Ground-state energy of charged quantum fluids in two dimensions

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(Received 24 March 1986; revised manuscript received 18 June 1986)

The ground state of a two-dimensional charged quantum system is studied using the method of correlated-basis functions. For particles obeying the Bose-Einstein statistics we compute the ground-state energy variationally for all particle densities using the Bijl-Dingle-Jastrow trial wave function. The Bose ground-state energy and wave function so determined are used next to study the Fermi system. We compute the Fermi ground-state energy using a cluster expansion approach, which is again valid for all particle densities, and find that the ground state is paramagnetic. While these calculations provide variational upper bounds to the ground-state energies, we also establish independent lower bounds to the ground-state energies.

I. INTRODUCTION

Recent discoveries of the quantized Hall effect,[1,2] especially of the fractional quantization, indicate that a two-dimensional (2D) electron gas in a strong magnetic field behaves as a many-body quantum system. To achieve a truly first-principles understanding of the quantized Hall effect, therefore, it is important to consider the electron gas as a many-body quantum system by taking the Coulomb interactions into consideration. As a first step toward achieving this goal, we consider in this paper the ground state of a 2D charged quantum system which can satisfy either the Fermi-Dirac (FD) or Bose-Einstein (BE) statistics, and in the absence of an external magnetic field. Indeed, the problem of a 2D electron gas has been of increasing recent interest. Its ground-state properties have been studied under the ring-diagram approximation,[3,4] and under the random phase, Hubbard, and the self-consistent approximations.[5] More recently, the problem of a 2D quantum electron gas has been studied under an effective-potential expansion[6] and under the ladder approximation.[7,8] Substantial differences appear to exist between these numerical results to warrant a further study of the problem. In this paper we study the ground-state energy of 2D charged Bose and Fermi systems using a variational correlated-basis-function (CBF) approach.[9]

The CBF approach to the study of quantum-mechanical many-particle systems is a first-principles formulation which, when used with a complete set of basis functions, does not involve uncontrolled approximations. The first step of the CBF approach is the use of a variational wave function (upon which a complete set of basis functions can be built). In this paper we carry out this variational calculation, and compare our results with prior results and a prior Monte Carlo study[10] using similar variational wave functions. Our study is a natural extension of applications of the variational CBF approach to three-dimensional (3D) charged Bose[11] and Fermi[12,13] systems. While the variational approach provides an upper bound to the ground-state energy, we also establish in this paper an independent lower bound for the ground-state energy.

The organization of this paper is as follows. In Sec. II, the quantum many-body problem at hand is defined and formulated, and a lower bound for the ground-state energy is obtained. In Sec. III, we use a variational wave function to evaluate the ground-state energy for the Bose system. The Bose ground-state energy and wave function so determined are used in Sec. IV to compute the ground-state energy of the Fermi system, and the results are compared with those previously obtained.

II. LOWER BOUND FOR THE GROUND-STATE ENERGY

Consider a system of N charged particles, each possessing mass m and charge $-e$, confined to a uniform neutralizing background of area A. We shall consider the limit of $N\to\infty$, $A\to\infty$, while holding the particle density $\sigma=N/A$ constant. The Hamiltonian of the system is given by

$$H=T+V\,, \tag{2.1}$$

where

$$T=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 \tag{2.2}$$

and

$$V=\tfrac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\(j\neq i)}}^{N}v(r_{ij})-\tfrac{1}{2}\sigma^2\int\int v(r_{12})d\mathbf{r}_1 d\mathbf{r}_2 \tag{2.3}$$

are, respectively, the kinetic- and potential-energy operators. Here, $v(r)=e^2/r$ is the Coulomb interaction between two particles at a distance r apart. The last term in (2.3) represents the interaction energy due to the presence of the uniform charge background. The particles obey either the Fermi-Dirac or the Bose-Einstein statistics.

Our goal is to compute the ground-state energy for the Hamiltonian (2.1). This means that, for particles of a given density and statistics, we seek for the lowest eigenvalue of H in the subspace of wave functions obeying the associated symmetry. Thus, the ground-state solutions of the Schrödinger equations

$$H\Psi_0^B = E_0^B \Psi_0^B \quad \text{(BE statistics)}, \tag{2.4}$$

$$H\Psi_0^F = E_0^F \Psi_0^F \quad \text{(FD statistics)}, \tag{2.5}$$

with respective symmetric and antisymmetric eigenfunctions, give rise to the ground-state energies E_0^B, E_0^F and wave functions Ψ_0^B, Ψ_0^F.

We first obtain a lower bound for the ground-state energy. For the Bose system we evaluate the expectation value of H using Ψ_0^B. This leads to the expression

$$E_0^B = \langle \Psi_0^B \mid T \mid \Psi_0^B \rangle + \langle \Psi_0^B \mid V \mid \Psi_0^B \rangle . \tag{2.6}$$

Now regarding Ψ_0^B as a trial wave function for each of the two terms on the right-hand side of (2.6), we obtain the inequality[14]

$$E_0^B \geq T_0^B + V_0^B , \tag{2.7}$$

where T_0^B and V_0^B, are, respectively, the lowest eigenvalues of T and V among the symmetric wave functions. Now

$$T_0^B = 0 \tag{2.8}$$

and V_0^B is given by the classical bound[15]

$$V_0^B = -N(1.9605)e^2\sqrt{\sigma} , \tag{2.9}$$

which can be more conveniently expressed in units of rydberg $=1$ Ry $= me^4/2\hbar^2$. Introducing a dimensionless quantity r_s defined by

$$\pi a_B^2 r_s^2 = \sigma^{-1} , \tag{2.10}$$

where $a_B = \hbar^2/me^2$ is the Bohr radius, one finds that

$$e^2\sqrt{\sigma} = \frac{2}{(\pi r_s)^{1/2}} \text{ Ry} . \tag{2.11}$$

It follows from (2.7) that a lower bound for E_0^B, in units of Ry, is given by

$$E_0^B \geq -N(2.2122)/r_s . \tag{2.12}$$

Repeating the same argument for the Fermi system and noting that a system of N charged fermions has the same lower bound (2.9) for its potential energy, we arrive at

$$E_0^F \geq T_0^F + V_0^B , \tag{2.13}$$

where T_0^F is the lowest eigenvalue of T among the antisymmetric wave functions. Allowing the possibility that the system may actually have different numbers of spin-up and spin-down electrons, we write

$$N_\pm = N(1 \pm x)/2 , \tag{2.14}$$

where N_+ and N_- are the respective electron numbers. A simple calculation of the energy of two filled Fermi circles (the ground state) leads to the following expression for T^F, in units of Ry [cf. (4.8) and (4.11) below]:

$$T_0^F(x) = N(1+x^2)/r_s^2 . \tag{2.15}$$

This leads to the following lower bound for the Fermi ground-state energy:

$$E_0^F(x) \geq N[(1+x^2)/r_s^2 - 2.2122/r_s] . \tag{2.16}$$

III. CHARGED BOSE GAS

We now use a variational approach to compute the ground-state energy E_0^B for the charged Bose system. The variational approach is based on the Bijl-Dingle-Jastrow-(BDJ-) type wave function in the form[9]

$$\Psi_0^B = \frac{\exp\left[\frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\(i<j)}}^{N} w(r_{ij})\right]}{\left[\int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N \exp\left[\sum_{i=1}^{N}\sum_{\substack{j=1\\(i<j)}}^{N} w(r_{ij})\right]\right]^{1/2}} , \tag{3.1}$$

where the function $w(r)$ is to be varied. The expectation value E_0^B of the Hamiltonian (2.1) computed using the wave function (3.1) can be written as[9]

$$\begin{aligned} E_0^B &= \int \cdots \int \Psi_0^B H \Psi_0^B d\mathbf{r}_1 \cdots d\mathbf{r}_N \\ &= N(\hbar^2\sigma/8m) \int \nabla w(r) \cdot \nabla g_B(r) d\mathbf{r} \\ &\quad + \tfrac{1}{2} N\sigma e^2 \int [g_B(r) - 1] d\mathbf{r}/r , \end{aligned} \tag{3.2}$$

where the pair-distribution function is defined by

$$g_B(r_{12}) = [N(N-1)/\sigma^2] \int \cdots \int (\Psi_0^B)^2 d\mathbf{r}_3 \cdots d\mathbf{r}_N . \tag{3.3}$$

We now introduce the hypernetted-chain (HNC) approximation[16]

$$w(r) = \ln g_B(r) - \frac{1}{(2\pi)^2\sigma} \int e^{i\mathbf{k}\cdot\mathbf{r}} [1 - S(k)]^2 d\mathbf{k}/S(k) , \tag{3.4}$$

where

$$S(k) = 1 + u(k) = 1 + \sigma \int e^{i\mathbf{k}\cdot\mathbf{r}} [g_B(r) - 1] d\mathbf{r} \tag{3.5}$$

is the boson structure factor. The introduction of (3.4) into (3.2) now permits us to regard E_0^B as a functional in g_B so that we may vary, instead of w, the function g_B to obtain a minimum for E_0^B. To this end we follow Lee[11] by adopting the ansatz

$$g_B(r) = 1 - \alpha \exp(-\pi\alpha\sigma r^2) \tag{3.6}$$

and consider $0 < \alpha < 1$ as the varying parameter. It must be emphasized at this point that while the variation of g_B appears to be a reasonable proposition, it should also be remembered that the definition (3.3) imposes certain necessary conditions on g_B that should be checked. One example is the inequality[17]

$$N\sigma e^2 \int [g_B(r) - 1] d\mathbf{r}/r \geq 2V_0^B , \tag{3.7}$$

which is indeed satisfied by (3.6).

The boson structure factor corresponding to (3.6) is

$$S(k) = 1 - \exp(-k^2/4\pi\alpha\sigma) . \tag{3.8}$$

Substituting (3.4) into (3.2) leads to

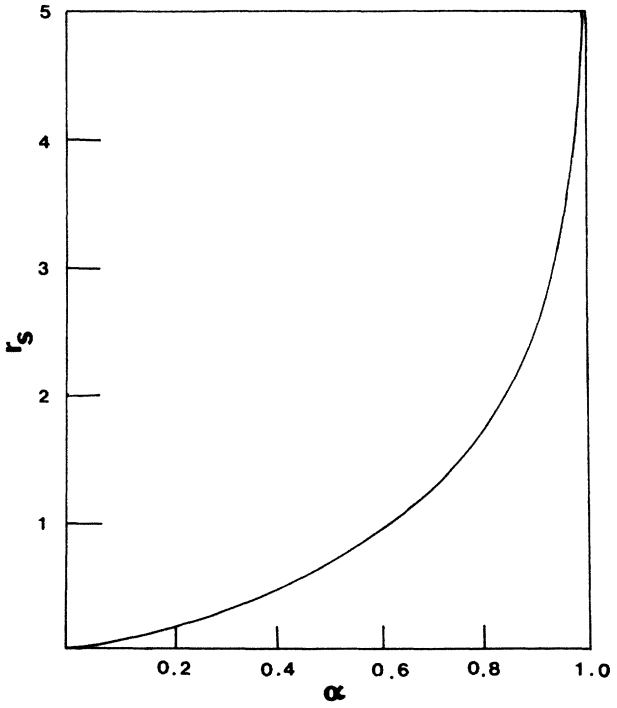

FIG. 1. Determination of α.

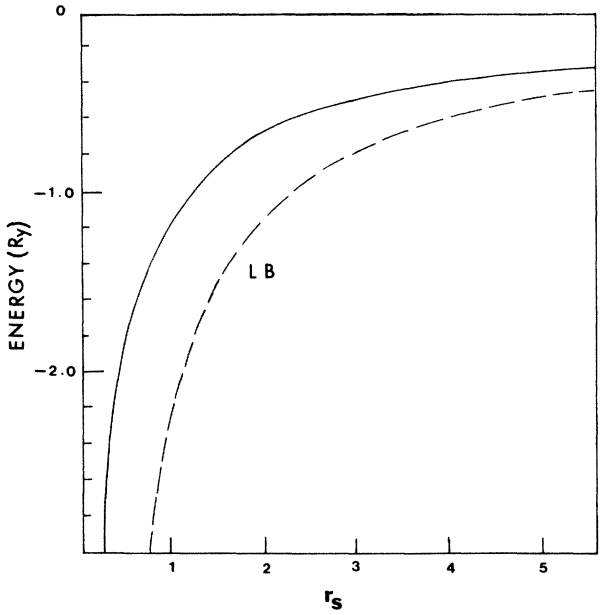

FIG. 2. Ground-state energy of the Bose system. Solid line: present calculation; LB: lower bound (2.12).

$$E_0^B = N\frac{\hbar^2\sigma}{8m}\int d\mathbf{r}[\nabla g_B(r)]^2/g_B(r) + N\frac{\hbar^2}{32\pi^2 m\sigma}\int d\mathbf{k}\,k^2[1-S(k)]^3/S(k) + \tfrac{1}{2}N\sigma e^2\int [g_B(r)-1]d\mathbf{r}/r\ . \tag{3.9}$$

Now using (3.6) and (3.8), and after some reduction, (3.9) becomes, in units of Ry,

$$E_0^B(\alpha)=N\left[\frac{\alpha^2}{r_s^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{(n+2)^2}+\frac{\alpha^2}{r_s^2}\left[\frac{\pi^2}{6}-\frac{5}{4}\right]-\frac{\sqrt{\pi}\alpha}{r_s}\right], \tag{3.10}$$

where the three terms on the right-hand side of (3.10) come from the evaluations of the corresponding integrals in (3.9).

It is now a simple matter to minimize $E_0^B(\alpha)$ with respect to α, yielding

$$\sqrt{\pi}r_s=2\alpha^{3/2}\{[-\alpha-\ln(1-\alpha)]/\alpha^2+2(\pi^2/6-\tfrac{5}{4})\}\ . \tag{3.11}$$

For fixed σ, or r_s, we determine α from (3.11) and, subsequently, E_0^B from (3.10). It turns out that it is most convenient using (3.11) to evaluate r_s as a function of α. The result of this calculation is shown in Fig. 1. Results of numerical evaluation of E_0^B are presented in Fig. 2 (and also Table I below) where the classical bound (2.12) is also shown for comparison. Note that in the low-density limit ($r_s\to\infty$) we have

$$\alpha\cong 1-e^{-\sqrt{\pi}r_s/2} \tag{3.12}$$

and

$$E_0^B\cong -N\sqrt{\pi}/r_s\ , \tag{3.13}$$

while in the high-density limit ($r_s\to 0$) we find

TABLE I. Evaluation of E_0^F ($x=0$) (in units of rydbergs).

r_s	σ (10^{15}/cm^2)	α	E_0^B/N	E_{01}^F/N	E_{02}^F/N	E_{03}^F/N	E_0^F/N
1.0	11.3671	0.6417	−1.1062	1.000	−0.2576	−0.0378	−0.4016
2.0	2.8418	0.8527	−0.6631	0.2500	−0.0859	−0.0112	−0.5102
3.0	1.2630	0.9404	−0.4818	0.1111	−0.0417	−0.0052	−0.4176
4.0	0.7104	0.9759	−0.3796	0.0625	−0.0242	−0.0030	−0.3443
5.0	0.4547	0.9902	−0.3133	0.0400	−0.0157	−0.0019	−0.2909
6.0	0.3158	0.9960	−0.2666	0.0278	−0.0109	−0.0013	−0.2510
8.0	0.1776	0.9993	−0.2053	0.0156	−0.0062	−0.00074	−0.1966
10.0	0.1137	0.999 89	−0.166 85	0.0100	−0.003 95	−0.000 476	−0.1613
20.0	0.02842	0.999 999	−0.086 024	0.0025	−0.000 987	−0.000 119	−0.084 63

$$\alpha \cong \left[\frac{3\sqrt{\pi} r_s}{2(\pi^2-6)}\right]^{2/3} = 0.7786 r_s^{2/3} \tag{3.14}$$

and

$$E_0^B \cong -1.1730 N r_s^{-2/3} . \tag{3.15}$$

IV. CHARGED FERMI GAS

For a charged Fermi system we look for the ground-state solution of (2.5) with a ground-state wave function Ψ_0^F antisymmetric in the N-particle coordinates. Following Wu and Feenberg[18] we choose the trial wave function Ψ_0^F to be a product of two factors:

$$\Psi_0^F = \Psi_0^B \phi_0 . \tag{4.1}$$

In (4.1) the factor Ψ_0^B accounts for the correlation between particles and is taken to be the ground-state wave function of the corresponding boson system, namely, the solution of (2.4).[19] The factor ϕ_0 in (4.1) is the model function taking into account the statistics of particles; we choose ϕ_0 to be the $N \times N$ determinant consisting of the N plane-wave orbitals

$$\phi_0 = \det | e^{i\mathbf{k}_m \cdot \mathbf{r}_n} s_m(\sigma_n) | , \tag{4.2}$$

where $\mathbf{k}_m$ are 2D wave vectors satisfying periodic boundary conditions and $s_m(\sigma_n)$ are spin functions. Furthermore, for each up or down spin component, the wave vectors are confined to a Fermi circle with the Fermi momentum

$$k_F^{\pm} = k_F(1 \pm x)^{1/2} , \tag{4.3}$$

where

$$k_F = \sqrt{2\pi\sigma} . \tag{4.4}$$

The expectation value H in Ψ_0^F can be evaluated using a cluster expansion method. Following a standard procedure[10,18] and using (2.4), we obtain

$$E_0^F(\mathbf{k}_1\sigma_1;\ldots;\mathbf{k}_N,\sigma_N) = \int (\Psi_0^F)^* H \Psi_0^F \Big/ \int (\Psi_0^F)^* \Psi_0^F = E_0^B + E_{01}^F + E_{02}^F + E_{03}^F + \cdots , \tag{4.5}$$

where the integrations extend over the N particle and spin coordinates. Terms in (4.5) are given by

$$E_{01}^F = \frac{\hbar^2}{2m} \sum_{\text{spin}} \sum_n k_n^2 ,$$

$$E_{02}^F = \frac{\hbar^2}{4mN} \sum_{\text{spin}} \sum_{l,n} k_{\ln}^2 u(k_{\ln}) \delta_{\ln} , \tag{4.6}$$

$$E_{03}^F = -\frac{\hbar^2}{4mN^2} \sum_{\text{spin}} \sum_{q,l,n} k_{ql}^2 S(k_{ql}) u(k_{\ln}) u(k_{nq}) \delta_{qln} ,$$

where $\delta_{\ln} = \delta_{\mathrm{Kr}}(\sigma_l, \sigma_n)$, $\delta_{qln} = \delta_{ql}\delta_{\ln}$, $k_{\ln} = |\mathbf{k}_l - \mathbf{k}_n|$, and $S(k)$ and $u(k)$ are given by (3.5) in terms of the pair-distribution function $g_B(r)$. Substituting (3.6) into (3.5) and (4.6), we obtain the following explicit expression for the ground-state energy as a function of x:

$$E_0^F(\sigma,x) = E_0^B(\sigma) + E_{01}^F(\sigma,x) + E_{02}^F(\sigma,x) + E_{03}^F(\sigma,x) + \cdots , \tag{4.7}$$

where

$$E_{01}^F(\sigma,x) = \frac{N\hbar^2}{8\pi^3\sigma m}\left[\int_{k<k_F^+} d\mathbf{k}\, k^2 + \int_{k<k_F^-} d\mathbf{k}\, k^2\right] = \frac{N}{2}\varepsilon_F(1+x^2) , \tag{4.8}$$

$$E_{02}^F(\sigma,x) = -\frac{N\hbar^2}{64\pi^4\sigma^2 m} \sum_{k=k_F^{\pm}} \int_{k_1<k} \int_{k_2<k} k_{12}^2 e^{-k_{12}^2/4\pi\alpha\sigma} d\mathbf{k}_1 d\mathbf{k}_2$$

$$= -\frac{4N}{\pi}\varepsilon_F \sum_{z=\pm x} (1+z)^3 \int_0^1 [2\cos^{-1}y - y(1-y^2)^{1/2}] y^3 e^{-2y^2(1+z)/\alpha} dy , \tag{4.9}$$

$$E_{03}^F(\sigma,x) = \frac{-N\hbar^2}{256\pi^6\sigma^3 m} \sum_{k=k_F^{\pm}} \int_{k_1<k} \int_{k_2<k} \int_{k_3<k} k_{12}^2 (1-e^{-k_{12}^2/4\pi\alpha\sigma}) e^{-(k_{23}^2+k_{31}^2)/4\pi\alpha\sigma} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$

$$= -N(\varepsilon_F/2\pi)[(1+x)^4 I_+ + (1-x)^4 I_-] , \tag{4.10}$$

and

$$I_\pm = \int_0^1 dy_1 \int_0^1 dy_2 \int_0^1 dy_3 \int_0^\pi d\theta_{y_1y_2y_3}\, y_{12}^2 \{1 - \exp[-(1\pm x)y_{12}^2/2\alpha]\} \times \exp[-(1\pm x)(y_1^2+y_2^2+2y_3^2)/2\alpha] \times I_0[(1\pm x)\alpha^{-1}(y_1^2y_3^2 + y_2^2y_3^2 + 2y_1y_2y_3^2\cos\theta)^{1/2}] ,$$

where I_0 is the modified Bessel function of the first kind. The Fermi energy ε_F is given by

$$\varepsilon_F = \hbar^2 k_F^2/2m = 2/r_s^2 \text{ Ry} . \tag{4.11}$$

In obtaining expressions on the right-hand side of (4.9) and (4.10), the following identities have been used:

$$\int_{-\pi}^{\pi} e^{x\cos\theta} d\theta = 2\pi I_0(x) , \tag{4.12}$$

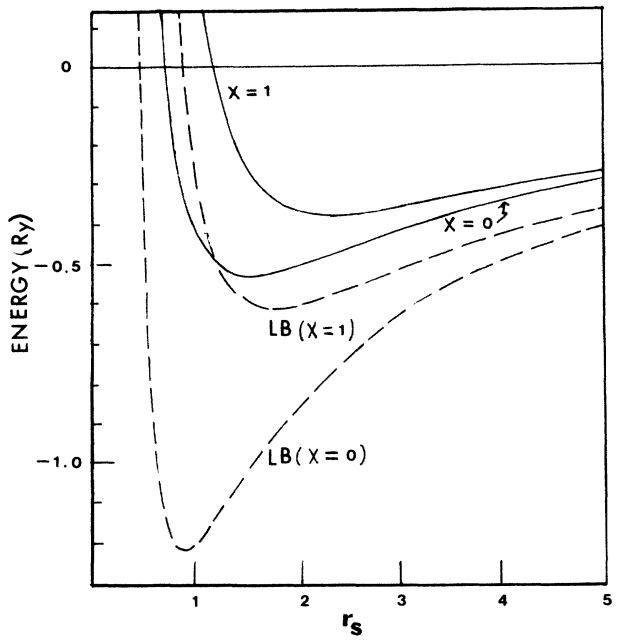

FIG. 3. Ground-state energy of the Fermi system. Solid lines: present calculation; LB: lower bounds (2.16).

$$\int_{k_1\le k_F}\int_{k_2\le k_F} f(k_{12})d\mathbf{k}_1 d\mathbf{k}_2 = 8\pi k_F^4 \int_0^1 f(2yk_F)[2\cos^{-1}y - y(1-y^2)^{1/2}]y\,dy \ . \tag{4.13}$$

We have carried out numerical evaluations of E^F given by (4.7)–(4.10) for both the paramagnetic ($x=0$) and ferromagnetic ($x=1$) states, and the results are shown in Fig. 3 together with the lower bounds (2.16). It is seen that the paramagnetic ($x=0$) state has a lower energy for all densities, agreeing with a similar conclusion drawn on the 3D system,[13] but in contrast with Ceperley's finding[10] that the ferromagnetic ($x=1$) state is preferred at low densities. However, the difference of the two energies in Ceperley's result is very small, and the finding reported by him is based on the use of a correlation factor determined under an (uncontrolled) random-phase approximation. It appears that the present finding is more likely indicative of the true nature of the ground state, and is certainly in line with the conclusion of a noninteracting system.

TABLE II. Comparison of the ground-state energy with prior results (in units of rydbergs).

r_s	E_0^F/N	Ref. 7	Ref. 8	Ref. 10
1.0	−0.4016	−0.4204	−0.45	−0.422
2.0	−0.5102	−0.5102	−0.53	
4.0	−0.3443	−0.3476		
8.0	−0.1966	−0.1984		
10.0	−0.1613			−0.1670
16.0	−0.10454	−0.10812		
20.0	−0.08463			−0.0916

Detailed numerical results of our calculation are summarized in Table I. Our results show that the series (4.7) converges rapidly, appearing to support the validity of the cluster expansion procedure used in the present study. Our results are also compared in Table II with those obtained by Freeman,[7] by Nagano, Singwi, and Ohnishi,[8] and by Ceperley,[10] and it is seen that in most cases our energy values are slightly higher than the prior results. We remark however, that, the errors of the prior studies are uncontrolled and, therefore, difficult to assess, while our study provides an estimated upper bound to the true ground-state energy. It should be noted in this connection that one version of Ceperley's Monte Carlo study, which uses a genuine overall variational approach in conjunction with a Yukawa-type correlation factor $w(r)$, also provides an upper bound. Indeed, for the few density values reported by Ceperley (cf. Table II), his Monte Carlo study does provide slightly better upper bounds. This may very well indicate that further improvement of our results can be achieved by adopting an overall variational approach for the Fermi system.

ACKNOWLEDGMENTS

We would like to thank Y. Takada for calling our attention to Refs. 5–8, 10, and 14. R.T. was supported in part by a grant from Northeastern University's Research and Scholarship Development Fund. The work of F.Y.W. was supported in part by National Science Foundation (NSF) Grant No. DMR-82-19254.

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