\ln r_s + C$ at large density, or as $a_0 \to \infty$. It can be seen that the second term in Eq. (5.7) approaches

$$c_2 = -1/9\pi^2. \tag{5.10}$$

We introduce a parameter $\theta = 2\pi a_0/3$ and put $k^2 = 12x$ in the first term to obtain

$$\begin{aligned}c_1 &= 2\left(\frac{9\theta}{\pi}\right)^2\int_0^{1/3}\frac{x}{1-x}\left[\left(1 + \frac{1}{6\theta x}(1-x)^2\right)^{1/2} - 1 - \frac{(1-x)^2}{12\theta x}\right]dx \\ &= 2\left(\frac{9\theta}{\pi}\right)^2\left(A + \tfrac{1}{3} + \ln\tfrac{2}{3} - \frac{5}{216\theta}\right).\end{aligned} \tag{5.11}$$

The integral represented by A can be transformed to

$$\begin{aligned}A &= \frac{2}{\pi}\int_0^\infty dz\int_0^{1/3}\frac{x}{1-x}\left(1 + \frac{(1-x)^2}{6\theta x}\right)\left(z^2 + 1 + \frac{(1-x)^2}{6\theta x}\right)^{-1}dx \\ &= \frac{2}{\pi}\int_0^\infty dz\left\{\ln\tfrac{3}{2} - \tfrac{1}{3} - \frac{z^2}{1+z^2}\left[\ln\tfrac{3}{2} - \tfrac{1}{2}(2b+1)\ln(\tfrac{2}{3}b + \tfrac{10}{9}) + \frac{2b^2+b-1}{2(b^2-1)^{1/2}}\ln\left(\frac{b+\frac{1}{3}-(b^2-1)^{1/2}}{b-(b^2-1)^{1/2}}\,\frac{b+(b^2-1)^{1/2}}{b+\frac{1}{3}+(b^2-1)^{1/2}}\right)\right]\right\}\end{aligned}$$

where $b = 3\theta(1+z^2) - 1$.

As $\theta \to \infty$, $b \to \infty$ for all z in the range of integration. We therefore expand the integrand for large b; because of the factor θ^2 outside the integral it is necessary to determine the integrand to terms in b^{-2} to obtain the logarithmic term and the constant in the result. It is found that

$$A \cong \frac{2}{\pi}\int_0^\infty dz\left[\ln\tfrac{3}{2} - \frac{1}{3} - \frac{z^2}{1+z^2}\left(\ln\tfrac{3}{2} + \frac{1}{4b^2}\ln\tfrac{2}{3}b - \frac{1}{3} - \frac{5}{36b} - \frac{47}{648b^2}\right)\right].$$

The terms in b^{-1} and b^{-2} can now be expanded in $[3\theta(1+z^2)]^{-1}$ and the integration on z performed. When all the results are assembled it is found that the quadratic and linear terms in θ drop out and that

$$\frac{E}{N} \cong -\frac{9}{16\pi^2}\ln(\tfrac{4}{3}\pi a_0) - \frac{9}{8\pi^2}\ln 2 + \frac{31}{48\pi^2}$$
$$\cong 0.0570\ln r_s - 0.1324. \qquad (5.12)$$

The latter numerical result has also been given by Gaskell.[12] The corresponding result of Gell-Mann and Brueckner is

$$E/N \cong 0.0622\ln r_s - 0.142.$$

The lack of agreement between the coefficients of the $\ln r_s$ term indicates that the Jastrow wave function is incapable of giving an exact description of the system, since it appears that we have summed all the terms that contribute logarithmically.

VI. EXCHANGE CORRECTIONS AND RESULTS

We now consider the other lowest-order contributions to the energy corresponding to Figs. 4(c), 4(d), and 4(f) and given by Eqs. (3.13) and (3.14). The various integrals can be written down in spherical coordinates and are listed as follows as energies per particle.

$$e_1 = -(3/\pi)a_0^2\int_0^\infty j_1(r)^2\phi'(r)^2\,dr, \qquad (6.1)$$

$$e_2 = (2a_0^2/\pi^2)\int_0^\infty r\,dr\int_0^\infty r'\,dr'\,j_1(r)j_1(r') \times g_1(r,r')\phi'(r)\phi'(r'), \qquad (6.2)$$

$$e_3 = -(12/\pi)a_0\int_0^\infty (1/r)j_1(r)^2\phi(r)\,dr, \qquad (6.3)$$

$$e_4 = (48a_0/\pi^2)\int_0^\infty r\,dr\int_0^\infty dr'\,j_1(r)j_1(r') \times g_0(r,r')\phi(r), \qquad (6.4)$$

$$e_5 = -(48a_0/\pi^3)\int_0^\infty r^2 I(r)\phi(r)\,dr, \qquad (6.5)$$

where

$$g_l(r,r') = \int_0^1 p^2 j_l(pr)j_l(pr')\,dp$$
$$= \frac{1}{r^2 - r'^2}\left[r' j_l(r)j_{l-1}(r') - r j_l(r')j_{l-1}(r)\right], \qquad (6.6)$$

$$I(r) = 2\int_0^\infty dr_1\int_0^{r_1} r_2\,dr_2\,j_1(r_1)j_1(r_2) \times \sum_l [r_2/r_1]^l g_l(r,r_1)g_l(r,r_2). \qquad (6.7)$$

The five contributions to the exchange energy correction have been computed numerically for various values of r_s. Although the five terms vary considerably with r_s, the sum is essentially constant in the range considered, and is 0.039 ± 0.002 for $0.1 < r_s < 6.0$. This is close to the result 0.046 quoted by Gell-Mann and Brueckner for the analogous second-order exchange contribution in perturbation theory. The asymptotic behavior of the exchange contributions for $r_s \to 0$ has not, however, been ascertained so that no firm conclusion should be drawn from this result.

The result given by Eq. (5.7) for the correlation energy per particle has been calculated numerically for various values of the density. These results, together with the results of the exchange energy calculation are given in Table I. The result at highest density is given within 1% by the asymptotic expression of Eq. (5.12). The results are also plotted in Fig. 7 together with the results of three other recent calculations.

VII. CONCLUSION

We have presented a linked-cluster–type expansion which is suitable for Jastrow-type wave functions. In this expansion each term is explicitly proportional to the particle number or system

TABLE I. Correlation energies per particle (in Ry). Δe_r is the contribution of the ring diagrams, Δe_{ex} is the exchange contribution and Δe_{corr} is the net result.

r_s	Δe_r	Δe_{ex}	Δe_{corr}
0.096	−0.269	0.040	−0.229
0.152	−0.244	0.040	−0.203
0.241	−0.219	0.041	−0.178
0.382	−0.195	0.041	−0.154
0.605	−0.171	0.041	−0.130
0.960	−0.149	0.041	−0.108
1.52	−0.128	0.041	−0.087
2.41	−0.108	0.040	−0.068
3.82	−0.090	0.039	−0.051
6.05	−0.074	0.037	−0.037

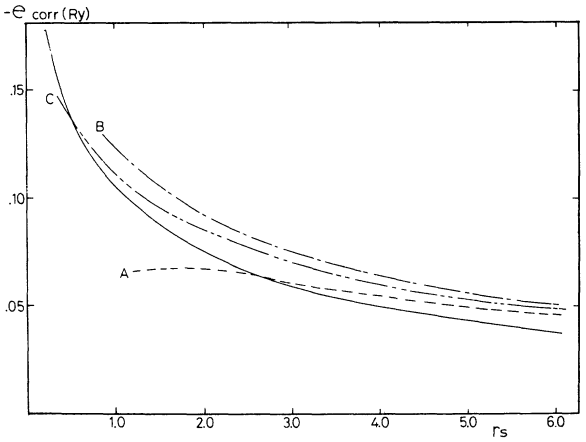

FIG. 7. Correlation energy as a function of r_s, including the exchange energy (solid curve). The other curves A, B, and C are the results of Lee and Ree (Ref. 12), Singwi *et al.* (Ref. 10) and Pokrant and Stevens (Ref. 12), respectively.

volume for uniform systems. This analysis can then be applied to make variational calculations for many-body problems, although such a procedure cannot provide rigorous upper bounds since it is not possible to sum the series for the energy beyond the first few terms.

The result has been applied to calculate the lowest-order corrections to the interaction energy in the case of a weakly interacting system and the variational equations for the correlation function have been obtained. It was shown in this case that the correlation function differs from unity by a term of order r^{-2} for large r.

The problem of a system interacting via potentials with a strong repulsive core has not been fully worked out. It has been seen that the results to lowest order in the density resemble those for the weakly interacting system and the variational equations for the correlation function have been determined. These resemble the Schrödinger equation, and reduce to the equations for the weakly interacting system under the approximation $f(r)=1$ in the potential-energy term.

A systematic approach to the problem of calculating higher-order correction terms to the low-density approximation has not so far been found. There are several problems that may be noted. The first of these is the complete elimination of the ϕ vertices in favor of f vertices, as has been done in the case of the two hole-line graphs. This problem must apparently be resolved by summing contributions of graphs with a fixed number of particle lines running through them connected by arbitrary numbers of ϕ vertices, permuted in all possible ways. The sum over permutations has the effect of replacing factors such as $[(p_1+p_2+\cdots p_n)!]^{-1}$ by $(p_1!p_2!\cdots p_n!)^{-1}$ and permits the elimination of ϕ vertices.

There are, however, a number of difficulties in connection with this. The first of these is to take into account corrections for the closure approximation made in summing over particle states. It appears that it is impossible to eliminate $\phi(r)$ completely from these correction terms but that it appears in a innocuous way, i.e., in a denominator, after the particle sums have been carried out. It may be that other cluster expansions for the fermion problem, in terms of the function f alone, are of necessity slowly convergent, because of the apparent necessity of the occurrence of the slowly convergent $\ln f$ in the expansion.

A second problem is to take into account systematically other corrections such as those of the exclusion principle violating diagrams. It seems that this problem is related to a third, the general question of convergence of the integrals arising in the calculation. Some of the integrals arising from diagrams with more than two particle lines running through them are divergent, but the divergences appear to be removed by the exclusion principle violating diagrams. The fact that $f(\vec{r})-1=O(r^{-2})$ is also important in this connection. It is hoped that these questions will be clarified in a future article.

The results given for the application to the electron-gas problem must be regarded as somewhat preliminary. There are a number of ways in which the result can be improved. One of these is to include the exchange energy in the variational calculation by considering different correlation functions between electrons of parallel and antiparallel spin. Another is to include higher-order contributions, perhaps of the ladder type as discussed in Sec. IV. It might be hoped that contributions could be isolated so that the result would approximate the correct asymptotic behavior at low densities as well as at large densities.

As was mentioned the results obtained here are similar to those of Gaskell. It appears, though, that the approach is quite different, and that the approach introduced here has the advantage of permitting systematic calculations of the higher-order corrections. For example, the exchange correction could be calculated in a straightforward manner. The method followed here may also be of interest in illuminating the correspondence between the variational method and the perturbation theory of Gell-Mann and Brueckner.

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