

Ground-state correlation energy for the homogeneous electron gas calculated by the transcorrelated method

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(Received 17 September 2003; revised manuscript received 25 November 2003; published 2 April 2004)

We have investigated the correlation energy for the homogeneous electron gas given by the transcorrelated (TC) method. In the TC method, the energy is defined by an expectation value of an effective Hamiltonian constructed by similarity transformation of the original Hamiltonian with respect to a Jastrow factor. In our calculation, a two-body Jastrow factor, which is the simplest function representing the electronic correlation effects, was adopted. Two parameters in the Jastrow factor are determined by the cusp conditions, which restricts the short-range electronic interactions and the long-range asymptotic condition resulted from the random-phase approximation. The energy is expressed within three-body integrals using the two-body Jastrow factor and so it is easily applied to the homogeneous electron gas without Monte Carlo sampling. We found that the TC method yields a fairly good estimate of the correlation energy, and so that of the total energy, especially for near the region of metallic densities ($2 < r_s < 10$) in spite of our simple formulation.

DOI: 10.1103/PhysRevB.69.165102

PACS number(s): 71.10.Ca, 05.30.Fk

I. INTRODUCTION

The study of the electron gas has long history initiated by Wigner.¹ Since it is characterized only by a constant density in the case of unpolarized electron gas, a variety of methods have been applied to the system in order to understand fundamental properties of the electronic interactions. High-density limit of the electronic correlation energy was well studied in 1950s to 1960s (Refs. 2–8) by means of the perturbation theory. However, it is known that the analytical formula derived by the perturbation theory is incapable of reproducing the correct correlation energy in the region of metallic densities ($1.8 < r_s < 6$).⁸

An alternative approach is based on the variational method,^{9–18} in which the wave function is assumed to be a specific form such as the Jastrow-Slater-type wave function, and then the trial function is optimized according to the variational principle. The variational method has been combined with the modern computational developments, which enable us to carry out direct evaluations of the energy expectation values using the correlated wave functions. This approach, called the variational Monte Carlo (VMC) method, was pioneered by Ceperley¹⁷ for fermion systems. In his work, both the polarized and unpolarized electron gases were studied over the wide range of densities in detail. The more sophisticated stochastic approach, so-called Green's-function Monte Carlo (GFMC) method, was also applied to the homogeneous electron gas in order to investigate its phase diagram.¹⁹ The data have been interpolated with analytical functions' fitted parameters by Vosko *et al.*²⁰ and Perdew and Zunger.²¹ In the latest work, modifications for the functional form and its parameters have been proposed by Perdew and Wang.²² Since the Monte Carlo method requests a periodic boundary condition representing the infinite electron gas, it

always contains uncertainty. Ortiz and Ballone have recalculated the electron-gas correlation energy by the VMC (Ref. 18) and the GFMC (Ref. 23) method using a periodic cell larger than those taken in the previous work by Ceperley *et al.*^{17,19} Recently, improvements over the trial wave function have been studied by Kwon *et al.*²⁴ They adopted a function that includes backflow and three-body correlations for the high-density region of the homogeneous three-dimensional electron gas. The same trial wave function has also been applied to the low-density electron gas.²⁵ The Fermi hypernetted-chain (FHNC) method^{26,27} is also variational approach, where the Euler-Lagrange equation for the pair-correlation function constructed from the Jastrow-Slater-type wave function is approximately solved. The FHNC method reproduced the results given by the VMC calculation¹⁷ and then it is known as a reliable approach for the electron gas.

Takada combined the perturbation theory with the variational method in order to make use of the advantages of both the approaches, and proposed the effective-potential expansion (EPX) method.²⁸ It was found that the correlation energies given by the EPX method are in very good agreement with those obtained from the GFMC method.¹⁹

The coupled-cluster (CC) method, which is well known as an accurate quantum chemical calculation, was also applied to calculate the electron-gas correlation energy and gave very similar results to the GFMC method.^{29,30}

The transcorrelated (TC) method^{31–42} is another promising approach to deal with strongly correlated electronic systems. The basic idea of the TC method was given by Boys and Handy,^{31–35} that is, the correlation effects are efficiently incorporated into the many-body Hamiltonian by means of a similarity transformation with respect to the Jastrow factor. A trial function is optimized so as to satisfy the transformed

eigenequation. Since the effective Hamiltonian, which we call TC Hamiltonian, already contains some electronic correlation effects, a simple trial function such as a single Slater determinant is enough to obtain accurate energy estimates. The TC method has been successfully applied to atoms and molecules.³³⁻⁴¹ The ground-state energy for the homogeneous electron was also calculated by Armour⁴² following the original formalism of the TC method given by Boys and Handy.³¹⁻³⁴ In his work, it was shown that the TC method can reproduce the results given by Gaskell's variational approach for both the wave function and ground-state energy of the electron gas.

In this paper, we examine the electron gas limit of the energy given by the TC method as a preliminary work for the solid-state calculation. We adopted a simple two-body Jastrow factor including two parameters. These parameters are determined by the two asymptotic conditions: the cusp conditions and the random-phase approximation, and so no parametrization is required in our formalism. This is the main difference from the previous work of Armour where parameters are optimized so as to satisfy the transformed eigenequation. We compare our correlation energy estimates for the homogeneous electron gas with those given by a variety of modern methods introduced in this section. In Sec. II, we briefly address the theory of the TC method and show the formula for the electron-gas correlation energy. In Sec. III, we will show our numerical results of the correlation energy and total energy for the homogeneous electron gas. In Sec. IV, we will give our conclusions.

II. THEORY

Since we have addressed the detailed theory of the TC method in our previous paper,⁴¹ here we only show its important concepts. The Hartree atomic units ($m = e^2 = \hbar = 1$) are used in this section. In the TC method, the eigenequation for the many-body electronic system,

$$\mathcal{H}\Psi = E\Psi, \quad (1)$$

is transformed into

$$\mathcal{H}_{\text{TC}}\Phi = E\Phi, \quad (2)$$

$$\mathcal{H}_{\text{TC}} = \frac{1}{F}\mathcal{H}F. \quad (3)$$

Ψ is the exact eigenfunction and F is the Jastrow factor representing the correlation effects, which depends on the relative position and spin of electrons. Φ is defined by a division of these two functions, $\Phi = \Psi/F$. Since the similarity transformation does not change the eigenvalues, one can solve the transformed eigenequation (2) instead of the original eigenequation (1) in order to obtain eigenenergies E . Although Φ is generally described by a linear combination of the Slater determinants, relatively smaller number of determinants are enough to attain accurate energies because the TC Hamiltonian \mathcal{H}_{TC} already contains some correlation effects originated from the Jastrow factor. In our calculation, a normalized single Slater determinant D was simply adopted

for Φ . Since \mathcal{H}_{TC} is non-Hermitian operator, variational treatment of the total energy is not applicable. Hence, a variance of the local energy $E_L = \mathcal{H}_{\text{TC}}D/D$ is introduced by^{35,41}

$$\sigma^2 = \int |D|^2 |E_L - E|^2 d^{3N}x = \int |\mathcal{H}_{\text{TC}}D - ED|^2 d^{3N}x. \quad (4)$$

Here x contains both of the space and spin coordinates (\mathbf{r}, γ) and $d^{3N}x$ denotes the $3N$ -dimensional integration where N is the number of electrons. The variance σ^2 is minimized with respect to D , F , and E for general systems so that Eq. (2) is satisfied as much as possible within the trial function D .⁴¹

We have simply adopted plane waves for the elements of D representing the unpolarized and metallic region of the homogeneous electron gas. Hence the system is characterized by a constant density n or the Wigner radius defined by $r_s = (3/4\pi n)^{1/3}$. Moreover, F is determined by two asymptotic conditions as we will show in the following discussions. Therefore, σ^2 should be minimized only with respect to E :

$$\frac{\partial \sigma^2}{\partial E} = 2E - \int D^* \mathcal{H}_{\text{TC}} D d^{3N}x - \int D \mathcal{H}_{\text{TC}}^* D^* d^{3N}x = 0. \quad (5)$$

E is then written as

$$\begin{aligned} E &= \text{Re} \int D^* \mathcal{H}_{\text{TC}} D d^{3N}x \\ &= \frac{1}{2} \int D^* (\mathcal{H}_{\text{TC}} + \mathcal{H}_{\text{TC}}^\dagger) D d^{3N}x \\ &= \int D^* \mathcal{H} D d^{3N}x - \sum_{i=1}^N \int D^* \left| \frac{\nabla_i F}{F} \right|^2 D d^{3N}x. \end{aligned} \quad (6)$$

Here Re denotes the real part. This is the definition of the energy in the TC method. Equation (6) yields the exact ground-state energy if D is the eigenfunction of \mathcal{H}_{TC} . In general, since D is not the exact eigenfunction, Eq. (6) is an approximation of the energy which is different from the expectation value of the original Hamiltonian \mathcal{H} with respect to the same wave function FD :

$$\frac{\langle FD | \mathcal{H} | FD \rangle}{\langle FD | FD \rangle} \neq E. \quad (7)$$

Therefore, the variational principle is not available to the energy given by Eq. (6) and so it might be lower than the exact ground-state energy. The second term of Eq. (6) is considered to be the correlation energy in our formalism.

We adopt the following standard function for a two-body Jastrow factor:

$$F = \exp \left(-\frac{1}{2} \sum_{i=1}^N \sum_{j=1(\neq i)}^N u_{\sigma_i \sigma_j}(|\mathbf{r}_i - \mathbf{r}_j|) \right), \quad (8)$$

$$u_{\sigma \sigma'}(R) = \frac{A_{\sigma \sigma'}}{R} (1 - e^{-R/F_{\sigma \sigma'}}), \quad (9)$$

where σ_i denotes the spin of the i th electron, $\sigma_i = \sigma(\gamma_i)$. It has been used in the Monte Carlo calculation for the electron gas and solids.^{17,43,44} The two parameters in Eq. (9) are determined by the cusp conditions,

$$\frac{A_{\sigma\sigma'}}{2F_{\sigma\sigma'}^2} = \alpha_{\sigma\sigma'}, \quad (10)$$

where $\alpha_{\uparrow\uparrow} = 1/4$ and $\alpha_{\uparrow\downarrow} = 1/2$, and the random-phase approximation (RPA),^{44,45}

$$A_{\uparrow\uparrow} = A_{\uparrow\downarrow} = \frac{1}{\omega_p} = \frac{1}{\sqrt{4\pi n}}, \quad (11)$$

where ω_p is the plasma frequency. Therefore, $A_{\sigma\sigma'}$ and $F_{\sigma\sigma'}$ in Eq. (9) are completely determined by Eqs. (10) and (11), and so no variational parameter exists in our formulation. Now the correlation energy is explicitly written using the second term of Eqs. (6) and (8) as

$$\begin{aligned} E_c &= - \sum_{i=1}^N \int D^* \left| \frac{\nabla_i F}{F} \right|^2 D d^{3N}x \quad (12) \\ &= - \frac{1}{2} \sum_{\mu=1}^N \sum_{\nu=1}^N \int \phi_\mu^*(x) \phi_\nu^*(x') |\nabla u_{\sigma,\sigma'}(|\mathbf{r}-\mathbf{r}'|)|^2 \\ &\quad \times [\phi_\mu(x) \phi_\nu(x') - \phi_\mu(x') \phi_\nu(x)] dx dx' \\ &\quad - \frac{1}{2} \sum_{\mu=1}^N \sum_{\nu=1}^N \sum_{\eta=1}^N \int \phi_\mu^*(x) \phi_\nu^*(x') \phi_\eta^*(x'') \\ &\quad \times \nabla u_{\sigma\sigma'}(|\mathbf{r}-\mathbf{r}'|) \cdot \nabla u_{\sigma\sigma''}(|\mathbf{r}-\mathbf{r}''|) R_{\mu\nu\eta}(x, x', x'') \\ &\quad \times dx dx' dx'', \quad (13) \end{aligned}$$

where

$$R_{\mu\nu\eta}(x, x', x'') = \begin{vmatrix} \phi_\mu(x) & \phi_\nu(x) & \phi_\eta(x) \\ \phi_\mu(x') & \phi_\nu(x') & \phi_\eta(x') \\ \phi_\mu(x'') & \phi_\nu(x'') & \phi_\eta(x'') \end{vmatrix}. \quad (14)$$

Here, orthonormality conditions for the one-body wave functions $\phi_\mu(x)$ are utilized. Therefore, the correlation energy is calculated within three-body integrals in general. In the case of homogeneous electron gas with not so large r_s , that is, if we can reasonably assume that $\phi_\mu(\mathbf{r})$ is a plane wave, Eq. (13) is reduced into the following simple form:

$$E_c[n] = E_c^{(2)}[n] + E_c^{(3)}[n], \quad (15)$$

$$E_c^{(2)}[n] = \Omega n \varepsilon_c^{(2)}(n),$$

$$\begin{aligned} \varepsilon_c^{(2)}(n) &= -\pi n \int_0^\infty [u'_{\uparrow\uparrow}(R)^2 + u'_{\uparrow\downarrow}(R)^2] R^2 dR \\ &\quad + 9\pi n \int_0^\infty \varrho(k_F R)^2 u'_{\uparrow\uparrow}(R)^2 R^2 dR, \quad (16) \end{aligned}$$

$$E_c^{(3)}[n] = \Omega n \varepsilon_c^{(3)}(n)$$

$$\begin{aligned} \varepsilon_c^{(3)}(n) &= \frac{k_F^2}{\pi^2} \left(\frac{1}{2} \int_0^\infty \int_0^\infty [u'_{\uparrow\uparrow}(R)u'_{\uparrow\uparrow}(R') + u'_{\uparrow\downarrow}(R)u'_{\uparrow\downarrow}(R')] \right. \\ &\quad \times [B_1(x_1, x_2) - k_F^2 a^2 B_2(x_1, x_2)] dR dR' \\ &\quad - 3 \int_0^\infty \int_0^\infty u'_{\uparrow\uparrow}(R)u'_{\uparrow\uparrow}(R') \varrho(k_F R) \varrho(k_F R') \\ &\quad \left. \times [B_3(x_1, x_2) - k_F^2 a^2 B_4(x_1, x_2)] dR dR' \right), \quad (17) \end{aligned}$$

where $E_c^{(2)}[n]$ and $E_c^{(3)}[n]$ are the contributions from the two-body and three-body terms in Eq. (13), respectively. $u'_{\sigma\sigma'}(R)$ is the derivative of $u_{\sigma\sigma'}(R)$ with respect to R :

$$u'_{\sigma\sigma'}(R) = -\frac{A_{\sigma\sigma'}}{R^2} + A_{\sigma\sigma'} \left(\frac{1}{R^2} + \frac{1}{F_{\sigma\sigma'} R} \right) e^{-R/F_{\sigma\sigma'}}, \quad (18)$$

and the functions in Eqs. (16) and (17) are defined as follows:

$$\varrho(x) = -\frac{\cos x}{x^2} + \frac{\sin x}{x^3}, \quad (19)$$

$$B_1(x_1, x_2) = \int_{x_1}^{x_2} \varrho(x)^2 x^3 dx = [b_1(x)]_{x_1}^{x_2},$$

$$b_1(x) = \frac{\cos 2x}{4x^2} - \frac{1 + 2x^2 \text{Ci}(2x)}{4x^2} + \frac{\ln x}{2} + \frac{\sin 2x}{2x},$$

$$\text{Ci}(x) = -\int_x^\infty \frac{\cos y}{y} dy, \quad (20)$$

$$B_2(x_1, x_2) = \int_{x_1}^{x_2} \varrho(x)^2 x dx = [b_2(x)]_{x_1}^{x_2},$$

$$b_2(x) = -\frac{1 + 2x^2}{8x^4} + \frac{\cos 2x}{8x^4} + \frac{\sin 2x}{4x^3}, \quad (21)$$

$$B_3(x_1, x_2) = \int_{x_1}^{x_2} \varrho(x) x^3 dx = [b_3(x)]_{x_1}^{x_2},$$

$$b_3(x) = -x \sin x - 2 \cos x, \quad (22)$$

$$B_4(x_1, x_2) = \int_{x_1}^{x_2} \varrho(x) x dx = [b_4(x)]_{x_1}^{x_2},$$

$$b_4(x) = -\frac{\sin x}{x}. \quad (23)$$

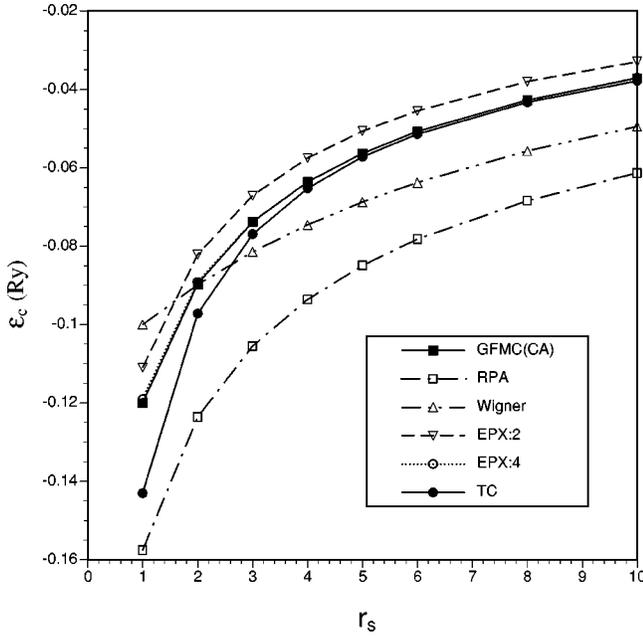


FIG. 1. The correlation energy estimates per electron for the unpolarized electron gas as a function of the Wigner radius r_s given by a variety of methods: the present work based on the transcorrelated method (TC), the Green's-function Monte Carlo method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)], the random-phase approximation (RPA), the Wigner's interpolation (Wigner),^{1,2} and the effective-potential expansion method²⁸ containing the second (EPX:2) and the fourth (EPX:4) power of the expansion. GFMC(CA) and EPX:4 are almost identical. Our results (TC) and the exact values given by GFMC(CA) are in good agreement at intermediate densities ($2 < r_s < 10$).

Here Ω is the volume of the system and k_F is the Fermi wave number obtained by

$$k_F = (3\pi^2 n)^{1/3}, \quad (24)$$

and a^2 , x_1 , and x_2 are defined by

$$a^2 = R^2 + R'^2, \quad (25)$$

$$x_1 = k_F(R + R'), \quad (26)$$

$$x_2 = k_F|R - R'|. \quad (27)$$

It is understood from Eqs. (16) and (17) that the electron-gas correlation energy is easily evaluated within two-dimensional integrals. This is the great advantage of our method. We will show the results for the electron-gas correlation energy given by the formulas Eqs. (15)–(17) in comparison with those given by a variety of other methods in the following section.

III. RESULTS

In Figs. 1 and 2, the correlation energy estimates per electron given by the present work based on the TC are shown as a function of the Wigner radius r_s . A variety of correlation energy estimates given by the Green's-function Monte Carlo

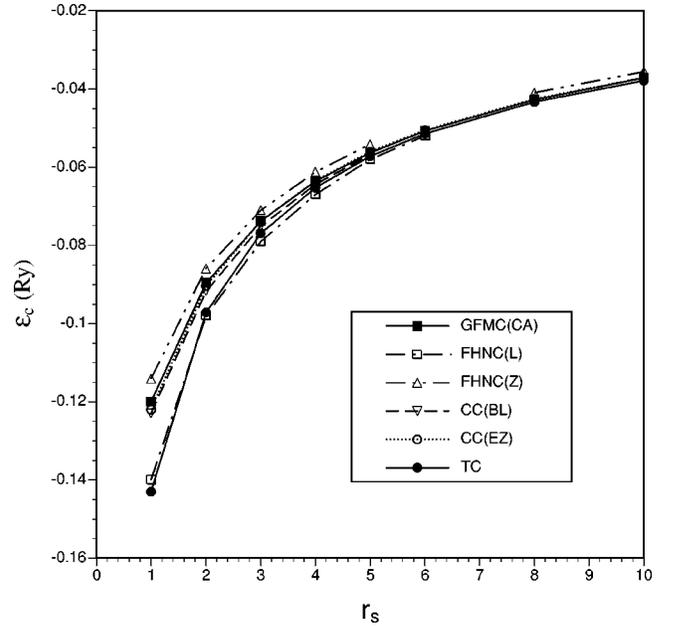


FIG. 2. The correlation energy estimates per electron for the unpolarized electron gas as a function of the Wigner radius r_s given by a variety of methods: the present work based on the transcorrelated method (TC), the Green's-function Monte Carlo method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)], the Fermi hypernetted-chain (FHNC) method given by Zabolitzky²⁶ [FHNC(Z)] and Lanto [FHNC(L)],²⁷ and the coupled cluster method given by Bishop and Lührmann²⁹ [CC(BL)] and Emrich and Zabolitzky³⁰ [CC(EZ)].³⁰ GFMC(CA) and CC(EZ) are almost identical. Our results (TC) are very close to those of FHNC(L).

method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)], RPA, the Wigner's interpolation (Wigner),^{1,2} the effective-potential expansion method²⁸ containing the second (EPX:2) and the fourth (EPX:4) power of the expansion, the FHNC method given by Zabolitzky²⁶ [FHNC(Z)] and Lanto [FHNC(L)],²⁷ and the coupled cluster method given by Bishop and Lührmann²⁹ [CC(BL)] and Emrich and Zabolitzky³⁰ [CC(EZ)] are also shown. Here the values of GFMC(CA) are considered to be exact. The present results (TC) become very close to the exact values at intermediate densities ($2 < r_s < 10$). Furthermore, the results given by TC and FHNC(L) are almost identical despite that our approach is much simpler than the FHNC method.

In Table I, the correlation energy estimates given by these methods are listed. The discrepancy between TC and GFMC(CA) becomes larger again as r_s increases over 10. However, it is remarkable that we were able to obtain relatively accurate values in the region ($2 < r_s < 10$) within our simple formulation as we explained in Sec. II. The reason for the disagreement in the large r_s limit is that the RPA itself becomes an inadequate approximation. Moreover, since the Jastrow factor (8) contains only the two-body terms, three-body or four-body terms might improve the discrepancy. It should be mentioned that the differences in the correlation energies between GFMC(CA) and the recent GFMC calculations given by Ortiz *et al.*,²³ Kwon *et al.*,²⁴ and Zong

TABLE I. Correlation energy estimates per electron for the unpolarized electron gas as a function of the Wigner radius r_s given by the present work based on the transcorrelated method (TC), the random-phase approximation (RPA), the effective-potential expansion method²⁸ containing the second (EPX:2) and the fourth (EPX:4) power of the expansion, the coupled cluster method given by Bishop and Lüthmann²⁹ [CC(BL)] and Emrich and Zabolitzky [CC(EZ)],³⁰ the Fermi hypernetted-chain (FHNC) method given by Zabolitzky²⁶ [FHNC(Z)] and Lantto [FHNC(L)],²⁷ and the Green's-function Monte Carlo method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)]. All energies are in Rydberg ($m = \frac{1}{2}$, $e^2 = 2$, $\hbar = 1$).

r_s	RPA	EPX:2	EPX:4	CC(BL)	CC(EZ)	FHNC(L)	FHNC(Z)	TC	GFMC(CA)
0.01	-0.2864	-1.7748	-0.3807
0.1	-0.2876	-0.251	-0.502	-0.243
1.0	-0.1576	-0.111	-0.119	-0.123	-0.122	-0.140	-0.1141	-0.143	-0.120
2.0	-0.1236	-0.0821	-0.0891	-0.0917	-0.0904	-0.098	-0.0859	-0.0971	-0.0896
3.0	-0.1055	-0.0671	-0.0737	-0.0751	-0.0738	-0.079	-0.0710	-0.0769	-0.0738
4.0	-0.0936	-0.0575	-0.0636	-0.0644	-0.0634	-0.067	-0.0612	-0.0653	-0.0636
5.0	-0.0849	-0.0506	-0.0563	-0.0568	-0.056	-0.058	-0.0541	-0.0572	-0.0563
6.0	-0.0782	-0.0455	-0.0507	...	-0.0505	-0.052	...	-0.0514	-0.0507
8.0	-0.0684	-0.0380	-0.0427	...	-0.0425	...	-0.0409	-0.0433	-0.0427
10.0	-0.0613	-0.0329	-0.0370	...	-0.037	-0.037	-0.0355	-0.0378	-0.0371
20.0	-0.04276	-0.0236	-0.023	-0.0218	-0.0246	-0.0231
50.0	-0.02536	-0.011	...	-0.0137	-0.0114
100.0	-0.01660	-0.0062	...	-0.0087	-0.0064

*et al.*²⁵ are much smaller than the discrepancy between TC and GFMC(CA).

In Fig. 3, we show the total energies for the unpolarized electron gas estimated by the present work based on the TC,

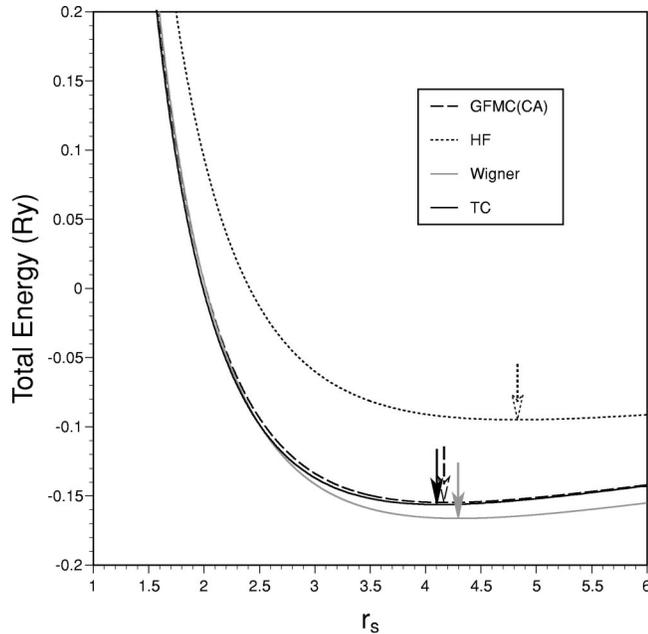


FIG. 3. The total energy estimates per electron for the unpolarized electron gas given by the present work based on the transcorrelated method (TC), the Green's-function Monte Carlo method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)], the Hartree-Fock method (HF), and the Wigner's interpolation (Wigner),^{1,2} as a function of the Wigner radius r_s . The arrow indicates the minimum point of each energy. The total energy given by the present work (TC) and its minimum point are very close to those of GFMC(CA).

the Green's-function Monte Carlo method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)], the Hartree-Fock method (HF), and the Wigner's interpolation (Wigner).^{1,2} The difference between GFMC(CA) and HF is the total correlation energy. The arrow indicates the minimum point of each energy. As we can see easily, the total energy obtained by the present work (TC) and its minimum point are very close to those given by GFMC(CA). In Table II, the minimum of each energy and the corresponding r_s value are listed.

IV. CONCLUSIONS

We have investigated the electron-gas limit of the energy given by the transcorrelated method. In our method, two parameters in the Jastrow factor are determined by the two asymptotic conditions: the cusp conditions and the random-phase approximation. It was found that the correlation energy for the unpolarized electron gas given by our method shows fairly good agreement with the exact results especially

TABLE II. The minimum values of the total energy E_{\min} per electron for the unpolarized electron gas and the corresponding r_s values given by the present work based on the transcorrelated method (TC), the Green's-function Monte Carlo method calculated by Ceperley and Alder¹⁹ and its interpolations²⁰ [GFMC(CA)], the Hartree-Fock method (HF), and the Wigner's interpolation^{1,2} (Wigner) are listed. All energies are in Rydberg ($m = \frac{1}{2}$, $e^2 = 2$, $\hbar = 1$).

	HF	Wigner	TC	GFMC(CA)
r_s	4.82	4.30	4.10	4.18
E_{\min}	-0.0950	-0.1663	-0.1563	-0.1548

for the region of metallic densities $2 < r_s < 10$, and its total energy is almost identical with the exact result in $1 < r_s < 10$. It is remarkable that we could achieve these successful results within our simple formulation, which is computationally less demanding than conventional methods. These results indicate that the transcorrelated approach is very promising not only for finite systems but also for bulk system. We

will further study these issues in order to carry out practical transcorrelated calculation for solids.

ACKNOWLEDGMENTS

We would like to thank Professor M. Imada, Professor Y. Takada, and Professor H. Aoki for meaningful discussions and advice.

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