in Eq. (5.3), while in the time integration over the velocity correlation function we have to include the diffusion relaxation factor $e^{-\Gamma^c_{k'}|t_{21}|}$ for the concentration fluctuation of wave number k'. This brings in the ratio $\gamma = k'/k$, in the notation of Eq. (3.1). The resulting integral is

$$\int_{-\infty}^{+\infty} dt_{21}\, e^{-\Gamma^c_{k'}|t_{21}|} \langle v_{\vec{k}\mu}(t_2) v^{*}_{\vec{k}\mu}(t_1)\rangle$$

$$= \frac{2T}{k^2}\left\{\frac{1}{\eta(0,k,0)} - \frac{1}{\eta(0,k,0)^2} \times \left[\eta\left(0,k,\frac{k'}{k}\right) - \eta(0,k,0)\right]\right\}$$

$$\simeq \frac{2T}{k^2\eta(0,k,k'/k)} \qquad \text{(B13)}$$

and appears in the integrand of Eq. (5.3).

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Electron Gas at Metallic Densities*

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The ground-state properties of an electron gas at metallic densities are investigated using the Wu–Feenberg theory of Fermi liquids. The correlation energy, the low-temperature specific heat, and the spin susceptibility are computed, and the ground state is found to be paramagnetic. The perturbative correction to the correlation energy owing to the particle-hole excitations in a correlated-basis-function formulation is found to be insignificant.

I. INTRODUCTION

The problem of a quantum electron gas in its ground and low excited states has been a subject of interest for many years. The study was initiated by Wigner[1] in a calculation of the correlation energy which he defined to be the difference between the true ground-state energy and that given by the Hartree-Fock approximation. The correlation energy is a function of the electron density which is measurable in terms of the dimensionless parameter r_s, the average interparticle distance in unit of Bohr radius. At high densities ($r_s \ll 1$), the correlation energy is expressed in a series expansion in r_s. The leading coefficients of this expansion were first obtained by Macke, [2] and the calculation was later extended by Gell-Mann and Brueckner and others. [3] In the low-density limit ($r_s \gg 1$), the electrons tend to form a stable lattice. [1] The correlation energy at low densities is expressible in a series expansion in r_s^{-1}. [4]

It is considerably more difficult to carry out studies on the electron gas in the physically more interesting metallic density range $1 < r_s < 6$. This corresponds to the densities of electrons in metals. The main difficulty lies in the lack of a useful expansion parameter which necessitates careful considerations. Many approximate treatments have been applied to the electron gas in this density range. They include, among others, the random phase approximation (RPA), [5] a dielectric formulation, [6] a method of Green's function, [7] and variational approaches. [8]

One approach that has not been fully tried in its application to an electron gas is the method of correlated basis functions (CBF). [9] The CBF method has been successful in dealing with strongly interacting many-particle systems such as liquid and solid helium and certain nuclear systems. It has also been proven to be successful for the charged Bose gas whose interaction is long ranged. It is therefore natural to extend the region of its application to an electron gas, especially in the intermediate density range for which the CBF method is best fitted for numerical calculations. We wish to emphasize at this point that the CBF method is a self-contained perturbative treatment, as opposed to the variational calculations that have previously been carried out using the same type of wave functions. [8]

In this paper we report on the results of a preliminary application of the CBF method to an electron gas in the intermediate density range. Here we are primarily interested in extending the Wu-Feenberg theory[10] of fermion systems, which has proven to be successful for liquid He^3, [11] to the problem of an electron gas. As in the case of liquid He^3, perturbative calculations will be carried out by considering particle-hole excitations. The correction to the correlation energy is found to be very small. The low-temperature specific heat and the ground-state spin susceptibility are also computed.

II. BASIC THEORY

Consider a system of N electrons of mass m confined in a uniform neutralizing background of volume Ω. The Hamiltonian takes the form

$$\mathcal{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + V(\vec{r}_1, \ldots, \vec{r}_N) , \tag{1}$$

where the potential energy $V(\vec{r}_1, \ldots, \vec{r}_N)$ includes the Coulomb energy between the particles and that between the particles and the background. We shall consider the limit of $N \to \infty$, $\Omega \to \infty$, while holding the electron density $\rho = N/\Omega$ constant. We are interested in the ground-state solution of the Schrödinger equation

$$\mathcal{H} \Psi_0^F = E_0^F \Psi_0^F \tag{2}$$

for a given density ρ and antisymmetric wave functions.

A conventional, although in principle not necessary, starting point of the CBF method is an educated guess on the ground-state wave function. The expectation value of the Hamiltonian in this state is then taken to be the zeroth-order approximation to the ground-state energy. Higher-order corrections to this approximation can be obtained in a perturbative treatment using a set of properly chosen basis functions. For fermion systems a convenient choice of the basis is the set

$$\psi_i^F = \psi_0 \varphi_i , \quad i = 0, 1, 2, \ldots . \tag{3}$$

In (3), $\psi_0 = \psi_0(\vec{r}_1, \ldots, \vec{r}_N)$ is a correlation factor which accounts for the correlation between the particles, and $\varphi_i = \varphi_i(\vec{r}_1\sigma_1, \ldots, \vec{r}_N\sigma_N)$, the model function which is antisymmetric in the N spatial and spin coordinates $(\vec{r}_j, \sigma_j)$, accounts for the required statistics. Note that these basis functions differ only in the choice of the model functions.

Following the lead of Wu and Feenberg, [10] we take the correlation factor to be the ground-state solution of (2) among the boson-type (symmetric) wave functions:

$$\psi_0 = \psi_0^B(\vec{r}_1, \ldots, \vec{r}_N), \tag{4}$$

$$\mathcal{H} \psi_0^B = E_0^B \psi_0^B . \tag{5}$$

Furthermore, the model function is taken to be a determinant of plane-wave orbitals:

$$\varphi_i = \det \left| e^{i\vec{k}_m \cdot \vec{r}_n} s_m(\sigma_n) \right| . \tag{6}$$

In (6), the wave vectors $\vec{k}_m$ are determined by the usual periodic boundary conditions and $s_m(\sigma_n)$ is the spin wave function. The basis set is therefore characterized by the quantum numbers $\{\vec{k}_m, s_m\}$. The zeroth-order approximation to the ground-state wave function is written as, according to (3),

$$\psi_0^F = \psi_0^B \varphi_0 , \tag{7}$$

in which the wave vectors in φ_0 are confined within a Fermi sphere for each component of the spin. The wave function (7) forms the basis of the theory of Fermi liquids formulated by Wu and Feenberg. [10] Other basis functions can be generated by extending the range of the wave vectors in the model functions. Examples are states with two or more electrons excited outside the Fermi sea. A perturbative calculation using these "particle-hole-excitation" wave functions has been formulated by Woo.[11]

We begin our study by stating some basic relations occurring in the theory. The boson pair-distribution function is defined by

$$g_B(r_{12}) = \frac{N(N-1)}{\rho^2} \int \psi_0^{B^2}\, d\vec{r}_3 \ldots d\vec{r}_N\ , \tag{8}$$

where ψ_0^B is taken to be normalized. The boson liquid-structure factor is defined in terms of the Fourier transform of $g_B - 1$ as

$$S(k) \equiv 1 + u(k) = 1 + \rho \int e^{i\vec{k}\cdot\vec{r}} [g_B(r) - 1]\, d\vec{r}\ . \tag{9}$$

The expectation value of the Hamiltonian $\mathcal{H}$ in the state ψ_0^F takes the following expression[10]:

$$E^{(0)}(\vec{k}_1\sigma_1, \ldots, \vec{k}_N\sigma_N) \equiv \int \psi_0^{F*} \mathcal{H} \psi_0^F \Big/ \int \psi_0^{F*} \psi_0^F = E_0^B + E_1^F + E_2^F + E_3^F + \cdots\ , \tag{10}$$

where the integrations extend over all the N configurational and spin coordinates. Also,

$$E_1^F = \frac{\hbar^2}{2m} \sum_n k_n^2\ ,$$

$$E_2^F = \frac{\hbar^2}{4mN} \sum_{mn} k_{mn}^2 u(k_{mn}) \delta_{mn}\ , \tag{11}$$

$$E_3^F = -\frac{\hbar^2}{4mN^2} \sum_{lmn} k_{lm}^2 S(k_{lm}) u(k_{mn}) u(k_{nl})\, \delta_{lmn}\ ,$$

where

$\delta_{mn} = 1$ for $s_m = s_n$,

$\delta_{mn} = 0$ for $s_m \neq s_n$,

$\delta_{lmn} = 1$ for $s_l = s_m = s_n$

$\delta_{lmn} = 0$ otherwise,

and the summations extend over all momenta contained in φ_0.

Identifying $E^{(0)}$ as the unperturbed ground-state energy, one can next perform the Rayleigh-Schrödinger perturbation using the set of nonorthogonal basis (3) (with ψ_0^B in place of ψ_0). A formal formulation of this procedure can be found in Ref. 11. The exact ground-state energy is thus given by

$$E_0^F = E^{(0)} + \Delta E^{(2)} + \Delta E^{(3)} + \cdots\ , \tag{12}$$

where $\Delta E^{(2)}$, $\Delta E^{(3)}$, etc., are the contributions from successive perturbative expansions. In practice, it is feasible to compute only the leading one or two terms in the perturbative expansion. The usefulness of the theory will then depend on the convergence of the series, which in turn depends on how well ψ_0^F approximates the exact ground-state wave function Ψ_0^F. An explicit expression of $\Delta E^{(2)}$ generated by considering the set of basis functions with a pair of electrons excited outside the Fermi sea is included in Appendix B.[11]

As we shall see in Sec. IV, the ground state of an electron gas is paramagnetic. For this state, the pair-distribution function defined by ψ_0^F can be expressed in terms of g_B as[10]

$$g_F(r_{12}) = g_B(r_{12}) \big[1 - \tfrac{1}{2} h^2(k_F r_{12}) - \rho \int g_B(r_{23}) f(r_{31})\, h^2(k_F r_{23})\, d\vec{r}_3 + \tfrac{1}{2} \rho\, h(k_F r_{12}) \times \int g_B(r_{23}) f(r_{31})\, h(k_F r_{23})\, h(k_F r_{31})\, d\vec{r}_3 + \cdots \big]. \tag{13}$$

In (13),

$$f(r) \equiv g_B(r) - 1\ ,$$
$$h(k_F r) \equiv (2/N) \sum_{k<k_F} e^{i\vec{k}\cdot\vec{r}} = 3(\sin k_F r - k_F r \cos k_F r)/(k_F r)^3\ , \tag{14}$$

and the Fermi momentum is given by $k_F = (3\pi^2\rho)^{1/3}$. The Wu–Feenberg theory also permits the calculation of the low-temperature specific heat C and the spin susceptibility χ. The results for the paramagnetic state turn out to be best interpreted in terms of the Landau parameter defined by

$$f(\vec{k}_1, \vec{k}_2) = \frac{\hbar^2}{4m} k_{12}^2 u(k_{12}) - \frac{\hbar^2}{32 m \pi^3 \rho} \times \int [k_{12}^2 S(k_{12}) u(k_{13}) u(k_{23}) + k_{23}^2 S(k_{23}) u(k_{21})\ u(k_{13}) + k_{13}^2 S(k_{13}) u(k_{23}) u(k_{12})]\, d\vec{k}_3 + \cdots\ . \tag{15}$$

Letting

$$f_0(k_F, \cos(\vec{k}_1, \vec{k}_2)) \equiv f(\vec{k}_1, \vec{k}_2)_{k_1 = k_2 = k_F} \tag{16}$$

one has[10]

$$C_0/C = 1 - (3/4e_F) \int_{-1}^{1} f_0(k_F, y) y\, dy\ , \tag{17}$$

$$\chi_0/\chi = 1 + (3/4e_F) \int_{-1}^{1} f_0(k_F, y)(1 - y)\, dy\ , \tag{18}$$

where $e_F = \hbar^2 k_F^2/2m$, and C_0, χ_0 refer to, respectively, the low-temperature specific heat and the Pauli spin susceptibility for an ideal Fermi gas. Perturbative corrections are not included in (13)–(18).

III. GROUND STATE OF THE CHARGED BOSE GAS

Since our results for the fermion system are expressed in terms of $S(k)$ and $g_B(r)$ defined by the exact boson-type wave function ψ_0^B, our first concern is to solve the problem of a charged Bose gas. For this problem we use a variational approach based on the Bijl–Dingle–Jastrow (BDJ) -type wave function of the form[12]

$$\psi_0^B = \exp\Big(\tfrac{1}{2} \sum_{i<j} u(r_{ij})\Big) \Big/ \Big[\int d\vec{r}_1 \ldots d\vec{r}_N \exp\Big(\sum_{i<j} u(r_{ij})\Big)\Big]^{1/2}\ , \tag{19}$$

TABLE I. Optimum values of α and the boson ground-state energy.

r_s	α	E_0^B/N (Ry)
1.0	0.4421	−0.7691
2.0	0.6655	−0.4478
3.0	0.8078	−0.3237
4.0	0.8981	−0.2557
5.0	0.9530	−0.2120
6.0	0.9835	−0.1813
10.0	1.000	−0.1148
20.0	1.000	−0.0597

and follow closely the procedures of Ref. 12. Instead of varying $u(r)$ directly, Lee[12] introduced the variational pair-distribution function

$$g_B(r) = 1 - \alpha \exp[-\pi(\alpha\rho)^{2/3} r^2] \tag{20}$$

with α to be varied. The corresponding boson liquid-structure factor is

$$S(k) = 1 - \exp[-k^2/4\pi(\alpha\rho)^{2/3}] \ . \tag{21}$$

The function $u(r)$ can be expressed in terms of $g_B(r)$ either as a series expansion in the parameter[12] α or through the solution of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) equation in conjunction with the Kirkwood superposition approximation for the three-particle distribution function.[13] Numerical results obtained by Lee in the intermediate density range show very little difference between these two approaches when the variational pair-distribution function (20) is used. In fact, in the density range $0.01 < r_s < 30$, the first two terms alone in the series expansion are sufficient to yield the resulting energy values to within 0.1%. These two terms are known as the hypernetted-chain (HNC) approximation[14]:

$$u(r) = \ln g_B(r) - \frac{1}{(2\pi)^3\rho} \int e^{i\vec{k}\cdot\vec{r}} \frac{[1-S(k)]^2}{S(k)} d\vec{k} \ . \tag{22}$$

Therefore we shall simply use (22) in extending the ground-state calculation to other values of electron density not considered by Lee.

The expectation value of the Hamiltonian operator (1) in the BDJ wave function (19),

$$E^B(\alpha) \equiv \int \psi_0^B \mathcal{H} \psi_0^B \, d\vec{r}_1 \cdots d\vec{r}_N$$

$$= N \frac{\hbar^2 \rho}{8m} \int \nabla u(r) \cdot \nabla g_B(r) \, d\vec{r} + \tfrac{1}{2} N\rho e^2 \int \frac{1}{r} [g_B(r) - 1] \, d\vec{r} \ ,$$

becomes, after introducing (22),

$$E^B(\alpha) = N \frac{\hbar^2\rho}{8m} \int \frac{1}{g_B(r)} [\nabla g_B(r)]^2 d\vec{r} + \frac{N\hbar^2}{(4\pi)^3 m\rho} \int \frac{[1-S(k)]^3}{S(k)} k^2 d\vec{k} + \tfrac{1}{2} N\rho e^2 \int \frac{1}{r} [g_B(r) - 1] \, d\vec{r}$$

$$= N \frac{\pi^2}{r_s^2} \left(\frac{3\alpha}{4\pi}\right)^{5/3} \left(2 \sum_{n=0}^{\infty} \frac{\alpha^n}{(n+2)^{5/2}} + \sum_{n=0}^{\infty} \frac{1}{(n+3)^{5/2}}\right) - 2N \left(\frac{3\alpha}{4\pi}\right)^{1/3} \frac{1}{r_s} \ , \quad \alpha \leq 1. \tag{23}$$

The last expression in (23) is obtained by substituting (20) and (21) for $g_B(r)$ and $S(k)$, and is expressed in rydberg units $(me^4/2\hbar^2)$. It is then a simple matter to minimize $E^B(\alpha)$ by varying α. Results in the density range $1 < r_s < 20$ are given in Table I. For $r_s = 1$, 3, and 10 our result agrees with that of Lee.

IV. NUMERICAL RESULTS FOR ELECTRON GAS

Having considered the ground-state problem for the charged Bose gas, we are now ready to carry out numerical computations for the electron gas. The first question of interest is the nature of the ground state: Is the ground state of an electron gas ferromagnetic or paramagnetic? That is, are the spins parallel or antiparallel? We can answer this question by comparing the energies in the two states. Let the number of electrons in the spin + and − states be N_+ and N_-, respectively, and write $N_\pm = \frac{1}{2}N(1 \pm x)$. In the ground state (7), the momenta of the electrons will fill two Fermi spheres of radii $k_F^\pm = k_F(1 \pm x)^{1/3}$. The ground-state energy (12) now becomes

$$E(\rho, x) = E_0^B(\rho) + E_{01}^F(\rho, x) + E_{02}^F(\rho, x) + E_{03}^F(\rho, x) + \cdots + \Delta E^{(2)}(\rho, x) + \cdots \ , \tag{24}$$

where

$$E_{01}^F(\rho, x) = \tfrac{3}{10} N e_F [(1+x)^{5/3} + (1-x)^{5/3}] \ ,$$

$$E_{02}^F(\rho, x) = 12 N e_F \Big[(1+x)^{8/3} \int_0^1 (y^4 - \tfrac{3}{2} y^5 + \tfrac{1}{2} y^7) u(2k_F^+ y) \, dy + (1-x)^{8/3} \int_0^1 (y^4 - \tfrac{3}{2} y^5 + \tfrac{1}{2} y^7) u(2k_F^- y) \, dy\Big] \ , \tag{25}$$

$$E_{03}^F(\rho, x) = -\tfrac{1}{2} N e_F \left(\frac{3}{8\pi}\right)^3 \Big[(1+x)^{11/3} \int_{y_i<1} y_{12}^2 S(k_F^+ y_{12}) \times u(k_F^+ y_{23}) u(k_F^+ y_{31}) \, d\vec{y}_1 d\vec{y}_2 d\vec{y}_3 + (1-x)^{11/3} \int_{y_i<1} y_{12}^2 S(k_F^- y_{12}) \times u(k_F^- y_{23}) u(k_F^- y_{31}) \, d\vec{y}_1 d\vec{y}_2 d\vec{y}_3\Big] \ .$$

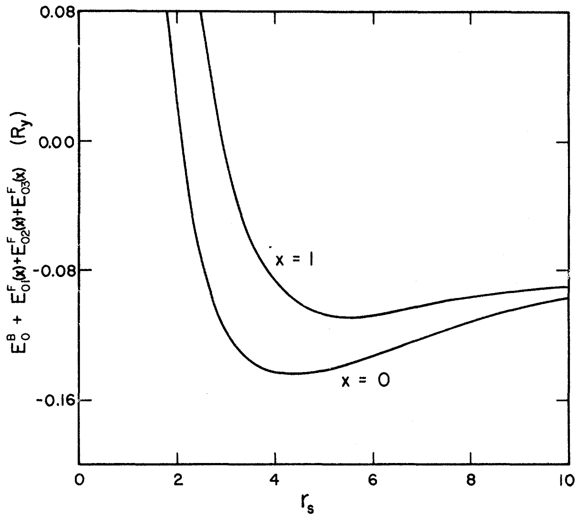

FIG. 1. Comparison of the paramagnetic ($x=0$) and ferromagnetic ($x=1$) ground-state energies of an electron gas. The perturbative corrections are not included.

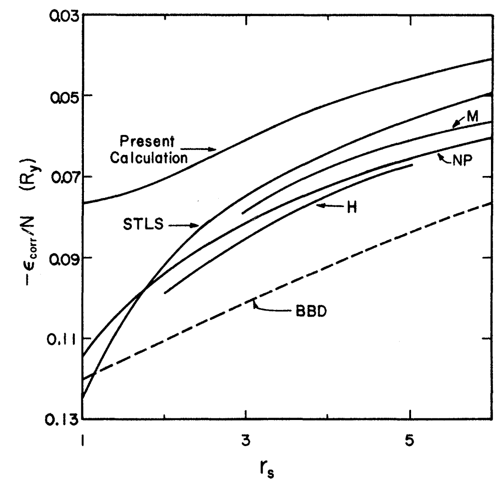

FIG. 2. Comparison of the correlation energy. STLS (Singwi *et al.*, Ref. 6), H (Hubbard, Ref. 5), NP (Nozières and Pines, Ref. 5), BBD (Becker *et al.*, Ref. 8), M (Monnier, Ref. 15).

As we shall see presently, $E_{0n}^F(\rho, 0)$ converges well in n and $\Delta E^{(2)}(\rho, 0)$ is very small. Therefore, for the purpose of comparing energies, it is sufficient to consider only the first four terms in (24). $E_{02}^F(\rho, x)$ can be evaluated in a closed form, while $E_{03}^F(\rho, x)$ has to be computed numerically. The detailed expressions of E_{02}^F and E_{03}^F suitable for numerical calculations are given in Appendix A. The numerical results are presented in Fig. 1. We see that the paramagnetic state has a lower energy at all densities. This is in agreement with the conclusion reached by Carr[4] and by Hedin.[7] Numerical values for $E_{02}^F(\rho, 0)$ and $E_{03}^F(\rho, 0)$ are also included in Table II.

To compute the paramagnetic ground-state energy more accurately, we must include the perturbative corrections $\Delta E^{(2)}$, $\Delta E^{(3)}$, ... An explicit expression of $\Delta E^{(2)}$ from considering the pair-excited states is given in Appendix B. This expression was first derived and put in a form suitable for numerical calculations by Woo.[11] We have further simplified Woo's procedures and evaluated this correction term for the electron gas. The results are also presented in Table II with the details reported in Appendix B. Because of the prohibitive amount of labor involved in the higher-order calculations, we shall omit the corrections $\Delta E^{(3)}$, etc. Furthermore, since the series E_{0n}^F converges reasonably well in n, the terms with $n \geq 4$ are also neglected. Combining these together, we obtain the correlation energy ϵ_{corr}, defined as the difference between the true ground-state energy and the Hartree-Fock energy $E_{HF} = N[2.2099/r_s^2 - 0.9163/r_s]$:

$$\epsilon_{corr} \approx N(0.9163/r_s) + E_0^B + E_{02}^F(\rho, 0) + E_{03}^F(\rho, 0) + \Delta E^{(2)}(\rho, 0) . \quad (26)$$

Numerical results are tabulated in Table II and compared in Fig. 2 with those obtained by others. It appears that our procedure yields a somewhat higher correlation energy. However, there is evidence that this discrepancy may be owing largely to the inadequacy in the evaluation of E_0^B. Monnier[15] has recently performed a Monte Carlo cal-

TABLE II. Ground-state and correlation energies (in rydberg).

r_s	E_0^B/N	E_{01}^F/N	E_{02}^F/N	E_{03}^F/N	$\Delta E^{(2)}(0)/N$	E_0^F/N	ϵ_{corr}/N
1	−0.7691	2.2099	−0.1863	−0.0329	−0.0043	1.2173	−0.0763
2	−0.4478	0.5525	−0.0662	−0.0126	−0.0022	0.0039	−0.0706
3	−0.3237	0.2455	−0.0340	−0.0066	−0.0014	−0.1202	−0.0603
4	−0.2557	0.1381	−0.0207	−0.0040	−0.0010	−0.1433	−0.0523
5	−0.2120	0.0884	−0.0318	−0.0027	−0.0007	−0.1408	−0.0460
6	−0.1813	0.0614	−0.0097	−0.0019	−0.0005	−0.1320	−0.0407
10	−0.1148	0.0221	−0.0035	−0.0007	−0.0002	−0.0971	−0.0276
20	−0.0597	0.0055	−0.0009	−0.0002	−0.00005	−0.0553	−0.0150

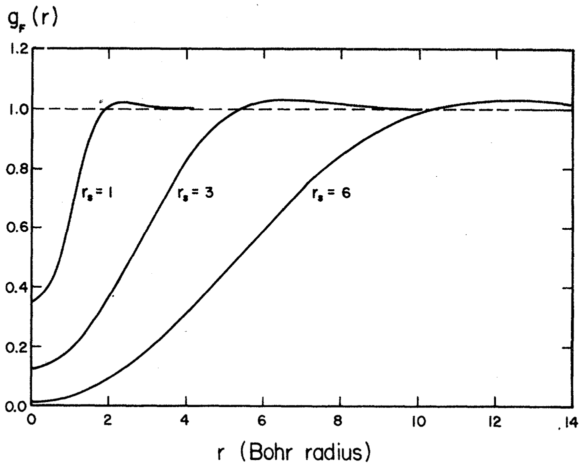

FIG. 3. Pair-distribution function $g_F(r)$ at three different densities. The distance r is in units of Bohr radius.

culation on the correlation energy of an electron gas based also on the Wu–Feenberg formulation and a variational calculation of E_0^B. While his numbers on the electron correlation energy are about 0.015 Ry lower than those of ours (see Fig. 2), his values on E_0^B are approximately 0.03 Ry below the best existing results, including those tabulated in Table I, in the density range under consideration. Accepting his values as an upper bound,[15] this would indicate the possibility of further improvement in the evaluation of E_0^B, although we have found it extremely difficult to achieve this based on the variational form of E^B given by (23). On the other hand, we have used correlation factors suggested by Becker *et al.*[8] in a variational calculation for the electron gas, but have been unable to reproduce their values for the correlation energy. It therefore seems that the values given by Becker *et al.*[8] may actually be on the lower side. Based on these considerations, it is reasonable to conclude that the Wu–Feenberg theory is adequate for an electron-gas system provided that the problem of the corresponding charged Bose gas can be solved with sufficient accuracy. Now our result shows that the correction to the correlation energy due to the particle-hole excitation is negligible in the density range considered. As a preliminary application of the Wu–Feenberg theory we shall not further consider these perturbative corrections in this paper. It must be emphasized, however, that these corrections may very well play an important role in the computation of the transport properties, which would be a topic for further investigation.

The pair-distribution function $g_F(r)$ can be computed using (13). We show in Fig. 3 the result for three different densities. For large and intermediate r the behavior of our $g_F(r)$ is close to that obtained by Singwi *et al.*[6] We have also computed the low-temperature specific heat and the spin susceptibility using (17) and (18). First from (16) and (21), we have

$$f_0(k_F, y) = e_F(y-1)\exp[(9\pi/8\alpha^2)^{1/3}(1-y)] + (\text{higher-order terms})\,. \tag{27}$$

Stopping at the three-particle term given explicitly in (15), we find

$$C/C_0 = (1 + a_2 + a_3)^{-1}\,, \qquad \chi/\chi_0 = (1 + b_2 + b_3)^{-1}\,, \tag{28}$$

with

$$a_2 = (3/16p^2)[1 - 1/p + (4p + 3 + 1/p)e^{-4p}]\,,$$

$$b_2 = -(3/16p^3)[1 - (1 + 4p + 8p^2)e^{-4p}]\,,$$

where

$$p = \tfrac{1}{4}(9\pi/\alpha^2)^{1/3}\,.$$

The numbers a_3 and b_3 are given in terms of multidimensional integrals obtained by substituting the second term in (15) and (16) into (17) and (18). These integrals have been evaluated numerically using the Monte Carlo method. Results are presented in Tables III and IV where they are also compared with those obtained by others. The specific heat is compared in Table III with the values obtained by Hedin,[7] Rice,[16] and by Silverstein.[17] These results do not differ much and all lead to effective masses close to 1. For $r_s < 1$, our re-

TABLE III. Specific heat $C/C_0 = (1 + a_2 + a_3)^{-1}$.

r_s	a_2	a_3	C/C_0	Hedin[a]	Rice[b]	Silverstein[c]
1	0.031	0.008	0.962	0.961	0.96	
2	0.028	0.007	0.967	0.969	0.99	1.02
3	0.022	0.007	0.971	0.979	1.02	1.05
4	0.017	0.006	0.976	0.987	1.06	1.10
5	0.014	0.005	0.980	0.993		
6	0.013	0.002	0.985	0.998		

[a]Reference 7. [b]Reference 16. [c]Reference 17.

TABLE IV. Spin susceptibility $\chi/\chi_0 = (1 + b_2 + b_3)^{-1}$.

r_s	b_2	b_3	χ/χ_0	Rice[a]	Silverstein[b]	Dupree and Geldart[c]
1	−0.069	−0.045	1.14	1.15		
2	−0.142	−0.087	1.30	1.26	1.26	1.31
3	−0.188	−0.114	1.44	1.40	1.28	1.48
4	−0.218	−0.132	1.54	1.48	1.29	1.65
5	−0.235	−0.142	1.61			1.83
6	−0.244	−0.152	1.65			2.05

[a]Reference 16. [b]Reference 17. [c]Reference 19.

sults coincide with those of Hedin.[7] The situation is somewhat different in the calculation of the spin susceptibility. It is well known[18] that the many-body interaction leads to an enhancement of the paramagnetic susceptibility of an electron gas. As shown in Table IV, our calculation shows a greater enhancement than the values obtained by Rice[16] and Silverstein.[17] However, the recent calculations by Dupree and Geldart[19] and by Pizzimenti *et al.*[20] lead to values that are further enhanced in the high-r_s region. The results of Dupree and Geldart[19] are also included in Table IV. The main difference lies in the fact that our values, like those of Rice and Silverstein, tend to saturate for high r_s, while those of Refs. 19 and 20 lead to curves that bend upward for larger r_s. It is of interest to note that the experimental points, as reported in Refs. 19 and 20, also show the tendency of flattening out at high r_s.

V. CONCLUSIONS

We have carried out calculations on the ground state of an electron gas in the intermediate density range $1 \leq r_s \leq 6$. The calculations are based on the Feenberg–Wu–Woo theory of Fermi liquids and a variational approach to the charged Bose gas. While it appears that the variational calculation of the Bose system may be inadequate, a number of other possibilities exist to improve upon this calculation. The first possibility is to treat the correlation factor variationally; it is hopeful that the correlation energy can be lowered if a variational calculation is carried out for the Fermi system. One possible approach is then to treat the momentum distribution in φ_0 variationally, since it is known[21] that in an interacting Fermi system the momentum distribution does not vanish outside the Fermi level. Another possibility is to improve upon the perturbative calculations. Whil it is in principle possible to obtain the ground-state energy by computing the perturbative corrections to all orders using the basis set (3) and (6), it is in practice impractical to go beyond two or three terms in the series. This then precludes the possibility of describing the collective excitations, known to exist in an electron system, by the basis set (3) and (6). To properly take these collective excitations into consideration, it is necessary to introduce a basis set containing the collective coordinates explicitly. Progress is being made in formulating the perturbative theory using these wave functions.[22]

After the completion of this work we received a preprint from Ree and Lee[23] in which they reported a similar calculation on the correlation energy of an electron gas. While their results on the correlation energy are comparable to ours, we have gone further in this paper to include the second-order perturbative corrections and compute other ground-state properties.

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APPENDIX A: EVALUATION OF $E_{02}^F(\rho,x)$ AND $E_{03}^F(\rho,x)$

The integrals in $E_{02}^F(\rho, x)$, given in (25), can be evaluated straightforwardly upon using (21) for $S(k)$:

$$\int_0^1 (y^4 - \tfrac{3}{2}y^5 + \tfrac{1}{2}y^7)\, u(2k_F^+ y)\, dy = (3/2D_+^4)\,[1 - D_+ - e^{-D_+} + \tfrac{1}{4}\pi^{1/2} D_+^{3/2}\,\mathrm{erf}(D_+^{1/2})]\,, \quad \text{(A1)}$$

where $D_\pm = (9\pi/\alpha^2)^{1/3}(1 \pm x)^{2/3}$. We then find

$$E_{02}^F(\rho, x) = -18N\epsilon_F(\alpha^2/9\pi)^{4/3}\,\{2 - D_+ - D_- - e^{-D_+} - e^{-D_-} + \tfrac{1}{4}\pi^{1/2}[D_+^{3/2}\,\mathrm{erf}(D_+^{1/2}) + D_-^{3/2}\,\mathrm{erf}(D_-^{1/2})]\}\,, \quad \text{(A2)}$$

where $\mathrm{erf}(x) = (2/\pi^{1/2})\int_0^x e^{-t^2}dt$ is the error function.

The ninefold integration in $E_{03}^F(\rho, x)$ can be reduced to a sixfold integration as follows:

$$\int y_{12}^2 S(k_F^+ y_{12})\, u(k_F^+ y_{23})\, u(k_F^+ y_{31})\, d\vec{y}_1\, d\vec{y}_2\, d\vec{y}_3 = 8\pi^2 \int_0^1 dy_1 \int_0^1 dy_2 \int_0^1 dy_3 \int_{-1}^1 d\omega \int_{-1}^1 d\mu \int_0^{2\pi} d\varphi \times [\, y_1^2 y_2^2 y_3^2 y_{12}^2 S(k_F^+ y_{12})\, u(k_F^+ y_{23})\, u(k_F^+ y_{31})] \quad \text{(A3)}$$

with

$$y_{12}^2 = y_1^2 + y_2^2 - 2y_1 y_2 \omega\,, \quad y_{31}^2 = y_1^2 + y_3^2 - 2y_1 y_3 \mu\,,$$
$$y_{23}^2 = y_2^2 + y_3^2 - 2y_3 y_2[(1-\omega^2)^{1/2}(1-\mu^2)^{1/2}\cos\varphi + \omega\mu]\,, \quad \text{(A4)}$$

and $\omega \equiv \cos(\vec{y}_1, \vec{y}_2)$ and $\mu \equiv \cos(\vec{y}_1, \vec{y}_3)$. This then gives us

$$E_{03}^F(\rho, x) = -\tfrac{1}{2}N\epsilon_F\,(3/8\pi)^3\, 8\pi^2 \int_0^1 dy_1 \int_0^1 dy_2 \times \int_0^1 dy_3 \int_{-1}^1 d\omega \int_{-1}^1 d\mu \int_0^{2\pi} d\varphi\, y_1^2 y_2^2 y_3^2 y_{12}^2 \times [(1+x)^{11/3} S(k_F^+ y_{12})\, u(k_F^+ y_{23})\, u(k_F^+ y_{31}) + (1-x)^{11/3} S(k_F^- y_{12})\, u(k_F^- y_{23})\, u(k_F^- y_{31})]\,. \quad \text{(A5)}$$

We have evaluated the integral (A5) using the Monte Carlo method. As an independent check on the accuracy of our evaluation, we have also evaluated $E_{03}^F(\rho, 0)$ at $r_s = 1$ with a six-dimensional Simpson's rule. The two results agree to within 3%.

APPENDIX B: EVALUATION OF $\Delta E^{(2)}$

The second-order perturbative correction to the ground-state energy, $\Delta E^{(2)}$, from the consideration of the pair-excited states has been derived in Ref. 11. With some minor change of notations, the expression is

$$\Delta E^{(2)} = Ne_F(3/8\pi)^3 \int_{x_i<1,x_{i'}>1} d\vec{x}_1 d\vec{x}_2 d\vec{x}_{1'} d\vec{x}_{2'}\, \delta(\vec{x}_1+\vec{x}_2-\vec{x}_{1'}-\vec{x}_{2'}) \times [f_1(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'}) + f_2(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'}) - f_3(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'})] , \tag{B1}$$

where

$$\begin{aligned} f_1(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'}) &\equiv (x_{11'}^2 - \tfrac{1}{4}A_{1'2';12} - x_{11'}^4/A_{1'2';12})u^2(k_F x_{11'}) , \\ f_2(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'}) &\equiv (x_{1'2}^2 - \tfrac{1}{4}A_{1'2';12} - x_{1'2}^4/A_{1'2';12})u^2(k_F x_{1'2}) , \\ f_3(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'}) &\equiv (\tfrac{1}{2}(x_{11'}^2 + x_{1'2}^2) - \tfrac{1}{4}A_{1'2';12} - x_{11'}^2 x_{1'2}^2/A_{1'2';12})u(k_F x_{11'})u(k_F x_{1'2}) , \\ A_{1'2';12} &\equiv (1/e_F)[E^{(0)}(\vec{k}_{1'},\vec{k}_{2'},\vec{k}_3,\ldots,\vec{k}_N) - E^{(0)}(\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots,\vec{k}_N)] , \end{aligned} \tag{B2}$$

and $\vec{x}_i \equiv \vec{k}_i/k_F$.

We first consider an integral of the form

$$I \equiv \int_{x_{i'}>1} d\vec{x}_{1'} d\vec{x}_{2'}\, \delta(\vec{x}_1+\vec{x}_2-\vec{x}_{1'}-\vec{x}_{2'}) f(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{2'}) = \int_{\substack{x_{1'}>1 \\ |\vec{x}_1+\vec{x}_2-\vec{x}_{1'}|>1}} d\vec{x}_{1'} f(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_1+\vec{x}_2-\vec{x}_{1'})$$
$$= \int_0^{2\pi} d\varphi \int_{-1}^{1} d\mu \int_1^\infty x_{1'}^2\, dx_{1'}\, f(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_1+\vec{x}_2-\vec{x}_{1'}) , \quad |\vec{x}_1+\vec{x}_2-\vec{x}_{1'}|>1 \tag{B3}$$

where we have introduced the spherical coordinates with the vector $\vec{x}=\vec{x}_1+\vec{x}_2$ pointing in the z direction and $\mu \equiv \cos(\vec{x},\vec{x}_{1'})$. The integral (B3) has been evaluated by Woo[11] using a rather complicated geometrical construction. A simpler procedure is as follows. The restriction $|\vec{x}_1+\vec{x}_2-\vec{x}_{1'}|>1$ may be written as

$$\mu < F \equiv (x^2 + x_{1'}^2 - 1)/2x x_{1'} , \tag{B4}$$

where $x \equiv |\vec{x}_1+\vec{x}_2|$. Now, for $0<x<2$ and $x_{1'}>1$, the ranges of F are

$$\begin{aligned} F &> 1 \quad \text{for } x_{1'} > x+1 , \\ -1 < F &< 1 \quad \text{for } 1 < x_{1'} < x+1 . \end{aligned} \tag{B5}$$

The range of μ is therefore restricted to $\{-1, F\}$ for $x_{1'}<x+1$. The integral (B3) now reduces to

$$I = \int_0^{2\pi} d\varphi \left(\int_1^{x+1} dx_{1'} \int_{-1}^{F} d\mu + \int_{x+1}^{\infty} dx_{1'} \int_{-1}^{1} d\mu \right) f(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_1+\vec{x}_2-\vec{x}_{1'}) . \tag{B6}$$

The expression (B6) is considerably simpler than the one derived by Woo. Substituting (B6) into (B1) and making use of the relation

$$\int_{x_i<1} d\vec{x}_1 d\vec{x}_2 = 8\pi^2 \int_0^1 x_1^2\, dx_1 \int_0^1 x_2^2\, dx_2 \int_{-1}^{1} d(\cos(\vec{x}_1,\vec{x}_2)) = 8\pi^2 \int_0^1 x_1^2\, dx_1 \int_0^1 x_2^2\, dx_2 \int_{|x_1-x_2|}^{x_1+x_2} x\, dx/x_1 x_2 , \tag{B7}$$

we obtain

$$\Delta E^{(2)} = Ne_F(3/8\pi)^3\, 8\pi^2 \int_0^1 x_1\, dx_1 \int_0^1 x_2\, dx_2 \int_{|x_1-x_2|}^{x_1+x_2} x\, dx \int_0^{2\pi} d\varphi \left(\int_1^{x+1} dx_{1'} \int_{-1}^{F} d\mu + \int_{x+1}^{\infty} dx_{1'} \int_{-1}^{1} d\mu \right)(f_1+f_2-f_1) \tag{B8}$$

Here,

$$f_i = f_i(\vec{x}_1,\vec{x}_2,\vec{x}_{1'},\vec{x}_{1'}-\vec{x}_1-\vec{x}_2) ,$$

$$\vec{x}=\vec{x}_1+\vec{x}_2 , \qquad \mu=\cos(\vec{x},\vec{x}_{1'}) ,$$

and φ is the azimuthal angle of $\vec{x}_{1'}$ in a plane perpendicular to $\vec{x}$.

In our evaluation of (B8), the expression of $A_{1'2';12}$ is approximated by[11]

$$\begin{aligned} A_{1'2';12} &\approx [E_1^F(\vec{k}_{1'},\vec{k}_{2'},\vec{k}_3,\ldots,\vec{k}_N) - E_1^F(\vec{k}_1,\vec{k}_2,\ldots,\vec{k}_N)](1/e_F) \\ &= x_{1'}^2 + x_{2'}^2 - x_1^2 - x_2^2 . \end{aligned} \tag{B9}$$

The key formulas which give $x_{11'}$ and $x_{1'2}$ in terms of the integration variables can be found in Ref. 11. The remaining six-dimensional integral in (B8) is then carried out using the Monte Carlo method.

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Translational Hydrodynamics and Light Scattering from Molecular Fluids*

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The density fluctuations in a molecular fluid are studied by treating the fluid as a multicomponent reacting mixture. The *ordinary* hydrodynamic equations for a reacting mixture form the starting point of the present derivation. The description is then contracted to that appropriate for the one-component molecular fluid. The resulting *translational hydrodynamics* theory contains memory effects due to the internal relaxation process. The results are compared with a recent kinetic model and with two previous theories of Mountain. The dynamic structure factor $S(k, \omega)$ and the roots of the dispersion relation are computed for parahydrogen gas and studied as a function of density. The results indicate that the treatment of the thermal-diffusivity mode in the theories by Mountain breaks down in the low-density region. It is suggested that Rayleigh–Brillouin scattering experiments on dilute parahydrogen gas at room temperature and densities between 5 and 30 amagats can quantitatively verify the predictions of translational hydrodynamics.

I. INTRODUCTION

In this article we consider the calculation of density fluctuations in a single-component molecular fluid, and the interpretation of light scattering experiments which can be used to probe these fluctuations. For simple liquids, it is natural to attempt such calculations by using the linearized hydrodynamic equations.[1] However, it is well known from ultrasonics[2] and light scattering experiments[3] that for molecular fluids these equations do not correctly describe the frequency dependence of the sound absorption coefficient or the spectrum of the scattered light. If the molecular fluid is a dilute gas, the appropriate kinetic equations are well known and have been used to interpret the Brillouin spec-