Correlation Energy of an Electron Gas in the Quantum Strong-Field Limit*

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The ground state of an electron gas in an intense magnetic field is studied using a wave function of the product form $\psi_0^B\Phi$. The correlation factor ψ_0^B is taken to be the ground-state solution of a charged Bose gas and Φ a determinant of single-particle Landau states. In the quantum strong-field limit so that only the lowest Landau state is populated, the correlation energy is computed using the cluster-expansion technique and a variational determination of the boson energy. Numerical results obtained are lower than those derived under the random-phase approximation.

I. INTRODUCTION

The correlation energy of a quantum-mechanical electron gas has been a subject under intensive study for many years.[1] The major effort in the past has been the calculation of the correlation energy in zero magnetic field, which depends only on the density of the system. Quite recently, attention has been focused on the effect of a magnetic field, in particular, that of a strong field under which only the lowest Landau state is populated, known as the quantum strong-field limit (QSFL).[2-5] This problem is of astrophysical interest for gravitationally collapsed bodies, such as white dwarfs and pulsars, which are characterized by high densities ($\sim 10^{31}$ cm^{-3}) and intense magnetic fields ($\sim 10^{12}$ G).[6] The QSFL can also be realized in semiconductors such as indium antimonide, with mobile carriers of effective mass $\sim 10^{-29}$ G and densities $\sim 10^{17}$ cm^{-3}, at relatively low fields ($\sim 10^5$ G).[7] The inclusion of the additional parameter of a magnetic field makes the problem of considering the electron-electron interactions more complicated. The evaluation of the exchange energy E_{ex} has been considered by a number of authors,[8] and was treated correctly only recently.[2] Kaplan and Glasser[3] argued that in extreme magnetic fields a high-density electron gas undergoes a transition to an ordered structure of charged rods, and they estimated the energy on this basis using the Hartree-Fock approximation. More recently Horing *et al.*[5] computed the correlation energy in the QSFL under the random-phase approximation (RPA). An expansion of the ground-state energy for high fields has also been derived by Isihara and Tsai[4] under the ring-diagram approximation. The extent to which these approximations are valid is not known. In this paper we carry out what we believe to be a more realistic calculation of the correlation energy in the QSFL. Our approach is based upon the Wu-Feenberg theory of fermion liquids[9] and is along the lines of the method of correlated basis functions.[10] This method has recently been used to study the ground state of an electron gas in zero field.[1,11] Here, as we shall see, the method leads to improved values of the correlation energy in the QSFL.

II. FORMULATION

Consider a system of N electrons of mass m each confined in a uniform neutralizing background of cubic volume L^3. A constant magnetic field H is applied in the z direction. We adopt the atomic units in which all distances are measured in units of the Bohr radius $a_0=\hbar^2/me^2$, energies in $\mathcal{R}_\infty=e^2/2a_0=me^4/2\hbar^2$, and magnetic fields in $H_0=\mathcal{R}_\infty/\mu_B=e^3m^2c/\hbar^3=2.350405\times10^9$ G, where $\mu_B=e\hbar/2mc$ is the Bohr magneton. Useful dimensionless parameters in these units include the size of the box, $l=L/a_0$, the field strength $h=H/H_0$, and the inverse density $r_s=(3l^3/4\pi N)^{1/3}$. We shall eventually take the limit of $N\to\infty$, $l\to\infty$ while holding r_s constant. Typical values of physical interest range from $h\sim1{,}000$, $r_s\sim0.1$ for astronomical systems to $h\sim1$, $r_s\sim1$ for semiconductors.

We shall also assume the validity of nonrelativistic quantum mechanics.[12] Using the Landau gauge $\vec{A}=(0,Ha_0x,0)$, the Hamiltonian takes the form

$$\mathcal{H}=\sum_{j=1}^{N}\mathcal{H}_{0j}+V-h\sum_{j=1}^{N}\sigma_j^z, \tag{1}$$

where

$$\mathcal{H}_{0j}=-\left[\frac{\partial^2}{\partial x_j^2}+\left(\frac{\partial}{\partial y_j}-ihx_j\right)^2+\frac{\partial^2}{\partial z_j^2}\right]. \tag{2}$$

Here the potential energy V includes the Coulomb energy between the electrons and that between the electrons and the background, and σ_j^z is the Pauli spin operator.

For the ground-state wave function of $\mathcal{H}$ we take the trial form

$$\psi_0^F = \psi_0^B \Phi\,, \tag{3}$$

where, following Ref. 1, the correlation factor ψ_0^B is taken to be the ground-state wave function of a charged Bose gas, namely,

$$\mathcal{H}_B \psi_0^B = E_0^B \psi_0^B\,, \tag{4}$$

with

$$\mathcal{H}_B = -\sum_{j=1}^{N} \nabla_j^2 + V\,. \tag{5}$$

The model function Φ in (3) takes the determinantal form

$$\Phi = (N!)^{-1/2} \det|\varphi_m(\vec{r}_j) s_m(\sigma_j)|\,, \tag{6}$$

where $\varphi_m(\vec{r}_j)$ is the single-particle Landau state satisfying

$$\mathcal{H}_{0j}\varphi_m(\vec{r}_j) = E_m \varphi_m(\vec{r}_j) \tag{7}$$

and $s_m(\sigma_j)$ is the spin function. Using (4)–(7), it can be easily shown that the expectation value of $\mathcal{H}$ in ψ_0^F leads to the expression

$$\langle \mathcal{H} \rangle_{\psi_0^F} = E_0^B + \sum_m E_m + h(N_+ - N_-) - \tfrac{1}{2}\left[\frac{\partial}{\partial\beta} \ln I(\beta)\right]_{\beta=0}\,, \tag{8}$$

where the summation $\sum_m$ extends over the N orbitals contained in Φ, N_+ and N_- are, respectively, the numbers of spins parallel and antiparallel to the applied field, and

$$I(\beta) = \int \psi_0^{B\,2} \exp(\beta \sum_j \nabla_j^2)(\Phi^* \Phi)\,, \tag{9}$$

with the integrations extending over all N sets of spatial and spin coordinates.

The last term in (8) can be evaluated by the cluster-expansion technique.[13] In the QSFL only the lowest Landau state is populated with all spins aligned antiparallel to the applied field. Thus we have

$$\varphi_m(\vec{r}) = \exp[i(p_m y + q_m z) - \tfrac{1}{2}h(x - p_m/h)^2]\,, \tag{10}$$

$$E_m = q_m^2 + h\,, \quad N_+ - N_- = -N. \tag{11}$$

The ranges of the momenta p and q in (10) are $|p| \le \frac{1}{2}hl$ and $|q| \le q_F = 3\pi/2hr_s^3$, where the Fermi momentum q_F is determined from the normalization $N = \sum_m 1 = \sum_p \sum_q 1$ in the QSFL. Using (9) we first obtain[9,13]

$$\ln I(\beta) = \sum_m \ln X_m + \sum_{m<n} x_{mn} + \sum_{m<n<p} (x_{mnp} - 3x_{mn}x_{np}) + \cdots\,, \tag{12}$$

where

$$x_{m\cdots p} = X_{m\cdots p}/X_m \cdots X_p\,,$$

$$X_m(\beta) = \int \psi_0^{B\,2} e^{\beta\nabla_1^2} \varphi_m^*(\vec{r}_1)\varphi_m(\vec{r}_1) = I_m(\beta)\,, \tag{13}$$

$$X_{mn}(\beta) = I_{mn}(\beta) - X_m(\beta)X_n(\beta)\,,$$

$$X_{mnp}(\beta) = I_{mnp}(\beta) - X_m(\beta)X_{np}(\beta) - X_n(\beta)X_{mp}(\beta) - X_p(\beta)X_{mn}(\beta) - X_m(\beta)X_n(\beta)X_p(\beta)\,,$$

etc.,

and $I_m, I_{mn}, I_{mnp}, \ldots$, are given by (9) with orbitals m; m,n; m,n,p; $\ldots$, in Φ.

The cluster integrals $X_m, X_{mn}, \ldots$, can be evaluated in terms of the n-particle distribution functions defined by ψ_0^B:

$$g_n^B(1,2,\ldots,n) = \frac{N!\, l^{3n}}{(N-n)!\, N^n} \times \int \psi_0^{B\,2}\, d\vec{r}_{n+1} \cdots d\vec{r}_N \Big/ \int \psi_0^{B\,2}\,. \tag{14}$$

Thus we find

$$X_m(0) = \frac{1}{l}\int_{-l/2}^{l/2} f_{1m}^2\, dx_1 \to \frac{1}{l}\left(\frac{\pi}{h}\right)^{1/2},$$

$$X_m'(0) = 0\,,$$

$$X_{mn}'(0) = \frac{-1}{2l}\int [g_2^B(r_{12}) - 1] \times \left[+2p_{mn}^2 + 2q_{mn}^2 - \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}\right] f_{1m} f_{1n} f_{2n} f_{2m} \times e^{i(p_{mn}y_{12} + q_{mn}z_{12})}\, d\vec{r}_1\, d\vec{r}_2\,, \tag{15}$$

etc.,

where

$$f_{jm} \equiv e^{-h(x_j - p_m/h)^2/2}.$$

In the following we shall use the normalized variational form of g_2^B:

$$g_2^B(r_{12}) = 1 - a e^{-(9a^2\pi/16)^{1/3}(r/r_s)^2}\,, \tag{16}$$

where a is the variational parameter. With this expression for g_2^B the y and z integrations in (15) can be performed using, e.g.,

$$\int_{-l/2}^{l/2} dy_1 \int_{-l/2}^{l/2} dy_2\, e^{-by_{12}^2 + ip_{mn}y_{12}} \to l(\pi/b)^{1/2} e^{-p_{mn}^2/4b}\,. \tag{17}$$

In both (15) and (17) the arrow denotes the leading result expected in the bulk limit. It must be emphasized here that these integrals are rather complicated for finite l because the range of p_m is also l dependent. Combining (8), (11), and (12), we find

$$\langle H \rangle_{\psi_0^F} = E_0^B + \sum_m q_m^2 + E_2^F + E_3^F + \cdots\,, \tag{18}$$

where

$$E_2^F = -\tfrac{1}{2}\sum_{m<n} x'_{mn}(0),$$

$$E_3^F = -\tfrac{1}{2}\sum_{m<n<p} [x'_{mnp}(0) - 6x'_{mn}(0)x_{np}(0)],$$

etc.,

are the successive cluster contributions. The summations $\sum_m$ may be replaced by integrations:

$$\sum_m \to \left(\frac{l}{2\pi}\right)^2 \int_{-hl/2}^{hl/2} dp_m \int_{-q_F}^{q_F} dq_m . \tag{19}$$

Using (15) and (17), E_2^F is thus given by a six-fold integral which, after some steps, can be evaluated in a closed form to yield

$$E_2^F = -N\frac{2ath}{(1+2t)^2}\left[(3+2t)\,\mathrm{erf}(2\sqrt{\pi}\,t/a) - \frac{2a}{\pi t}(1+t)(1-E)\right], \tag{20}$$

with

$$t = \frac{\pi}{hr_s^2}\left(\frac{3a}{4\pi}\right)^{2/3}, \quad E = e^{-4\pi t^2/a^2},$$

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt .$$

The term E_3^F can be similarly evaluated in a closed form if the three-particle distribution function g_3^B arising therein is approximated by the convolution form.[10,14] The algebra is straightforward, although quite tedious. The resulting expression is[15]

$$E_3^F = -N\frac{a^2h}{2}\left\{\frac{3-t-84t^2-176t^3-64t^4}{(1+2t)^4(1+4t)^2} I + \frac{2tJ}{3+6t+4t^2} + \frac{4(1+t)}{\pi(1+2t)^2}(1-E) - \frac{8t^2E}{a^2(1+2t)}\right.$$
$$- \frac{a(1-4t)(1-E)}{\pi(1+4t)(1+2t)^2}\,\mathrm{erf}\left(\frac{2\sqrt{\pi}\,t}{a}\right) - \frac{a\sqrt{2}}{4\pi}\frac{(11+22t+28t^2+16t^3)}{(1+4t)(1+2t)^2(3+6t+4t^2)}\,\mathrm{erf}\left(\frac{2\sqrt{(2\pi)}t}{a}\right)$$
$$\left. + \frac{a}{\pi}\left(\frac{E}{2}\right)^{1/2}\left[\frac{3-4t}{(1+2t)^2(1+4t)} + \frac{2E(1-6\pi t^2/a^2)}{3+6t+4t^2}\right]\mathrm{erf}\left(\frac{\sqrt{(2\pi)}t}{a}\right)\right\}, \tag{21}$$

where

$$I = \int_0^t \left[\mathrm{erf}\left(\frac{t+x}{a/\sqrt{\pi}}\right) + \mathrm{erf}\left(\frac{t-x}{a/\sqrt{\pi}}\right)\right]^2 dx,$$

$$J = \frac{1}{\sqrt{(2\pi)}}\int_0^{2\sqrt{\pi}\,t/a} e^{-3x^2/2}\left[\mathrm{erf}\left(\frac{x}{\sqrt{2}}\right) + \mathrm{erf}\left(\frac{2\sqrt{(2\pi)}t}{a} - \frac{x}{\sqrt{2}}\right)\right]dx .$$

In the above we have assumed a knowledge of the solution of the boson problem (4). To find E_0^B we follow the procedures of Ref. 1 by using the Jastrow wave function and the variational form (16) for g_2^B. Numerical results have been given in Ref. 1 for $1 < r_s < 20$. Further results for $0.5 < r_s < 0.6$ are included here in Table I. It is known[1] that in the density range $1 < r_s < 6$ this procedure yields E_0^B about 0.015 Ry higher than the Monte Carlo values. In the high-density limit the value of E_0^B so obtained is about 6% (~0.25 Ry at $r_s = 0.1$) below the exact value.[16] Anticipating these uncertainties to be less than 10% of the computed correlation energy, the variational form (16) appears to be reasonably adequate for our purposes of evaluating E_0^B.

III. CORRELATION ENERGY

The correlation energy, which is defined to be the difference between $\langle \mathcal{H} \rangle_{\psi_0^F}$ and the Hartree-Fock energy $E_{\mathrm{HF}} = \sum_m q_m^2 + E_{\mathrm{ex}}$, is finally given by

$$E_{\mathrm{corr}} = E_0^B - E_{\mathrm{ex}} + E_2^F + E_3^F + \cdots , \tag{22}$$

where

$$E_{\mathrm{ex}} = N\frac{hr_s^3}{3\pi^2}\left[\ln Q + \gamma + e^Q\int_Q^\infty \frac{e^{-x}}{x}dx - 4Q\int_0^\infty e^{-Qx^2}\tan^{-1}\left(\frac{1}{x}\right)dx\right], \tag{23}$$

$Q = 9\pi^2/2h^3r_s^6$,

$\gamma = 0.5772\ldots =$ Euler const.

TABLE I. Optimum values of a and the boson ground-state energy. Results for higher values of r_s can be found in Ref. 1.

r_s	a	E_0^B/N (Ry)
0.05	0.0527	−7.448
0.06	0.0603	−6.494
0.07	0.0676	−5.783
0.08	0.0745	−5.230
0.09	0.0813	−4.786
0.10	0.0877	−4.422
0.20	0.1456	−2.621
0.30	0.1949	−1.928
0.40	0.2385	−1.550
0.50	0.2785	−1.308
0.60	0.3158	−1.138

TABLE II. Numerical results for some representative values of r_s and h. All energies are in rydbergs.

r_s	h	E_{HF}/N	E_{ex}/N	E_2^F/N	E_3^F/N	E_{corr}^{RPA}/N	E_{corr}/N
0.06	800	229.40	−18.50	−12.19	−1.81	−0.078	−1.99
	1000	140.34	−18.32	−11.87	−2.29	−0.147	−2.33
0.08	600	64.80	−13.64	−8.93	−2.05	−0.167	−2.57
	800	31.19	−12.93	−8.10	−2.60	−0.375	−3.00
	1000	16.10	−12.14	−7.19	−2.83	−0.699	−3.11
0.10	300	71.15	−11.10	−7.48	−1.35	−0.080	−2.15
	500	19.20	−10.41	−6.55	−2.19	−0.335	−2.75
	1000	−0.66	−8.16	−4.09	−2.01	−2.284	−2.36
1.0	1	6.599	−0.8036	−0.3997	0.0118	−0.002	−0.3534
	3	−0.2873	−1.1098	−0.5757	−0.1599	−0.043	−0.3949
	5	−0.7446	−1.0407	−0.4813	−0.2173	−0.162	−0.4270

is the exchange energy obtained by Danz and Glasser.[2] Numerical results of (22) are exhibited in Table II for some typical values of r_s and h of physical interest. We note that the cluster expansion converges reasonably well. Our results on the correlation energy are also compared in Table II with those obtained under the RPA.[17] It is seen that our values are lower.[18] Based on the variational nature of our approach, this then indicates improvements over the RPA. This is in contrast to the case of zero magnetic field, where the RPA energies are lower.[1] It appears from Table II that for high fields our results and those of the RPA approach each other. This conclusion is somewhat deceptive, for neither of these treatments are valid in the extreme high-field limit, which corresponds to the relativistic region.[12] On the other hand, the present formulation is restricted only to the QSFL limit. It is therefore extremely important to bear in mind the region of validity in comparing the results.

To summarize, we have made a realistic calculation of the ground-state energy of an electron gas in the QSFL using the product wave function (3). The variational determination of the boson energy and the convergence of the successive clusters in the expansion of the energy appear to be reasonably adequate. Our calculation leads to lower, and presumably better, values of the correlation energy as compared to those obtained under the random-phase approximation. The formulation can also be extended to study the magnetic properties such as the de Haas-van Alphen effect in the case of an intermediate magnetic field. Investigation in this direction is underway and the results will be reported in the future.

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[12]The limitations of the nonrelativistic theory can be briefly examined as follows: From the solution of the Dirac equation, the energy of an electron in a magnetic field is [M. H. Johnson and B. A. Lippmann, Phys. Rev. 76, 828 (1949)] $E=2\alpha^{-2}[1+(\alpha q)^2+2\alpha^2 h(n+r-1)]^{1/2}$, where $n=0, 1, 2, \cdots$, $r=1, 2$, and $\alpha=e^2/\hbar c=1/137$ is the fine-structure constant. This expression reduces to the nonrelativistic limit (11) for $n=0$ if $(\alpha q)^2 \ll 1$ and $\alpha^2 h \ll 1$. In the QSFL, these nonrelativistic conditions are realized for $r_s<1$ provided that $r_s^{-2}<h<10^3$.
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[15]Details of the steps leading to (21) can be found in the Ph.D. dissertation of G. Keiser (Northeastern University, 1973) (unpublished).
[16]In the high-density limit ($r_s \ll 1$) we keep only the first term in the summation in (23) of Ref. 1. This leads to

$E_0^B = -0.846/r_s^{3/4}$ as compared to the exact value $E_0^B = -0.8031/r_s^{3/4}$ (Ref. 10, Chap. 7).

[17] In the atomic units, the RPA value of the correlation energy [Eq. (10) of Ref. 5] reads $E_{\text{corr}}^{\text{RPA}}/N = -[F(r) - \ln 2 - 1/2]\, 2r_s^3\hbar^2/3\pi^2$, where $r = 1/\pi q_F$ and $F(r)$ is given by (13) of Ref. 5.

[18] Our values of the ground-state energy are also lower than the estimates made by Kaplan and Glasser in Ref. 3.