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Variational Calculation of the Electron-Gas Correlation Energy*

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The ground-state correlation energy of the electron gas is calculated in the region of intermediate densities using the variational method of Becker, Broyles, and Dunn for two trial wave functions. Each trial function is taken to be a product of two factors, one factor being the ground-state wave function for the ideal gas of spin-1/2 particles and the other being a product of pair functions in the relative coordinates of the electrons. In one trial function a single pair function is used; in the other, the pair functions between parallel and antiparallel spins are allowed to differ. The pair functions are parametrized and approximations to the energy minimized. The three-particle correlation functions appearing in the kinetic energy are replaced by either the Kirkwood superposition approximation (KSA) or the convolution approximation (CA) to give two approximate energy functionals for each wave function. The ideal-gas N-particle probability density is approximated by a Boltzmann factor with an effective pair potential. This effective potential is obtained by inverting the hypernetted chain equation for the known pair-correlation function of the ideal Fermi gas. The pair-correlation functions for the interacting system are then calculated by means of the hypernetted-chain equation. The CA correlation energies join smoothly with both the high- and low-density expansions. The CA and KSA correlation energies differ by less than 4% everywhere in the intermediate-density region. The pair-correlation functions exhibit generally reasonable physical behavior.

I. INTRODUCTION

Since the pioneering work of Wigner[1] many studies have been devoted to the problem of calculating the ground-state correlation energy of the electron gas. The correlation energy is defined by

$$\epsilon_c = \epsilon - \epsilon_{\mathrm{HF}}\,, \tag{1.1}$$

where ϵ is the ground-state energy per electron and ϵ_{HF} is the familiar Hartree-Fock approximation to ϵ given by[1,2]

$$\epsilon_{\mathrm{HF}} = \epsilon_I + \epsilon_x\,, \tag{1.2}$$

with

$$\epsilon_I = \tfrac{3}{5}\epsilon_F\,, \quad \epsilon_x = -3e^2k_F/4\pi\,,$$

where $\epsilon_F = \hbar^2k_F^2/2m$, $k_F = (3\pi^2\rho)^{1/3}$, and ρ denotes the mean density of electrons. In conventional units one has

$$\epsilon_{\mathrm{HF}} = 2.21/r_s^2 - 0.916/r_s\ \mathrm{Ry}\,,$$

where r_s is the ion-sphere radius (the radius of a sphere of volume $1/\rho$) in units of the Bohr radius.

Asymptotic expansions of ϵ_c are known in the limits of very high[2-4] and very low[5] densities. These expansions are presumed to give good approximations to ϵ_c in the regions $r_s \lesssim 0.5$ and $r_s \gtrsim 20$. By interpolating between the high- and low-density expansions Carr[5] and Isihara and Montroll[6] have obtained estimates of ϵ_c in the region of intermediate densities. Various attempts[7-16] to extend the high-density perturbation theories into the region of metallic densities ($2 \lesssim r_s \lesssim 6$) have been made. Paralleling these studies there have appeared several variational methods,[17-21] all based on the trial wave function

$$\Psi_{\underline{\sigma}} = D_{\underline{\sigma}} \exp\left(-\tfrac{1}{2} \sum_{i<j} u(r_{ij})\right), \tag{1.3}$$

where $D_{\underline{\sigma}}$ is the ground-state energy eigenfunction of an ideal Fermi gas written as a determinant of single-particle momentum-spin states and the subscript $\underline{\sigma}$ denotes the set of spin coordinates.

The purpose of the present work is to obtain correlation energies and spin-averaged correlation functions $g(r)$ in the range $0.5 \lesssim r_s \lesssim 20$ using the trial function in Eq. (1.3) and a modification of the variational calculation of Becker, Broyles, and Dunn[18]: a suitable parametrization of $u(r)$ is chosen and approximate forms of the associated mean-energy functional $\epsilon[u]$ are minimized by variation. Then, using a simple generalization of the above trial function, spin-spin correlation functions are calculated at metallic densities.

The choice of the second trial function rests on noting that because of the absence of spin-dependent terms in the Hamiltonian, electrons with opposite spin components are distinguishable and, hence, may be treated as different particles, say, types α (spin up) and β (spin down). To satisfy the Pauli principle, the wave function must be antisymmetrized with respect to exchange of coordinates of electrons with the same spin component. A trial function appropriate to this view is

$$\Psi = D_\alpha D_\beta \exp\left(-\tfrac{1}{2} \sum_{i<j} u_{ab}(r_{ij})\right), \tag{1.4}$$

where $u_{ab}(r_{ij})$ is a pair function between a type-a particle at $\vec{r}_i$ and a type-b particle at $\vec{r}_j$ and $D_\alpha D_\beta$ is the ideal-gas ground-state energy eigenfunction written as a product of determinants, each composed of the single-particle states of electrons with one spin component. Since the numbers of spin-up and spin-down electrons are assumed to be equal, it follows by symmetry that the functional equivalencies $D_\alpha \equiv D_\beta$ and $u_{\alpha\alpha} \equiv u_{\beta\beta}$ hold. Parametrizations of $u_{\alpha\alpha}(r)$ and $u_{\alpha\beta}(r)$ are chosen and the associated mean energy functional $\epsilon[u_{\alpha\alpha}, u_{\alpha\beta}]$ is minimized, yielding the spin-spin correlation functions $g_{\alpha\alpha}(r)$ and $g_{\alpha\beta}(r)$.

It is convenient to refer to the functionals $\epsilon[u]$ and $\epsilon[u_{\alpha\alpha}, u_{\alpha\beta}]$ as one- and two-component energy functionals, respectively. Of course, if one sets $u_{\alpha\alpha} \equiv u_{\alpha\beta} \equiv u$, then $\epsilon[u_{\alpha\alpha}, u_{\alpha\beta}] = \epsilon[u]$. We begin by introducing approximations to $\epsilon[u]$, since generalization of these approximations to $\epsilon[u_{\alpha\alpha}, u_{\alpha\beta}]$ is straightforward.

Dunn and Springer have developed a closely related method for treating this problem in which the ground state is approximated as in Eq. (1.3) or (1.4) and an approximation to the Schrödinger equation is solved for $u(r)$ or for $u_{\alpha\alpha}(r)$ and $u_{\alpha\beta}(r)$.[22] There exists a generalization of this method to nonzero temperatures in which the Slater sum is approximated by a Boltzmann factor with an effective pair potential.[23,24] An extension of the latter technique is currently under investigation to approximate the Slater sum and thermodynamic properties of a fluid by treating it as a mixture of nuclei and electrons with Coulomb interactions.[23,25-27]

II. ONE-COMPONENT ENERGY FUNCTIONAL

We consider a completely degenerate system of N electrons contained in a cube of volume Ω with a neutralizing uniform positive background. The Hamiltonian operator for this system is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(\vec{r}_{ij}), \tag{2.1}$$

where the electron-electron interaction (including the background) is

$$v(\vec{r}) = \Omega^{-1} \sum_{\vec{k} \neq 0} \frac{4\pi e^2}{k^2} e^{i\vec{k}\cdot\vec{r}} \tag{2.2}$$

and the usual periodic boundary conditions have been imposed. It is convenient to choose our unit of length to be k_F^{-1} so that henceforth we have $k_F = 1$ and $\rho = 1/3\pi^2$. Then $(\hbar^2/2m)\nabla^2$ is replaced by $\epsilon_F \nabla^2$.

For the trial function of Eq. (1.3) it is straightforward to show that the mean kinetic energy per particle can be written in the form

$$\epsilon_{\text{kin}} = \epsilon_I + \tfrac{1}{4}\epsilon_F Z_N^{-1} \int \sum_{\underline{\sigma}} |\Psi_{\underline{\sigma}}|^2 (\nabla_1 A)^2 d^{3N}r, \tag{2.3a}$$

where

$$Z_N = \int \sum_{\underline{\sigma}} |\Psi_{\underline{\sigma}}|^2 d^{3N}r, \tag{2.3b}$$

$$\sum_{\underline{\sigma}} |\Psi_{\underline{\sigma}}|^2 = \sum_{\underline{\sigma}} |D_{\underline{\sigma}}|^2 e^{-A}, \tag{2.3c}$$

$$A = \sum_{i<j} u(r_{ij}). \tag{2.3d}$$

Defining the n-body correlation function by

$$g^{(n)}(1,\ldots,n)=\frac{N!}{(N-n)!Z_N\rho^n}\int\sum_{\underline{Q}}|\Psi_{\underline{Q}}|^2 d(n+1)\cdots dN\,, \tag{2.4}$$

Eq. (2.3a) is easily reduced to

$$\epsilon_{\text{kin}}=\epsilon_I+\epsilon^{(2)}+\epsilon^{(3)}\,, \tag{2.5a}$$

where

$$\epsilon^{(2)}=\tfrac{1}{4}\epsilon_F\rho\int d^3r\,[\nabla u(r)]^2 g(r)\,, \tag{2.5b}$$

$$\epsilon^{(3)}=\tfrac{1}{4}\epsilon_F\rho^2\int d^3r_{12}\,d^3r_{13}\,\nabla_1 u(r_{12})\cdot\nabla_1 u(r_{13})g^{(3)}(1,2,3)\,, \tag{2.5c}$$

and we have set $g\equiv g^{(2)}$.

In the thermodynamic limit, i.e., $N\rightarrow\infty$ and $\Omega\rightarrow\infty$ with $\rho=N/\Omega$ held constant, one finds for ϵ_{int}, the mean interaction energy per particle,

$$\epsilon_{\text{int}}=\tfrac{1}{2}\rho\int d^3r(e^2/r)G(r)\,, \tag{2.6}$$

where

$$G(r)=g(r)-1 \tag{2.7}$$

is a short-ranged function. If we define the structure factor by

$$S(k)=1+\rho\tilde{G}(k)\,, \tag{2.8}$$

where $\tilde{G}(k)$ is the Fourier transform of $G(r)$, i.e.,

$$\tilde{G}(k)=\int d^3r\,e^{i\vec{k}\cdot\vec{r}}G(r)\,,$$

then Eq. (2.6) can be written in the form

$$\epsilon_{\text{int}}=\frac{1}{2}\int\frac{d^3k}{(2\pi)^3}\frac{4\pi e^2}{k^2}[S(k)-1]\,. \tag{2.9}$$

Throughout the present work, unless otherwise indicated, a tilde will be used to denote the Fourier transform of a function.

Our problem is to minimize the functional

$$\epsilon[u]=\epsilon_{\text{kin}}[u]+\epsilon_{\text{int}}[u] \tag{2.10}$$

by varying $u(r)$. Now the condition that $u(r)$ be an extremal of $\epsilon[u]$ is that it satisfies the Euler-Lagrange equation

$$\delta\epsilon[u]/\delta u(\vec{r})=0. \tag{2.11}$$

Studies[17,28] of this equation under various approximations show that for large r, in agreement with Bohm and Pines,[29]

$$u(r)\sim a/r\,, \tag{2.12a}$$

where

$$a=e^2/\tfrac{1}{2}\hbar\omega_{pl} \tag{2.12b}$$

and ω_{pl} is the plasma frequency,

$$\omega_{pl}=(4\pi\rho e^2/m)^{1/2}\,. \tag{2.12c}$$

It is also known that $u(0)$ is finite because of the quantum tunneling effect. Hence, following Becker *et al.*, we choose the one-parameter form

$$u(r)=(a/r)(1-e^{-br})\,, \tag{2.13}$$

with a given by Eq. (2.12b), and vary b to minimize $\epsilon[u]$. Actually, Becker *et al.* vary both a and b, but at $r_s=3.39$ and 5.65 they find values of a very close to those given by Eq. (2.12b). As is seen below, Eq. (2.12) ensures that our structure factor have the small-k behavior given by Pines and Nozières,[30] i.e.,

$$S(k)\rightarrow\hbar k^2/2m\omega_{pl}\quad\text{as } k\rightarrow 0\,. \tag{2.14}$$

III. APPROXIMATIONS TO $\epsilon[u]$

The expression for $\epsilon_{\text{kin}}[u]$ in Eq. (2.5) contains a three-body correlation function $g^{(3)}$. Starting from the same trial function the random-phase approximation (RPA)[29] of Bohm and Pines has been applied to obtain a kinetic-energy functional $\epsilon_{\text{kin}}^{\text{RPA}}[u]$[17,18] free of this difficulty, but the RPA may be used only at high densities. To eliminate $g^{(3)}$ from $\epsilon_{\text{kin}}[u]$ we use two approximations, each expressing $g^{(3)}$ as a functional of g: the Kirkwood superposition approximation (KSA),[31] first applied to this problem by Becker *et al.*, and the convolution approximation (CA).[32] In this way we obtain approximate kinetic-energy functionals $\epsilon_{\text{kin}}^{\text{KSA}}[u]$ and $\epsilon_{\text{kin}}^{\text{CA}}[u]$, which can easily be calculated given u and $g[u]$. Both $\epsilon_{\text{kin}}^{\text{KSA}}$ and $\epsilon_{\text{kin}}^{\text{CA}}$ can be written $\epsilon_{\text{kin}}^{\text{RPA}}$ plus correction terms. Comparison of the minimum values of the associated total-energy functionals $\epsilon^{\text{KSA}}[u]$ and $\epsilon^{\text{CA}}[u]$ gives an estimate of the error introduced into the energy by approximating $g^{(3)}$.

To enable us to calculate $g[u]$ we follow the work of Lado[33]: the ideal-gas configurational probability density is approximated by a Boltzmann factor with an ideal-gas effective pair potential $u_I(r)$. Hence by Eq. (2.3c) the probability density $\sum_{\underline{Q}}|\Psi_{\underline{Q}}|^2$ can be written approximately as a Boltzmann factor with an effective pair potential $u_t(r)=u(r)+u_I(r)$. An approximate integral equation from the classical pair theory of fluids can then be used to calculate $g[u]$ for a given $u(r)$.

A. Approximations to $g^{(3)}$ and $\epsilon_{\text{kin}}[u]$

If we denote the Fourier transform of $u(r)$ by $\phi(k)$ and use $g(r)=1+G(r)$, then Eq. (2.5b) can be rewritten

$$\epsilon^{(2)}=\epsilon_1^{(2)}+\epsilon_2^{(2)}\,, \tag{3.1a}$$

where

$$\epsilon_1^{(2)}=\tfrac{1}{4}\epsilon_F\rho\int\frac{d^3k}{(2\pi)^3}k^2\phi^2(k) \tag{3.1b}$$

and

$$\epsilon_2^{(2)} = \tfrac{1}{4}\epsilon_F \rho \int d^3r\,[u'(r)]^2 G(r) . \tag{3.1c}$$

Defining the function $\Delta g^{(3)}(1,2,3)$ by

$$g^{(3)}(1,2,3) = 1 + G(r_{12}) + G(r_{13}) + G(r_{23}) + G(r_{12})G(r_{13}) + G(r_{12})G(r_{23}) + G(r_{13})G(r_{23}) + \Delta g^{(3)}(1,2,3) , \tag{3.2}$$

Eq. (2.5c) can be written in the form

$$\epsilon^{(3)} = \tfrac{1}{4}\epsilon_F \rho^2 \int d^3r_{12}\, d^3r_{13}\, \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) \times [G(r_{23}) + 2G(r_{12})G(r_{23}) + \Delta g^{(3)}(1,2,3)] . \tag{3.3}$$

If we define the function

$$P(r) = [u'(r)/r]G(r) , \tag{3.4}$$

then Eq. (3.3) can be put in the form

$$\epsilon^{(3)} = \epsilon_1^{(3)} + \epsilon_2^{(3)} + \epsilon_3^{(3)} , \tag{3.5a}$$

where

$$\epsilon_1^{(3)} = \tfrac{1}{4}\epsilon_F \rho^2 \int \frac{d^3k}{(2\pi)^3}\, k^2 \phi^2(k) \tilde{G}(k) , \tag{3.5b}$$

$$\epsilon_2^{(3)} = \tfrac{1}{2}\epsilon_F \rho^2 \int \frac{d^3k}{(2\pi)^3}\, k \phi(k) \tilde{G}(k) \tilde{P}'(k) , \tag{3.5c}$$

$$\epsilon_3^{(3)} = \tfrac{1}{4}\epsilon_F \rho^2 \int d^3r_{12} d^3r_{13} \nabla_1 u(r_{12}) \cdot \nabla_1 u(r_{13}) \Delta g^{(3)}(1,2,3) . \tag{3.5d}$$

In Eq. (3.5c) we have written $\tilde{P}'(k)$ for $d\tilde{P}(k)/dk$.

Now it is well known that for our trial function the RPA gives

$$\epsilon_{\text{kin}}^{\text{RPA}} = \epsilon_I + \tfrac{1}{4}\epsilon_F \rho \int \frac{d^3k}{(2\pi)^3}\, k^2 \phi^2(k) S(k) . \tag{3.6}$$

But from Eqs. (3.1b) and (3.5b) we have

$$\epsilon_{\text{kin}}^{\text{RPA}} = \epsilon_I + \epsilon_1^{(2)} + \epsilon_1^{(3)} , \tag{3.7}$$

so that

$$\epsilon_{\text{kin}} = \epsilon_{\text{kin}}^{\text{RPA}} + \epsilon_2^{(2)} + \epsilon_2^{(3)} + \epsilon_3^{(3)} . \tag{3.8}$$

At this point our approximations to ϵ_{kin} appear as approximations to $\epsilon_3^{(3)}$. The integral in Eq. (3.5d) can be reduced to tractable forms using the Kirkwood superposition and the convolution approximations to $\Delta g^{(3)}(1,2,3)$ which give, respectively,[31,32]

$$\Delta g^{(3)}_{\text{KSA}}(1,2,3) = G(r_{12})G(r_{13})G(r_{23}) \tag{3.9}$$

and

$$\Delta g^{(3)}_{\text{CA}}(1,2,3) = \rho \int d4\, G(r_{14})G(r_{24})G(r_{34}) . \tag{3.10}$$

Substituting $\Delta g^{(3)}_{\text{KSA}}$ and $\Delta g^{(3)}_{\text{CA}}$ into Eq. (3.5d), one can show that $\epsilon_3^{(3)}$ is given within the KSA by

$$\epsilon_3^{(3)\,\text{KSA}} = \tfrac{1}{4}\epsilon_F \rho^2 \int \frac{d^3k}{(2\pi)^3}\, \tilde{G}(k) [\tilde{P}'(k)]^2 \tag{3.11}$$

and within the CA by

$$\epsilon_3^{(3)\,\text{CA}} = \tfrac{1}{4}\epsilon_F \rho \int d^3r G(r) [F'(r)]^2 , \tag{3.12}$$

where $F(r)$ is defined by

$$\tilde{F}(k) = \rho \phi(k) \tilde{G}(k) . \tag{3.13}$$

We can use Eq. (3.8) with Eqs. (3.11) and (3.12) to calculate $\epsilon_{\text{kin}}^{\text{KSA}}$ and $\epsilon_{\text{kin}}^{\text{CA}}$. However, if we note that $\epsilon_2^{(3)}$ is also given by

$$\epsilon_2^{(3)} = \tfrac{1}{2}\epsilon_F \rho \int d^3r\, G(r) u'(r) F'(r), \tag{3.14}$$

then for the CA we have the simpler form

$$\epsilon_{\text{kin}}^{\text{CA}} = \epsilon_{\text{kin}}^{\text{RPA}} + \tfrac{1}{4}\epsilon_F \rho \int d^3r\, G(r) [Q'(r)]^2 , \tag{3.15}$$

where $Q(r) = u(r) + F(r)$ or, by Eq. (3.13),

$$\tilde{Q}(k) = \phi(k) S(k) . \tag{3.16}$$

B. Calculation of $g[u]$

If the spin-averaged ideal-gas probability density is approximated as[33,34]

$$\sum_{\underline{\sigma}} |D_{\underline{\sigma}}|^2 \cong \exp\Big(-\sum_{i<j} u_I(r_{ij})\Big) \Big/ \int d^{3N}r \exp\Big(\sum_{i<j} u_I(r_{ij})\Big) , \tag{3.17}$$

then by Eqs. (2.3c) and (2.4) the pair correlation function is

$$g(r_{12}) = N(N-1)\rho^{-2} \int d3 \cdots dN \times \exp\Big(-\sum_{i<j} u_t(r_{ij})\Big) \Big/ \int d^{3N}r \exp\Big(-\sum_{i<j} u_t(r_{ij})\Big) , \tag{3.18}$$

where

$$u_t(r) = u(r) + u_I(r) . \tag{3.19}$$

We return to the problem of calculating u_I after discussing how best to perform the multidimensional integration in Eq. (3.18). Here we simply note that $u_I(r)$ is bounded everywhere and is of shorter range than $u(r)$. Thus $u(r)$ and $u_t(r)$ have the same asymptotic behavior given in Eq. (2.12).

Now it is shown in the classical theory of fluids that Eq. (3.18) can be developed into a diagrammatic expansion of the form[35,36]

$$g(r) = \exp[-u_t(r) + N(r) + B(r)] , \tag{3.20}$$

where $N(r)$ denotes the sum of the nodal diagrams and $B(r)$ the sum of the bridge (or elementary) diagrams. Introducing the direct correlation function C by

$$C(r) \equiv G(r) - N(r) , \tag{3.21}$$

it can further be shown that[36]

$$\tilde{N}(k)=\rho[\tilde{C}(k)]^2/[1-\rho\tilde{C}(k)]\,. \tag{3.22}$$

If the function $B(r)$ were known, then Eqs. (3.20)–(3.22) could be solved for the exact $g(r)$. But the only known representation of $B(r)$ is a formal infinite series. From Eqs. (3.21) and (3.22) we get

$$S(k)=1/[1-\rho\tilde{C}(k)]\,, \tag{3.23}$$

which is the Fourier transform of the Ornstein-Zernicke integral equation.[37,38]

To calculate g we use the hypernetted-chain (HNC) approximation[36,38–44] in which one neglects $B(r)$ in Eq. (3.20), i.e.,

$$g(r)=\exp[-u_t(r)+N(r)]\,. \tag{3.24}$$

The motivation for this choice is a recent study of the classical electron gas[22,45] in which it was found that the pair correlation functions obtained from the HNC equation are in remarkably close agreement with the Monte Carlo (MC) results of Brush, Sahlin, and Teller[46] over a large range of temperatures and densities. In these calculations the state of the system is described by the dimensionless parameter $\Gamma=e^2/kTr_0$, where k is Boltzmann's constant, T the absolute temperature, and r_0 the ion-sphere radius. In the range $1\lesssim\Gamma\lesssim 10$ the HNC and MC correlation functions are in excellent quantitative agreement and the potential energies agree to within about 1%.[47] By way of comparison, numerical calculations using the Percus-Yevick approximation[48] are in much greater disagreement with the MC results. For example, at $\Gamma=2.5$ the Percus-Yevick and MC potential energies differ by about 8%.[49]

We shall assume that the HNC equation yields a $g(r)$ for the quantum system with an accuracy comparable to that for a corresponding classical electron gas of the same density but at an effective temperature or, equivalently, an effective Γ. The latter is obtained by matching $u_t(r)$ and e^2/kTr at large r, i.e., by Eq. (2.12),

$$\Gamma=e^2/\tfrac{1}{2}\hbar\omega_{pl}r_0=(\tfrac{4}{3}r_s)^{1/2}\,. \tag{3.25}$$

Hence, for the range of densities $1\lesssim r_s\lesssim 20$ in the quantum system, the corresponding classical system falls in the range $1\lesssim\Gamma\lesssim 5$ within the region where the HNC equation is known to give very accurate correlation functions. Thus, our basic assumption is that the removal of the singularity at the origin in going from the classical Coulomb potential to the corresponding quantum effective potential does not adversely affect the accuracy of the HNC approximation.

The n-body correlation function of a completely degenerate ideal Fermi gas can be calculated by replacing $\Psi_{\underline{\sigma}}$ by $D_{\underline{\sigma}}$ in Eq. (2.4) and performing the integration. For $n=2$ one obtains the well-known result

$$g_I(r)=1-\tfrac{9}{2}[j_1(r)/r]^2\,, \tag{3.26}$$

where $j_1(r)=(\sin r-r\cos r)/r^2$. Note that $g_I(0)=\frac{1}{2}$. The ideal-gas structure factor is given by

$$\begin{aligned} S_I(k)&=\tfrac{3}{4}k-\tfrac{1}{16}k^3, \quad k\leqslant 2\\ &=1\,, \qquad\qquad k>2\,, \end{aligned} \tag{3.27}$$

where $S_I(k)=1+\tilde{G}(k)$ and $\tilde{G}_I(k)$ is the Fourier transform of $G_I(r)=g_I(r)-1$. Since $u_I(r)$ is shown in Ref. 34 to be insensitive to several methods used to obtain it, we invert the HNC equation using the exact $g_I(r)$ to obtain

$$u_I(r)=-C_I(r)+G_I(r)-\ln g_I(r)\,, \tag{3.28}$$

where

$$\tilde{C}_I(k)=\rho^{-1}\{1-[S_I(k)]^{-1}\}\,. \tag{3.29}$$

We find that $C_I(r)\sim -2r^{-2}+O(r^{-4})$ as $r\rightarrow\infty$ and, hence, that $u_I(r)\sim 2r^{-2}+O(r^{-4})$. We note further that $u_I(0)=1.06$ and that $u_I(r)$ is found numerically to be a strictly decreasing function.

Within the HNC approximation, Eq. (3.24), the short-range behavior of $G(r)$ implies that $N(r)$ has the same long-range behavior as $u_t(r)$ and, by Eq. (3.21), that $C(r)$ has the long-range behavior of $-u_t(r)$. We decompose $u_t(r)$ into long- and short-range parts by setting

$$u_t(r)=u_{lr}(r)+u_{sr}(r)\,, \tag{3.30a}$$

where

$$u_{lr}(r)=u(r)-C_I(r) \tag{3.30b}$$

and

$$u_{sr}(r)=G_I(r)-\ln g_I(r)\,. \tag{3.30c}$$

Since $G_I(r)\sim O(r^{-4})$, we see that $u_{sr}(r)\sim O(r^{-8})$ as $r\rightarrow\infty$. Defining the short-range functions $C_{sr}(r)$ and $N_{sr}(r)$ by

$$C_{sr}(r)\equiv C(r)+u_{lr}(r) \tag{3.31}$$

and

$$N_{sr}(r)\equiv N(r)-u_{lr}(r)\,, \tag{3.32}$$

we have the HNC equation in a form convenient for numerical solution:

$$C_{sr}(r)=e^{-u_{sr}(r)+N_{sr}(r)}-1-N_{sr}(r)\,, \tag{3.33a}$$

with

$$\tilde{N}_{sr}(k)=\frac{\rho[\tilde{C}(k)]^2}{1-\rho\tilde{C}(k)}-\tilde{u}_{lr}(k)\,, \tag{3.33b}$$

where

$$\tilde{C}(k)=\tilde{C}_{sr}(k)-\tilde{u}_{lr}(k)\,, \tag{3.34}$$

$$\tilde{u}_{lr}(k)=\phi(k)-\tilde{C}_I(k)\,, \tag{3.35}$$

and, for our parametrization,

$$\phi(k) = 4\pi a b^2/k^2(k^2+b^2)\,. \qquad (3.36)$$

Having solved Eqs. (3.33) we have $G(r) = C_{sr}(r) + N_{sr}(r)$ and $\tilde{G}(k) = \tilde{C}_{sr}(k) + \tilde{N}_{sr}(k)$.

Equations (3.33) were solved by iteration starting from the initial guess $C_{sr}(r) \equiv 0$ and computing successively $\tilde{C}_{sr}(k), \tilde{N}_{sr}(k), N_{sr}(r), C_{sr}(r)$ until the change in $N_{sr}(r)$ between consecutive iterations was on the order of or less than 1 part in 10^7. Although this process was rapidly convergent, the total number of iterations required was decreased by using Broyles's extrapolation method[50] on $N_{sr}(r)$.

The numerical Fourier transforms were calculated using Filon's method.[51] All calculations were performed to a precision of 15 digits using 512 points and the increment $\Delta r = 0.05(k_F^{-1})$. To check our numerical accuracy, we carried out range-increment tests at two widely separated densities. The range-increment test consisted of going to 1024 points and repeating the entire calculation with each of the increments $\Delta r = 0.05(k_F^{-1})$ and $\Delta r = 0.025(k_F^{-1})$. Our results were insensitive to this test.

Eliminating $\tilde{C}$ from Eq. (3.23) using Eqs. (3.34), (3.35), and (3.29) we obtain for the HNC structure factor

$$S(k) = \frac{S_I(k)}{1+\rho[\phi(k) - \tilde{C}_{sr}(k)]S_I(k)}\,. \qquad (3.37)$$

Our numerical solution has the large-r form

$$G(r) \sim -\tfrac{9}{4}(1+\delta)(\cos 2r)/r^4\,, \qquad (3.38)$$

where $\delta \ll 1$. We see from Eq. (3.37) that the oscillatory behavior of $G(r)$ arises from the discontinuity in $S_I''(k)$ at $k=2$. There is no r^{-4} term in Eq. (3.38), since the Coulomb interaction replaces the linear small-k dependence of $S_I(k)$ by $S(k) \to \hbar k^2/2m\omega_{pl}$. We can infer that δ is given by $(1+\delta) = [1-\rho\tilde{C}(2)]^{-2}$. The asymptotic behavior in Eq. (3.38) has been obtained elsewhere.[52]

Equation (3.37) is similar to the perturbation formula[17,53]

$$S(k) \cong \frac{S_I(k)}{1+\rho\phi(k)S_I(k)}\,, \qquad (3.39)$$

which is expected to be a good approximation at high densities where $u(r)$ can be treated as a weak long-range perturbation on $u_I(r)$.

IV. TWO-COMPONENT ENERGY FUNCTIONAL

Our treatment of the trial function in Eq. (1.4) is a straightforward generalization of the previous development. In this formulation spin-up (type-α) and spin-down (type-β) electrons are regarded as different particles. The total number of type-a electrons is N_a and the corresponding mean density is $\rho_a = N_a/\Omega$. The total number of electrons is $N = N_\alpha + N_\beta$, and the total mean density is $\rho = \rho_\alpha + \rho_\beta$.

Let us consider an arbitrary configuration of n_α spin-up and n_β spin-down electrons with an electron of type a at $\vec{r}_1$, type b at $\vec{r}_2, \ldots,$ and type d at $\vec{r}_n$. We define the associated n-body correlation function by

$$g_{ab\cdots d}(1,2,\ldots,n) = Z_N^{-1}\prod_c N_c!\,[(N_c - n_c)!\,\rho_c^{n_c}]^{-1} \times \int |\Psi|^2 d(n+1)\cdots dN\,, \qquad (4.1)$$

where $Z_N = \int |\Psi|^2 d^{3N}r$ and Ψ is given in Eq. (1.4). Let us define the function Δg_{abc} by

$$\begin{aligned} g_{abc}(1,2,3) = 1 &+ G_{ab}(r_{12}) + G_{ac}(r_{13}) + G_{bc}(r_{23}) \\ &+ G_{ab}(r_{12})G_{ac}(r_{13}) + G_{ab}(r_{12})G_{bc}(r_{23}) \\ &+ G_{ac}(r_{13})G_{bc}(r_{23}) + \Delta g_{abc}(1,2,3)\,, \end{aligned} \qquad (4.2)$$

where $G_{ab}(r) \equiv g_{ab}(r) - 1$. We further define the structure factors

$$S_{ab}(k) = \delta_{ab} + (\rho_a\rho_b)^{1/2}\tilde{G}_{ab}(k)\,. \qquad (4.3)$$

In precisely the same manner as in the one-component case we find for the mean kinetic energy per particle

$$\epsilon_{\rm kin} = \epsilon_{\rm kin}^{\rm RPA} + \epsilon_2^{(2)} + \epsilon_2^{(3)} + \epsilon_3^{(3)}\,, \qquad (4.4a)$$

where

$$\epsilon_{\rm kin}^{\rm RPA} = \epsilon_I + \tfrac{1}{8}\epsilon_F\rho\int\frac{d^3k}{(2\pi)^3}\,k^2[(\phi^2{}_{\alpha\alpha} + \phi^2{}_{\alpha\beta})S_{\alpha\alpha} + 2\phi_{\alpha\alpha}\phi_{\alpha\beta}S_{\alpha\beta}]\,, \qquad (4.4b)$$

$$\epsilon_2^{(2)} = \tfrac{1}{8}\epsilon_F\rho\int d^3r[(u'_{\alpha\alpha})^2G_{\alpha\alpha} + (u'_{\alpha\beta})^2G_{\alpha\beta}]\,, \qquad (4.4c)$$

$$\begin{aligned} \epsilon_2^{(3)} = \tfrac{1}{8}\epsilon_F\rho^2\int\frac{d^3k}{(2\pi)^3}\,k[&(\phi_{\alpha\alpha}\tilde{G}_{\alpha\alpha} + \phi_{\alpha\beta}\tilde{G}_{\alpha\beta})\tilde{P}'_{\alpha\alpha} \\ &+ (\phi_{\alpha\beta}\tilde{G}_{\alpha\alpha} + \phi_{\alpha\alpha}\tilde{G}_{\alpha\beta})\tilde{P}'_{\alpha\beta}]\,, \end{aligned} \qquad (4.4d)$$

$$\begin{aligned} \epsilon_3^{(3)} = \tfrac{1}{16}\epsilon_F\rho^2\int d^3r_{12}\,d^3r_{13} &\times[\nabla_1 u_{\alpha\alpha}(r_{12})\cdot\nabla_1 u_{\alpha\alpha}(r_{13})\Delta g_{\alpha\alpha\alpha}(1,2,3) \\ &+ 2\nabla_1 u_{\alpha\alpha}(r_{12})\cdot\nabla_1 u_{\alpha\beta}(r_{13})\Delta g_{\alpha\alpha\beta}(1,2,3) \\ &+ \nabla_1 u_{\alpha\beta}(r_{12})\cdot\nabla_1 u_{\alpha\beta}(r_{13})\Delta g_{\alpha\beta\beta}(1,2,3)]\,. \end{aligned} \qquad (4.4e)$$

We have set $\phi_{ab}(k) = \tilde{u}_{ab}(k)$ and $P_{ab}(r) = G_{ab}(r)u'_{ab}(r)/r$.

As before, we find approximate forms of $\epsilon_3^{(3)}$ using the Kirkwood superposition and the convolution approximation to $\Delta g_{abc}(1,2,3)$. The multicomponent KSA is just

$$\Delta g_{abc}^{\rm KSA}(1,2,3) = G_{ab}(r_{12})G_{ac}(r_{13})G_{bc}(r_{23})\,, \qquad (4.5)$$

which gives

$$\epsilon_3{}^{(3)\mathrm{KSA}} = \tfrac{1}{16}\epsilon_F\rho^2 \int \frac{d^3k}{(2\pi)^3}\{\tilde{G}_{\alpha\alpha}[(\tilde{P}'_{\alpha\alpha})^2 + (\tilde{P}'_{\alpha\beta})^2] + 2\tilde{G}_{\alpha\beta}\tilde{P}'_{\alpha\alpha}\tilde{P}'_{\alpha\beta}\}\,. \tag{4.6}$$

The two-component CA is derived in the Appendix. The CA gives

$$\epsilon^{\mathrm{CA}}_{\mathrm{kin}} = \epsilon^{\mathrm{RPA}}_{\mathrm{kin}} + \tfrac{1}{8}\epsilon_F\rho \int d^3r[G_{\alpha\alpha}(Q_1')^2 + G_{\alpha\beta}Q_2'(Q_2' + 2Q_3')]\,, \tag{4.7}$$

where

$$\tilde{Q}_1 = \phi_{\alpha\alpha}S_{\alpha\alpha} + \phi_{\alpha\beta}S_{\alpha\beta}\,, \qquad \tilde{Q}_2 = \phi_{\alpha\beta}S_{\alpha\alpha}\,, \quad \tilde{Q}_3 = \phi_{\alpha\alpha}S_{\alpha\beta}\,. \tag{4.8}$$

We now have two approximate kinetic-energy functionals which can readily be calculated given the u_{ab} and g_{ab}. In the thermodynamic limit the mean interaction energy per particle is simply

$$\epsilon_{\mathrm{int}} = \tfrac{1}{4}\rho \int d^3r(e^2/r)(G_{\alpha\alpha} + G_{\alpha\beta})\,. \tag{4.9}$$

To allow us to calculate the correlation functions, $|D_a|^2$ is approximated by a Boltzmann factor with an ideal-gas effective pair potential $u^I_{aa}(r)$. Thus $|\Psi|^2$ is written approximately as a Boltzmann factor with effective pair potentials $u^t_{ab} = u_{ab} + u^I_{ab}$, where $u^I_{\alpha\alpha} = u^I_{\beta\beta}$ (since $\rho_\alpha = \rho_\beta$) and $u^I_{\alpha\beta} = 0$. We obtain $u^I_{\alpha\alpha}$ by inverting the HNC equation for the exact $g^I_{\alpha\alpha}$, i.e.,

$$u^I_{\alpha\alpha}(r) = -C^I_{\alpha\alpha}(r) + G^I_{\alpha\alpha}(r) - \ln g^I_{\alpha\alpha}(r)\,, \tag{4.10}$$

where

$$\tilde{C}^I_{\alpha\alpha}(k) = \rho_\alpha^{-1}\{1 - [S_I(k)]^{-1}\} \tag{4.11}$$

and

$$g^I{}_{\alpha\alpha}(r) = 1 - 9[j_1(r)/r]^2\,. \tag{4.12}$$

Note that as $r \to 0$, we have $u^I_{\alpha\alpha}(r) \to -2\ln r$.

The two-component HNC equation is then used to compute the g_{ab}. The generalization of the HNC equation to multicomponent fluids has been given by Meeron.[38] For these calculations we chose the parametrization $u_{cd}(r) = ar^{-1}(1 - e^{-b_{cd}r})$, where a is given by Eq. (2.12b), and we varied $b_{\alpha\alpha}$ and $b_{\alpha\beta}$ to minimize the energy functional.

TABLE I. Correlation energies (in rydbergs) and minimizing parameters b (with $k_F = 1$) at various densities for the one-component convolution, Kirkwood superposition, and random-phase approximations.

r_s	$-\epsilon_c^{\mathrm{CA}}$	$-\epsilon_c^{\mathrm{KSA}}$	$-\epsilon_c^{\mathrm{RPA}}$	b_{CA}	b_{KSA}	b_{RPA}
0.565	0.136	0.131	0.126	0.50	0.50	0.45
1.13	0.107	0.104	0.097	0.60	0.60	0.50
3.39	0.0661	0.0635	0.0577	0.85	0.80	0.65
5.65	0.0499	0.0481	•••	0.95	0.95	•••
7.91	0.0407	0.0393	•••	1.00	1.00	•••
11.3	0.0322	0.0312	•••	1.05	1.05	•••
22.6	0.0196	0.0191	•••	1.15	1.20	•••

V. NUMERICAL RESULTS OF THE VARIATIONS

The correlation-energy functional $\epsilon_c[u]$ is defined by $\epsilon_c[u] = \epsilon[u] - \epsilon_{\mathrm{HF}}$, which for a given density differs from the mean-energy functional $\epsilon[u]$ by a constant. The correlation energy is the minimum value of $\epsilon_c[u]$. The CA, KSA, and RPA correlation energies are given in Table I with the minimizing parameters. For the whole intermediate range of densities $0.5 \lesssim r_s \lesssim 20$, we see that ϵ_c^{CA} and $\epsilon_c^{\mathrm{KSA}}$ never differ by more than 4% and the associated parameters are also in very close agreement. The increase in the relative deviation of the RPA energies and parameters from those of the CA and the KSA as r_s increases into the metallic region signals the breakdown of the RPA.

We now describe a method used by Dunn and Broyles[24] to calculate the correlation energy for an approximate wave function of the same form as the trial function given in Eq. (1.3). Setting

$$\hat{Z}_N = \langle D|\Psi\rangle\,, \tag{5.1}$$

it follows from the Schrödinger equation that the functional

$$\hat{\epsilon}_c[\Psi] = (N\hat{Z}_N)^{-1}\langle D|H|\Psi\rangle - \epsilon_{\mathrm{HF}} \tag{5.2}$$

is equal to the correlation energy when Ψ is the ground-state energy eigenfunction. Equation (5.2) is easily reduced to

$$\hat{\epsilon}_c = \tfrac{1}{2}\rho \int d^3r\, v(r)[\hat{g}(r) - 1] - \epsilon_x\,, \tag{5.3}$$

where

$$\hat{g}(r_{12}) = \frac{N(N-1)}{\hat{Z}_N\rho^2} \int d3 \cdots dN \sum_{\underline{\sigma}} D^*_{\underline{\sigma}}\Psi_{\underline{\sigma}}\,, \tag{5.4}$$

$v(r)$ is given in Eq. (2.2), and ϵ_x is the Hartree-Fock exchange energy given in Eq. (1.2). In the thermodynamic limit $v(r)$ is replaced by e^2/r in Eq. (5.3). Note that $\hat{g}$ is not a pair correlation function according to the definition of Eq. (2.4), but it is nevertheless a closely related function. If $\Psi_{\underline{\sigma}}$ is approximated as in Eq. (1.3), then Eq. (5.4) becomes

$$\hat{g}[u] = \frac{N(N-1)}{\hat{Z}_N\rho^2} \int d3 \cdots dN \sum_{\underline{\sigma}} |D_{\underline{\sigma}}|^2 \exp\Big(-\frac{1}{2}\sum_{i<j} u(r_{ij})\Big)\,. \tag{5.5}$$

From the definition of $g[u]$ in Eq. (2.4) it follows that $\hat{g}[u] = g[\tfrac{1}{2}u]$.

We refer to $\hat{\epsilon}_c[\Psi]$ as the Dunn-Broyles (DB) functional. The DB functional is not stationary for arbitrary variations about the ground state.

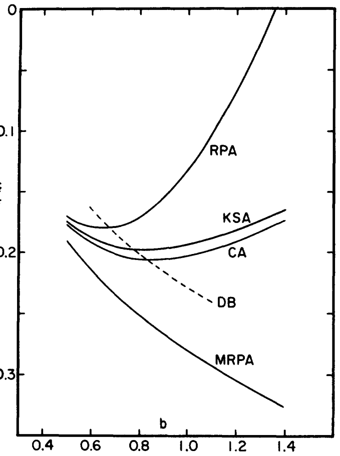

FIG. 1. Parameter variation at $r_s = 3.39$ for the random-phase, Kirkwood superposition, convolution, Dunn-Broyles, and modified-random-phase functionals (respectively denoted by RPA, KSA, CA, DB, and MRPA).

However, the correct correlation energy can be expected to lie on or near the DB curve $\hat{\epsilon}_c(b)$ obtained by introducing our parametrization of Ψ into Eq. (5.3) and varying b. To calculate $\hat{g}[u]$ we approximate the ideal-gas probability density by a Boltzmann factor with an effective pair potential u_I as in Eqs. (3.17) and (3.28) and perform the integration in Eq. (5.5) using the HNC equation for the pair potential $\hat{u}_t = \frac{1}{2}u + u_I$. Then $\hat{\epsilon}_c(b)$ may easily be calculated from Eq. (5.3). A parameter variation is shown in Fig. 1. We expect the DB curve to intersect our best correlation-energy functional quite close to its minimum. Since the RPA may be used only at high densities, we have only to choose between the CA and the KSA. It is seen that the DB curve intersects the CA curve closer to its minimum than to that of the KSA curve.

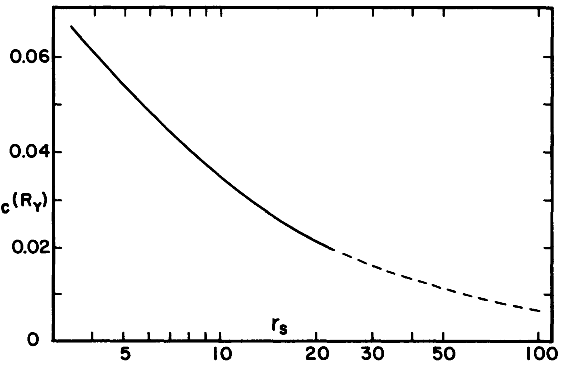

FIG. 2. Comparison of the CA correlation energies (solid curve) with the low-density expansion of Carr *et al.* (dashed curve) about $r_s \cong 25$.

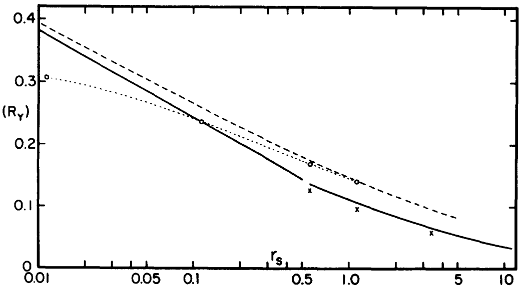

FIG. 3. Comparison of the CA correlation energies (solid curve with $r_s > 0.5$) with the high-density expansion of Gell-Mann and Brueckner, including the small correction term of Carr and Maradudin (solid curve with $r_s < 0.5$). The crosses denote our RPA correlation energies from Table I. The dashed curve is obtained from Gaskell's approximate correlation-energy functional evaluated for the solution to the associated Euler-Lagrange equation; the dotted curve is obtained by minimization of Gaskell's correlation-energy functional with our parametric form for $u(r)$, the circles locating the calculated points.

The MRPA (modified RPA) curve in Fig. 1 is calculated for the MRPA functional,[22] which may be obtained by replacing $g^{(3)}$ by $g(r_{23})$ in Eq. (2.5c). But we see that this functional has no minimum, at least for a reasonable value of the parameter. This behavior was found at all densities investigated. Hence, the MRPA appears to be fundamentally invalid so far as approximating the mean-energy functional is concerned.

Figures 2 and 3 show that the curve $\epsilon_c^{\mathrm{CA}}(r_s)$ joins smoothly at $r_s \cong 25$ with the low-density expansion of Carr *et al.*,[5]

$$\epsilon_c^{\mathrm{low}} = -0.876 r_s^{-1} + 2.65 r_s^{-3/2} - 2.94 r_s^{-2} + \cdots \qquad (5.6)$$

and at $r_s \cong 0.5$ with the high-density expansion of Gell-Mann and Brueckner[2]

$$\epsilon_c^{\mathrm{high}} = 0.0622 \ln r_s - 0.096 + 0.018 r_s \ln r_s + \cdots , \qquad (5.7)$$

where the coefficient of $r_s \ln r_s$ is that calculated by Carr and Maradudin.[4] At $r_s = 0.5$ the last term in Eq. (5.7) is only 4.3% of $\epsilon_c^{\mathrm{high}}$.

In Fig. 4 we compare ϵ_c^{CA} with other theories at intermediate densities. Monnier,[19] Lee and Ree[20] (LR), and Keiser and Wu[21] (KW) calculate ground-state energies and correlation functions of the charged-boson gas using variational methods and alter the statistics to those for the electron gas by means of the Wu-Feenberg formalism.[54] Using the fermion trial function $\Psi_F = D\Psi_B$, where $\Psi_B = \exp[-\frac{1}{2}\sum_{i<j} u(r_{ij})]$ is the boson trial function, Monnier minimizes the Wu-Feenberg expansion of $\langle\Psi_F|H|\Psi_F\rangle/\langle\Psi_F|\Psi_F\rangle$; but LR and KW minimize $\langle\Psi_B|H|\Psi_B\rangle/\langle\Psi_B|\Psi_B\rangle$ and then apply the Wu-Feenberg expansion. The discrepancy between

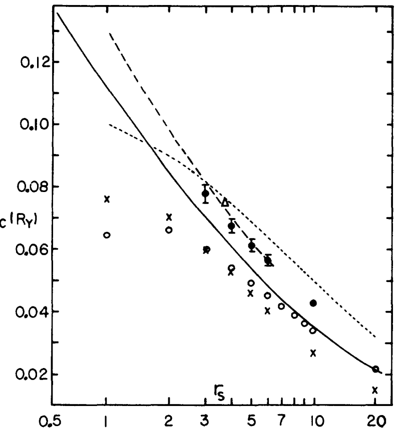

FIG. 4. Comparison of the CA correlation energies (solid curve) with those of other theories at intermediate densities: solid circles, Monnier; open circles, Lee and Ree; crosses, Keiser and Wu; triangle, Isihara and Montroll; dotted curve, Pines's alteration of Wigner's formula; dashed curve, Vashishta and Singwi.

the LR and KW correlation energies is due principally to their different charged-boson wave functions. It should also be noted that Monnier's boson energies are lower than those of LR, the differences being quite large with respect to the correlation energies (from about 50% to 30% of ϵ_c^{CA} as r_s increases from metallic to low densities). It is seen that the correlation energies of LR and KW do not have the proper behavior at smaller r_s. In contrast with the correct high-density expansion of Eq. (5.2), LR find the high-density form $\epsilon_c^{\text{LR}} = Ar_s^{-3/4} + Br_s^{-1/2} + \cdots$, where A and B are constants. Monnier did not extend his calculations to densities with $r_s < 3$.

The single point of Ishihara and Montroll[6] given in Fig. 4 occurs at the minimum of their total-energy curve, which they obtain by interpolating between the high- and low-density energy expansions using the method of two-point Padé approximants. Relative to our correlation energy at that density their result is about 20% low. The simple graphical interpolation of Carr *et al.*[5] gives correlation energies remarkably close to ϵ_c^{CA}.

Also included in Fig. 4 is Wigner's formula as altered by Pines,[55]

$$\epsilon_c = -0.88/(r_s + 7.8)\,, \qquad (5.8)$$

which has the correct behavior to $O(r_s^{-1})$ as $r_s \to \infty$. Nevertheless, Wigner's original formula (1938)[1]

$$\epsilon_c^{W} = -0.58/(r_s + 5.1) \qquad (5.9)$$

is in much closer agreement with ϵ_c^{CA} for $r_s > 2$. It is also interesting to note that at low densities unless the density is very low, i.e., unless $r_s \gg 100$, Eq. (5.9) is much closer to the low-density expansion in Eq. (5.6) than is Eq. (5.8).

The correlation energies computed by Lam[16] are not included in Fig. 4, since his correlation functions $g(r)$ take on relatively large negative values for small separations at low metallic densities.

At metallic densities Becker *et al.*[18] minimized the KSA energy functional for the trial form

$$u(r) = ar^{-1}(1 - e^{-br}) + c(r^2 + d^2)^{-1}\,, \qquad (5.10)$$

using the Percus-Yevick (PY) equation to compute g. Springer[22] then repeated this calculation at metallic and lower densities using the HNC equation instead of the PY equation. The PY equation gave correlation energies much lower than the HNC equation. In each case it was found that with a given by Eq. (2.12b), variation of b, c, and d gave energies differing negligibly from these obtained by variation of b alone, with $c = 0$. These results suggest that our simple one-parameter form for $u(r)$ is sufficiently flexible in the region $1 < r_s \lesssim 20$ so that more elaborate parametrizations would lower the energy by negligible amounts, independent of the approximation used to compute g.

Gaskell[17] has shown that if one uses the RPA energy functional

$$\epsilon^{\text{RPA}} = \epsilon_I + \frac{1}{4}\epsilon_F \rho \int \frac{d^3k}{(2\pi)^3}\, k^2 \phi^2 S + \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\, \frac{4\pi e^2}{k^2}\,(S - 1) \qquad (5.11)$$

and the perturbation formula introduced in Eq. (3.39), i.e.,

$$S = S_I(1 + \rho\phi S_I)^{-1}\,, \qquad (5.12)$$

then the Euler-Lagrange equation

$$\delta\epsilon^{\text{RPA}}/\delta\phi(\vec{k}) = 0 \qquad (5.13)$$

TABLE II. Correlation functions $g(r)$ at various densities determined by the one-component convolution approximation.

		g						
$k_F r$	g_I	$r_s = 0.565$	1.13	3.39	5.65	7.91	11.3	22.6
0	0.500	0.376	0.292	0.100	0.043	0.022	0.009	0.0008
0.4	0.516	0.419	0.350	0.172	0.100	0.065	0.038	0.0083
0.8	0.561	0.483	0.428	0.273	0.197	0.152	0.110	0.045
1.2	0.627	0.566	0.523	0.401	0.333	0.289	0.241	0.150
1.6	0.706	0.659	0.629	0.544	0.495	0.462	0.423	0.338
2.0	0.787	0.752	0.732	0.684	0.658	0.640	0.620	0.571
2.4	0.859	0.835	0.825	0.805	0.798	0.794	0.791	0.783
2.8	0.917	0.902	0.898	0.897	0.902	0.906	0.913	0.930
3.2	0.959	0.950	0.949	0.958	0.967	0.974	0.983	1.007
3.6	0.984	0.979	0.980	0.992	1.001	1.007	1.015	1.033
4.0	0.996	0.994	0.996	1.006	1.013	1.017	1.022	1.032
4.4	1.000	0.999	1.001	1.009	1.013	1.015	1.017	1.020
4.8	0.999	0.999	1.001	1.006	1.008	1.009	1.009	1.008

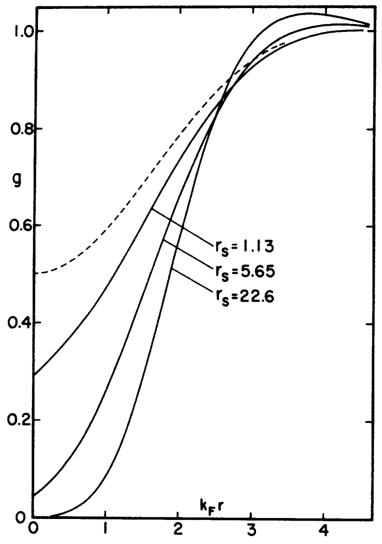

FIG. 5. Correlation functions g at various densities. The dashed curve is g_I.

has the solution

$$\phi = \gamma^2 S_I \{\rho k^2 [k^2 + (k^4 + \gamma^2 S_I^2)^{1/2}]\}^{-1}, \tag{5.14}$$

where $\gamma = \hbar\omega_{pl}/\epsilon_F$ and k is in units of k_F. [Since $\omega_{pl} = (4\pi\rho e^2/m)^{1/2}$, it follows from the definition of γ that $e^2 = 3\pi\gamma^2\epsilon_F/8k_F$.] In Fig. 3 we compare the correlation-energy curves calculated from Eqs. (5.11) and (5.12) for our parametric form $\phi = 4\pi a b^2[k^2(k^2+b^2)]^{-1}$ and for Gaskell's ϕ in Eq. (5.14). Disagreement between the correlation energy of Gaskell and that obtained by variation of the one-parameter form is interpreted to mean that the parametrization is inadequate at that density. We find that the one-parameter form is adequate (with error less than 3%) for $0.5 \lesssim r_s \lesssim 1$ but inadequate for $r_s \ll 0.5$, the difference increasing as $r_s \to 0$. This suggests that for a more judiciously chosen parametrization the curve $-\epsilon_c^{\text{CA}}$ would be raised slightly in the region $0.5 \lesssim r_s \lesssim 1$ so as to join more smoothly with the high-density expansion at $r_s \cong 0.5$. The close agreement between the one-parameter energy of Eqs. (5.11) and (5.12) and the high-density expansion at $r_s \cong 0.1$ is seen to be fortuitous.

TABLE III. Correlation energies (in rydbergs) and minimizing parameters $b_{\alpha\alpha}$, $b_{\alpha\beta}$ (with $k_F = 1$) at metallic densities for the two-component convolution and Kirkwood superposition approximations.

r_s	$-\epsilon_c^{\text{CA}}$	$-\epsilon_c^{\text{KSA}}$	$b_{\alpha\alpha}^{\text{CA}}$	$b_{\alpha\beta}^{\text{CA}}$	$b_{\alpha\alpha}^{\text{KSA}}$	$b_{\alpha\beta}^{\text{KSA}}$
3.39	0.0654	0.0633	0.65	0.95	0.60	0.90
5.65	0.0496	0.0481	0.75	1.05	0.70	1.05
7.91	0.0406	0.0393	0.75	1.15	0.75	1.10

It should be emphasized that the only purpose of the above comparison with Gaskell is to test the adequacy of our parametrization for $r_s \lesssim 1$. At metallic densities the perturbation formula Eq. (5.12) for $S(k)$ leads to unphysical overcorrelation manifested by correlation functions $g(r)$ which are negative for small interparticle separations and, hence, to energies which are much too low. Gaskell was only partially successful in his attempts to overcome these difficulties. Comparing with our ϵ_c^{RPA} energies in Fig. 3 (computed from the HNC equation), it is found that most of Gaskell's error in the region $0.5 \lesssim r_s$ is due not to the RPA but to the perturbation formula for $S(k)$—a not-too-surprising result. However, Gaskell has shown that at high densities Eqs. (5.11)–(5.14) yield the asymptotic expansion

$$\epsilon_c^G = 0.0570 \ln r_s - 0.132 + \cdots, \tag{5.15}$$

which has the correct form but incorrect coefficients [see Eq. (5.7)].

The correlation functions $g(r)$ at the CA minima are presented in Table II. At any density where the HNC equation has a solution it is obvious that $g(r) > 0$ for all r. As r_s increases, $g(0)$ decreases and $u(0)$ increases. Of course, at low densities $g(0)$ is practically zero. It is seen that the first maximum of $g(r)$ becomes more pronounced as the density decreases, and is located at $k_F r \cong 4$. Since $k_F r = (\frac{9}{4}\pi)^{1/3} r/r_0 \cong 1.92 r/r_0$, where r_0 is the ion-sphere radius, the first maximum is at $r \cong 2r_0$. The density dependence of the $g(r)$ is illustrated in Fig. 5. For the sake of exactness we should note that these calculations were performed with the density parameter γ^2 (where

TABLE IV. Correlation functions $g_{\alpha\alpha}(r)$ and $g_{\alpha\beta}(r)$ at metallic densities determined by the two-component convolution approximation.

		$r_s = 3.39$		$r_s = 5.65$		$r_s = 7.91$	
$k_F r$	$g_{\alpha\alpha}^I$	$g_{\alpha\alpha}$	$g_{\alpha\beta}$	$g_{\alpha\alpha}$	$g_{\alpha\beta}$	$g_{\alpha\alpha}$	$g_{\alpha\beta}$
0	0	0	0.149	0	0.0573	0	0.0200
0.4	0.0316	0.0154	0.281	0.0102	0.154	0.0090	0.0801
0.8	0.121	0.0746	0.444	0.0575	0.310	0.0540	0.210
1.2	0.255	0.186	0.612	0.160	0.502	0.156	0.404
1.6	0.413	0.340	0.759	0.313	0.689	0.314	0.617
2.0	0.573	0.513	0.870	0.494	0.839	0.500	0.799
2.4	0.718	0.678	0.944	0.669	0.939	0.679	0.926
2.8	0.835	0.814	0.986	0.813	0.995	0.823	0.996
3.2	0.918	0.910	1.006	0.914	1.019	0.922	1.026
3.6	0.968	0.968	1.013	0.973	1.024	0.978	1.032
4.0	0.992	0.996	1.013	1.000	1.022	1.001	1.028
4.4	1.000	1.004	1.011	1.006	1.016	1.006	1.021
4.8	0.999	1.002	1.009	1.003	1.011	1.001	1.014
5.2	0.995	0.997	1.007	0.998	1.008	0.996	1.009
5.6	0.993	0.994	1.005	0.994	1.006	0.992	1.006
6.0	0.993	0.994	1.004	0.994	1.004	0.992	1.005
6.4	0.995	0.995	1.003	0.995	1.003	0.994	1.004
6.8	0.997	0.998	1.002	0.998	1.002	0.997	1.003

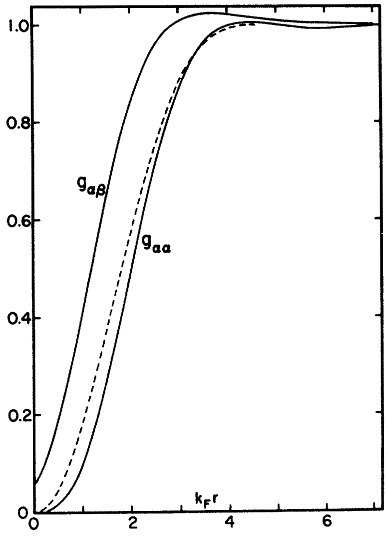

FIG. 6. Correlation functions $g_{\alpha\alpha}$ and $g_{\alpha\beta}$ at $r_s = 5.65$. The dashed curve is $g^I_{\alpha\alpha}$.

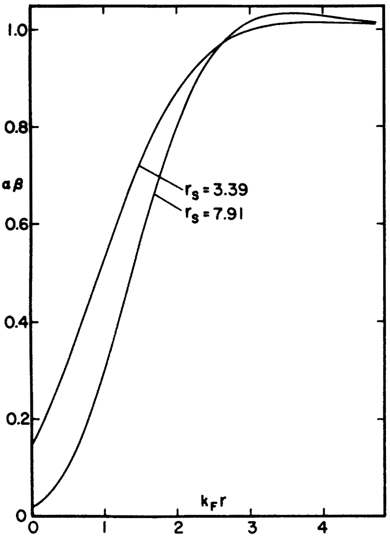

FIG. 7. Correlation functions $g_{\alpha\beta}$ at metallic densities.

$\gamma = \hbar\omega_{pl}/\epsilon_F$ as above) at the values $\gamma^2 = 0.5$, 1, 3, 5, 7, 10, and 20. The conventional r_s is related to γ^2 by $r_s = (\frac{3}{16}\pi)(\frac{9}{4}\pi)^{1/3}\gamma^2 \cong 1.130\gamma^2$.

The correlation energies determined by minimizing the energy functional $\epsilon[u_{\alpha\alpha}, u_{\alpha\beta}]$ at metallic densities are given in Table III. These energies are seen to differ negligibly from the corresponding energies in Table I. The correlation functions $g_{\alpha\alpha}(r)$ and $g_{\alpha\beta}(r)$ at the CA minima are given in Table IV. In accordance with the Pauli principle, $g_{\alpha\alpha}(0) = 0$ at all densities because $u^I_{\alpha\alpha}(r) \to +\infty$ as $r \to 0$. As the density decreases $g_{\alpha\beta}(0)$ decreases. In the presence of the Coulomb interaction the correlation hole between parallel spins is slightly wider than that of $g^I_{\alpha\alpha}(r)$ and the antiparallel spins are rather strongly correlated. The correlation functions at $r_s = 5.65$ are illustrated in Fig. 6, and the density variation of $g_{\alpha\beta}(r)$ is shown in Fig. 7.

VI. CONCLUSIONS

We have applied the variational principle to the electron-gas ground state in the region of intermediate densities. To compute the expectation value of the Hamiltonian for the trial functions in Eqs. (1.3) and (1.4) we introduced the following approximations:

(i) The three-particle correlation functions appearing in the mean kinetic-energy formulas are expressed as functionals of the pair correlation functions by means of the Kirkwood superposition and the convolution approximations. Thus, two approximate mean-energy functionals are obtained which may easily be calculated for either trial function, given u or the u_{ab} and the corresponding correlation functions.

(ii) The ideal-gas configurational probability density is approximated as a Boltzmann factor with an ideal-gas effective pair potential. This allows the correlation functions of the interacting system to be calculated in the same way as for a classical fluid with pairwise interactions.

(iii) The pair correlation functions are computed using the hypernetted-chain integral equation.

We find that the CA and KSA correlation energies differ by not more than 4% in the region $0.5 \lesssim r_s \lesssim 20$, the CA energies being lower everywhere. It is obvious that in comparing approximations to the mean-energy functional, a lower variational energy is not necessarily a better upper bound to the true energy since it may not be an upper bound at all. However, the Dunn-Broyles functional, which involves only approximations (ii) and (iii), intersects the CA energy functional closer to its minimum than to the minimum of the KSA energy functional (at least in the metallic region where the DB functional was computed). We conclude that the CA shows a slightly greater degree of consistency with the other approximations than does the KSA. This result leads us to prefer the CA correlation energies. The 4% relative difference between the CA and the KSA correlation energies provides an estimate of the error introduced by approximating $g^{(3)}$.

We must now estimate the accuracy of our other approximations. In the first place, having introduced approximation (ii), we must consider how accurately $g(r)$ is given by the HNC equation for the effective pair potential $u_t(r) = u(r) + u_I(r)$; in the second place, we must consider the very introduction of approximation (ii), without which the HNC equation could not have been used at all. At densities below the metallic region $u(r) \gg u_I(r)$, so that the Coulomb interaction dominates the effect of Fermi statistics. Thus one may expect that, at low densities, application of approximation (ii) introduces negligible error, the only remaining source of error being the HNC approximation. However, the remarkable accuracy of the HNC approximation for the classical electron gas and our assumption relating the quantum to a classical system by Eq. (3.25) suggest that at intermediate densities the HNC approximation itself introduces only a small error into the correlation energy. We assume that the latter error is comparable to that introduced by approximating $g^{(3)}$. For $r_s \lesssim 1$ and sufficiently small separations $u_I(r) > u(r)$, so that error introduced by approximation (ii) should become apparent at high densities. But the good agreement with the high-density expansion (Fig. 3) implies that approximation (ii) also introduces little error.

The variational calculations of Gaskell,[17] Becker *et al.*,[18] and Springer,[22] which were discussed in Sec. V, led us to the conclusion that more flexible parametrizations would lower our correlation energies by about 3% at $r_s \cong 0.5$ and by less than 1% for $r_s > 1$. An attempt to improve upon the present calculation by using more elaborate parametrizations would therefore appear to be illusory without further investigation of the basic approximations (i)–(iii).

In summary, then, we estimate the error in our CA correlation energies at metallic densities to be about 10%. But the close agreement with both the high- and low-density expansions suggests that the error may actually be less than this in the whole intermediate-density range.

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APPENDIX

The correlation functions for a two-component quantum fluid are defined by Eq. (4.1). The convolution approximation to g_{abc} is found in the same manner as for the one-component case. First, let us consider $g_{\alpha\alpha\beta}$. Substituting the expansion for $g_{\alpha\alpha\beta}$ given by Eq. (4.2) into each of the sequential relations

$$\int d1\, g_{\alpha\alpha\beta}(1,2,3) = (\Omega - 1/\rho_\alpha) g_{\alpha\beta}(r_{23}) \tag{A1}$$

and

$$\int d3\, g_{\alpha\alpha\beta}(1,2,3) = \Omega g_{\alpha\alpha}(r_{12}), \tag{A2}$$

it follows that $\Delta g_{\alpha\alpha\beta}$ must satisfy

$$\int d1\, \Delta g_{\alpha\alpha\beta}(1,2,3) = -\int d1\, G_{\alpha\alpha}(r_{12}) G_{\alpha\beta}(r_{13}) \tag{A3}$$

and

$$\int d3\, \Delta g_{\alpha\alpha\beta}(1,2,3) = -\int d3\, G_{\alpha\beta}(r_{13}) G_{\alpha\beta}(r_{23}), \tag{A4}$$

where use is made of

$$\int d^3r\, G_{ab}(r) = -\delta_{ab}/\rho_a. \tag{A5}$$

It is clear that $\Delta g_{\alpha\alpha\beta}(1,2,3) = \Delta g_{\alpha\alpha\beta}(2,1,3)$. A particular solution to Eqs. (A3) and (A4), which is symmetrical in coordinates 1 and 2, is the convolution form

$$\Delta g^{\mathrm{CA}}_{\alpha\alpha\beta}(1,2,3) = \rho_\alpha \int d4\, G_{\alpha\beta}(r_{14}) G_{\alpha\beta}(r_{24}) G_{\alpha\alpha}(r_{34}) + \rho_\alpha \int d4\, G_{\alpha\alpha}(r_{14}) G_{\alpha\alpha}(r_{24}) G_{\alpha\beta}(r_{34}). \tag{A6}$$

Now $\Delta g^{\mathrm{CA}}_{\alpha\beta\beta}(1,2,3)$ can be obtained at once from Eq. (A6) by interchanging indices α and β and coordinates 1 and 3.

Obviously

$$\Delta g^{\mathrm{CA}}_{\alpha\alpha\alpha}(1,2,3) = \rho_\alpha \int d4\, G_{\alpha\alpha}(r_{14}) G_{\alpha\alpha}(r_{24}) G_{\alpha\alpha}(r_{34}). \tag{A7}$$

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Observation of Amplitude Oscillation of Second-Harmonic Ion Acoustic Waves

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For the propagation of an ion acoustic wave, we observed an amplitude oscillation of the second-harmonic ion acoustic wave, which is qualitatively explained by nonlinear wave-wave-coupled theory with a fluid model.

I. INTRODUCTION

Since Malmberg and Wharton[1] observed an amplitude oscillation of an electron plasma wave, many authors have investigated the amplitude oscillations of the electron wave and an ion wave. Although the experimental result obtained by Malmberg and Wharton has been explained by nonlinear wave-particle interactions, the possibility of linear mixing[2] between a pseudowave and an ion acoustic wave has been pointed out as regards the amplitude oscillation of the ion wave.