PHYSICAL REVIEW B VOLUME 59, NUMBER 11 15 MARCH 1999-I

High-density expansion of correlation energy and its extrapolation to the metallic density region

T. Endo and M. Horiuchi
Department of Physics, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan

Y. Takada
Institute for Solid State Physics, University of Tokyo, Minato-ku, Tokyo 106-8666, Japan

H. Yasuhara
Department of Physics, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan

(Received 13 October 1998)

The r_s expansion of the correlation energy per electron for an electron liquid is completed exactly up to order r_s in units of Rydberg. A simple but accurate fitting formula for the correlation energy, which is a smooth extrapolation of the r_s expansion to the region of metallic densities is presented. [S0163-1829(99)07911-4]

I. INTRODUCTION

An electron gas, an assembly of electrons embedded in a uniform positive background is an important model to study the many-body effects in solids. The only parameter of this model, r_s defined by the radius of a sphere with the volume per electron scaled in units of the Bohr radius gives a measure of the ratio of the potential energy to the kinetic energy. Practically, energy-band calculations in the local density approximation rely on the numerical values of the correlation energy obtained from the Green's function Monte Carlo method.[1] Fundamentally, this model enables one to understand how the correlated motion of electrons is realized as a consequence of the delicate balance among the kinetic energy, the Pauli principle (the exchange effect), and the Coulomb interaction, avoiding further complications due to an external field of ions. At high densities corresponding to very small $r_s (r_s \lesssim 1)$, long-range parts of the Coulomb interaction between electrons determine their correlated motion predominantly. As r_s is increased to metallic levels $(1.8 \lesssim r_s \lesssim 5.6)$, intermediate- and short-range parts of the Coulomb interaction between electrons play an increasingly important role in the correlated motion as well. Analytic methods are desirable for the understanding of detailed features of correlation in the region of metallic densities. In this respect we think that the r_s expansion, the well-founded analytic approach from the high density limit deserves reconsideration in order to link to the available numerical results of the correlation energy at metallic densities.

The r_s expansion of the ground-state energy of the electron gas is originally an asymptotic expansion, and its radius of convergence is zero. This is a direct consequence of the fact that on a complex plane where the horizontal axis is the real part of the coupling constant e^2 and the vertical the imaginary part of e^2, there exists a branch cut along the line $\mathrm{Re}\, e^2 < 0$, indicating the instability of the normal Fermi liquid against the occurrence of superconductivity due to an arbitrarily weak attractive interaction.[2] The r_s expansion of the correlation energy per electron in units of Rydberg $\epsilon_c(r_s)$ includes nonanalytic terms such as $r_s{}^n \ln r_s$ with $n = 0,1,2,\cdots$,[3] besides powers of r_s. The appearance of these logarithmic factors in the expansion is ascribed to the long-range nature of the Coulomb interaction. The screening inherent in the Coulomb interaction can properly be described by a resummation of those perturbation terms, which are individually divergent owing to the piling up of the same small-wave-number component of the Coulomb interaction. Such a reordering of perturbation terms leads to a convergent result and gives rise to the nonanalytic terms above.

Carr and Maradudin[4] have attempted to evaluate the r_s expansion of $\epsilon_c(r_s)$ up to order r_s as

$$\epsilon(r_s) = 2.21 r_s{}^{-2} - 0.916 r_s{}^{-1} + 0.0622 \ln r_s - 0.096 + 0.018 r_s \ln r_s + (E_3' - 0.036) r_s + O(r_s{}^2 \ln r_s, r_s{}^2), \tag{1}$$

where r_s is related to the average electron density n through $4\pi/3(a_0 r_s)^3 = n^{-1}$; a_0 is the Bohr radius. The term of order r_s in Eq. (1), however, is not complete because E_3' remains unevaluated. E_3' comes from those third-order perturbation terms, which involve three different wave-number components of the Coulomb interaction. These third-order perturbation terms are closely related to intermediate- and short-range correlation, rather than the screening. In fact, the third-order particle-particle ladder diagram contributing to E_3' is indispensable for the proper description of short-range correlation. The importance of intermediate- and short-range correlation is enhanced with increasing r_s, and the proper evaluation of ϵ_c at metallic densities cannot possibly be achieved without it. In this regard the evaluation of E_3' has

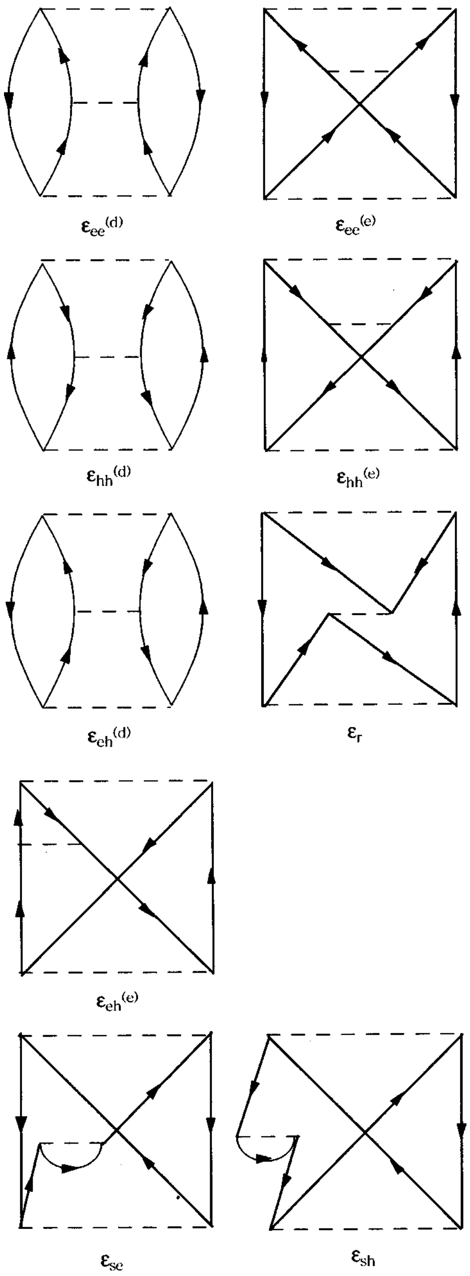

FIG. 1. Nine Feynman diagrams that make a contribution to E_{32}; $\epsilon_{\mathrm{ee}}^{(d)}$: electron-electron direct scattering, $\epsilon_{\mathrm{ee}}^{(e)}$: electron-electron exchange scattering, $\epsilon_{\mathrm{hh}}^{(d)}$: hole-hole direct scattering, $\epsilon_{\mathrm{hh}}^{(e)}$: hole-hole exchange scattering, $\epsilon_{\mathrm{eh}}^{(d)}$: electron-hole direct scattering, ϵ_r: doubly exchanged third-order RPA diagram, $\epsilon_{\mathrm{eh}}^{(e)}$: electron-hole exchange scattering, ϵ_{se}: exchange with electron self-energy, and ϵ_{sh}: exchange with hole self-energy.

the significant implication to link the high-density expansion of $\epsilon_c(r_s)$ with the available numerical results of $\epsilon_c(r_s)$ at metallic densities.

In this paper we shall first evaluate those third-order perturbation terms, which give E_3' in order to complete the r_s expansion up to order r_s. Next, we shall give a detailed explanation of how to improve on the random-phase approximation[5] (RPA) for the accurate evaluation of $\epsilon_c(r_s)$ at metallic densities, in connection with the strongly correlated features in the spin-antiparallel and the spin-parallel pair correlation functions $g^{\uparrow\downarrow}(r)$ and $g^{\uparrow\uparrow}(r)$. Finally, we present a simple but accurate fitting formula for $\epsilon_c(r_s)$, which is a smooth extrapolation of the r_s expansion to the region of metallic densities.

II. r_s EXPANSION

For the analysis of the r_s expansion it is convenient to use the notation[4] where each perturbation term is specified by $E_{m,2n}$ where m is the order of the Coulomb interaction and n the number of the interaction with the same wave-number component. In Eq. (1) the first term is the kinetic energy and the second the exchange energy specified by E_{12}. The third and higher order terms contribute to the correlation energy. The third term of order $\ln r_s$ that is predominant in the high-density limit can be derived from a summation of the most divergent series of perturbation terms, i.e., $\epsilon'=E_{24}+E_{36}+E_{48}+\cdots$. This was, for the first time, found by Macke.[3] The following constant term comes from both the second-order exchange term E_{22} and the higher order contribution of ϵ'. The second-order exchange was first evaluated numerically by the Monte Carlo method[6] and later analytically integrated by Onsager, Mittag, and Stephan.[7] The fifth term of order $r_s \ln r_s$ can be derived from a summation of the next most divergent series, i.e., $\epsilon''=E_{34}+E_{46}+E_{58}+\cdots$ and the higher order contribution of ϵ'. The expression for the sum of the next most divergent series was first derived by DuBois[8] from a careful examination of perturbation terms in the framework of the dielectric formulation. Its numerical coefficient was correctly evaluated by Carr and Maradudin.[4] The last term of order r_s comes from those third-order perturbation terms, which involve three different wave-number components of the Coulomb interaction, specified by E_{32} and the higher order contribution of ϵ' and ϵ''. Carr and Maradudin have calculated numerically such a contribution of order r_s as comes from ϵ' and ϵ'', leaving E_{32} unevaluated. E_{32} is the contribution from nine different types of Feynman diagrams drawn in Fig. 1, and can be written in the form of 12-dimensional integrals. The term E_{32} is nothing but $E_3'r_s$ in Eq. (1).

Note that three Coulomb interaction lines in each of the nine diagrams in Fig. 1 have different wave-number components. This implies that their contributions do not diverge because of the piling up of the same small wave-number component of the interaction. Three of the nine diagrams can be constructed by inserting one electron-electron or hole-hole or electron-hole interaction line between two separate bubbles in the second-order direct diagram. They are denoted by $\epsilon_{\mathrm{ee}}^{(d)}$, $\epsilon_{\mathrm{hh}}^{(d)}$, and $\epsilon_{\mathrm{eh}}^{(d)}$, respectively. Five of these diagrams can be constructed by inserting one interaction line in the second-order exchange diagram in all possible ways, i.e., one electron-electron or hole-hole or electron-hole interaction line or one self-energy interaction line in electron or hole lines. They are denoted by $\epsilon_{\mathrm{ee}}^{(e)}$, $\epsilon_{\mathrm{hh}}^{(e)}$, $\epsilon_{\mathrm{eh}}^{(e)}$, ϵ_{se}, and ϵ_{sh}, respectively. The remaining diagram can be constructed by exchanging each of two terminal interaction lines in the third order RPA, or ring diagram, which is denoted by ϵ_r. The expression for E_{32} is then given as follows:

$$
\begin{aligned}
E_{32}={}&\frac{3}{32\pi^7}\,\alpha r_s\int d^3\mathbf{p}_1 d^3\mathbf{p}_2\int d^3\mathbf{q}_1 d^3\mathbf{q}_2\frac{1}{\mathbf{q}_1^2}\,\frac{1}{\mathbf{q}_2^2}\left[\frac{2}{|\mathbf{q}_1-\mathbf{q}_2|^2}-\frac{1}{|\mathbf{p}_1+\mathbf{p}_2+\mathbf{q}_1+\mathbf{q}_2|^2}\right]\frac{1}{\mathbf{q}_1^2+\mathbf{q}_1\cdot(\mathbf{p}_1+\mathbf{p}_2)}\,\frac{1}{\mathbf{q}_2^2+\mathbf{q}_2\cdot(\mathbf{p}_1+\mathbf{p}_2)}\\
&-\frac{3}{16\pi^7}\,\alpha r_s\int d^3\mathbf{p}_1 d^3\mathbf{p}_2\int d^3\mathbf{q}_1 d^3\mathbf{q}_2\frac{1}{\mathbf{q}_1^2}\,\frac{1}{\mathbf{q}_2^2}\left[\frac{2}{|\mathbf{q}_1-\mathbf{q}_2|^2}-\frac{1}{|\mathbf{p}_1-\mathbf{p}_2|^2}\right]\frac{1}{\mathbf{q}_1\cdot(\mathbf{p}_2-\mathbf{p}_1)}\,\frac{1}{\mathbf{q}_2\cdot(\mathbf{p}_2-\mathbf{p}_1)}\\
&+\frac{3}{8\pi^7}\,\alpha r_s\int d^3\mathbf{p}_1 d^3\mathbf{p}_2 d^3\mathbf{p}_3\int d^3\mathbf{q}\,\frac{1}{\mathbf{q}^2}\,\frac{1}{|\mathbf{p}_1+\mathbf{p}_2+\mathbf{q}|^2}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_3|^2}\,\frac{1}{\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)}\,\frac{1}{\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_3)}\\
&+\frac{3}{16\pi^7}\,\alpha r_s\int d^3\mathbf{p}_1 d^3\mathbf{p}_2 d^3\mathbf{p}_3\int d^3\mathbf{q}\,\frac{1}{\mathbf{q}^2}\,\frac{1}{|\mathbf{p}_1+\mathbf{p}_2+\mathbf{q}|^2}\left[\frac{1}{|\mathbf{p}_1-\mathbf{p}_3+\mathbf{q}|^2}-\frac{1}{|\mathbf{p}_1-\mathbf{p}_3|^2}\right]\frac{1}{\{\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)\}^2}\,,
\end{aligned}
\tag{2}
$$

where wave numbers are measured in units of the Fermi wave number k_f and the corresponding Feynman diagrams are indicated. The first term in Eq. (2) comes from a direct and exchange pair of diagrams $\epsilon_{\rm ee}^{(d)}$, $\epsilon_{\rm ee}^{(e)}$, and another pair of diagrams $\epsilon_{\rm hh}^{(d)}$, $\epsilon_{\rm hh}^{(e)}$. The region of integration for $\epsilon_{\rm ee}^{(d)}$ and $\epsilon_{\rm ee}^{(e)}$ is

$$|\mathbf{p}_1+\mathbf{q}_1|>1,\quad |\mathbf{p}_1+\mathbf{q}_2|>1,\quad |\mathbf{p}_1|<1,$$

$$|\mathbf{p}_2+\mathbf{q}_1|>1,\quad |\mathbf{p}_2+\mathbf{q}_2|>1,\quad |\mathbf{p}_2|<1,$$

and the reversed inequalities for $\epsilon_{\rm hh}^{(d)}$ and $\epsilon_{\rm hh}^{(e)}$. The second term comes from diagrams $\epsilon_{\rm eh}^{(d)}$, ϵ_r, and the region of integration is

$$|\mathbf{p}_1+\mathbf{q}_1|>1,\quad |\mathbf{p}_1+\mathbf{q}_2|>1,\quad |\mathbf{p}_1|<1,$$

$$|\mathbf{p}_2+\mathbf{q}_1|<1,\quad |\mathbf{p}_2+\mathbf{q}_2|<1,\quad |\mathbf{p}_2|>1.$$

The third term comes from diagram $\epsilon_{\rm eh}^{(e)}$ and the region of integration is $|\mathbf{p}_i+\mathbf{q}|>1$, $|\mathbf{p}_i|<1$. The fourth term comes from diagrams $\epsilon_{\rm se}$, $\epsilon_{\rm sh}$, and the region of integration is $|\mathbf{p}_1+\mathbf{q}|>1$, $|\mathbf{p}_2+\mathbf{q}|>1$, $|\mathbf{p}_i|<1$.

We have evaluated the 12-dimensional integrals above by means of the following numerical technique. Replace every Coulomb interaction $\mathbf{q}_i^{-2}$ in the expression by the screened interaction $(\mathbf{q}_i^2+\lambda^2)^{-1}$ with an appropriate magnitude of λ. Then, the integrals can numerically be obtained by examining how they converge as λ is gradually approached to zero. There is a large amount of cancellation between the three integrals corresponding to direct diagrams $\epsilon_{\rm ee}^{(d)}$, $\epsilon_{\rm hh}^{(d)}$, and $\epsilon_{\rm eh}^{(d)}$; each of them is large in magnitude but finite. The sum of the three integrals above can be evaluated with an accuracy of double figures for $\lambda/2k_f<0.01$. The remaining six integrals corresponding to $\epsilon_{\rm ee}^{(e)}$, $\epsilon_{\rm hh}^{(e)}$, $\epsilon_{\rm eh}^{(e)}$, $\epsilon_{\rm se}$, $\epsilon_{\rm sh}$, and ϵ_r are nearly convergent for $\lambda/2k_f<0.01$. The sum of the six integrals above amounts approximately to zero because of mutual cancellation. As a result, the value of E_{32} is nearly equivalent to the contribution from the three direct diagrams $\epsilon_{\rm ee}^{(d)}$, $\epsilon_{\rm hh}^{(d)}$, and $\epsilon_{\rm eh}^{(d)}$. We have thus arrived at $E_{32}=0.015r_s$ with an accuracy of double figures. To sum up,

$$
\begin{aligned}
\epsilon'={}&0.0622\ln r_s-0.1422+0.00542r_s\ln r_s-0.0144r_s\\
&+O(r_s{}^2\ln r_s,r_s{}^2),
\end{aligned}
\tag{3}
$$

$$E_{22}=\frac{1}{3}\ln 2-\frac{3}{2\pi^2}\zeta(3)=0.04836\cdots, \tag{4}$$

where $\zeta(3)$ is the third-order Riemann zeta function,

$$\epsilon''=0.0130r_s\ln r_s-0.021r_s+O(r_s{}^2\ln r_s,r_s{}^2), \tag{5}$$

$$E_{32}=0.015r_s. \tag{6}$$

The r_s expansion exact up to order r_s is then given as follows:

$$\epsilon(r_s)\equiv 2.21r_s{}^{-2}-0.916r_s{}^{-1}+\epsilon_c(r_s), \tag{7}$$

$$
\begin{aligned}
\epsilon_c(r_s)={}&\epsilon'+E_{22}+\epsilon''+E_{32}=0.0622\ln r_s-0.0938\\
&+0.0184r_s\ln r_s-0.020r_s+O(r_s{}^2\ln r_s,r_s{}^2),
\end{aligned}
\tag{8}
$$

where the coefficients of order $r_s{}^0$, $r_s\ln r_s$ are written with available significant figures. The sum of the most divergent terms ϵ' overestimates the magnitude of the correlation energy at high densities. This is evident from a difference in the constant term between ϵ' and $\epsilon_c(r_s)$.

III. CORRELATION AT METALLIC DENSITIES

In its construction, the r_s expansion makes sense only at high densities ($r_s\lesssim 1$). It is quite useless for the evaluation of the correlation energy in the region of metallic densities ($1.8\lesssim r_s\lesssim 5.6$). Instead, we can adopt the RPA as a starting approximation in this region since it is the basic approximation for the description of two aspects characteristic of the Coulomb interaction: the existence of plasmon excitations and the screening as its counterpart effect. The RPA deals with the linear response to an external field in the framework of the linearized time-dependent Hartree approximation. As for the correlation energy, this approximation amounts to a summation of the most divergent series of perturbation terms for any r_s. Strictly, this is valid for high densities where long-range parts of correlation predominate over intermediate and short-range parts of correlation. Even in the region of metallic densities, however, the RPA gives the appropriate description of long-range correlation, since the RPA series make the most important contribution to small momentum-transfer interactions of all perturbation processes.

An apparent error in the RPA can be seen from the spin-parallel and the spin-antiparallel pair correlation functions $g^{\uparrow\uparrow}(r)$ and $g^{\uparrow\downarrow}(r)$, calculated in this approximation. Both of the two functions, which should, by definition, be positive incorrectly become negative at short distances, as r_s is increased to the values corresponding to metallic densities. That is, in this region the RPA overestimates those parts of correlation that are associated with intermediate and large momentum-transfer interactions, thus leading to a considerable overestimate in the magnitude of the correlation energy.[9]

We shall give an explanation of how to improve on the RPA. First, the RPA deals with the spin-antiparallel correlation and the spin-parallel correlation in quite the same way. In other words, $g^{\uparrow\downarrow}(r)-1$ and $\Delta g^{\uparrow\uparrow}(r)[=g^{\uparrow\uparrow}(r)-g^{\uparrow\uparrow}_{\mathrm{HF}}(r)]$ are evaluated with the same Feynman diagrams where $g^{\uparrow\uparrow}_{\mathrm{HF}}(r)$ is the spin-parallel pair correlation function in the Hartree-Fock approximation, or $g^{\uparrow\uparrow}(r)$ in the limit $r_s\rightarrow 0$. It neglects the second- and higher-order exchange terms and violates the requirement due to the Pauli principle $g^{\uparrow\uparrow}(0)=0$. Such an approximation is not correct except for the high-density limit. So far as the leading term of order $\ln r_s$ is concerned, both of the two correlations come from the same very small momentum transfer interactions and can be treated in quite the same way. Generally, there is a remarkable difference between the two correlations. In fact, the second-order exchange term not included in the RPA cancels, by half, large momentum-transfer interactions of the same order direct term. That is, spin-parallel electrons are forbidden to interact via large momentum transfers because of the Pauli principle; such interactions are allowed only between spin-antiparallel electrons. Thus, the inclusion of the exchange counterparts corrects the RPA's overestimate in the correlation energy from interactions between spin-parallel electrons.

Second, the RPA deals with short-range correlation to lowest order. This is not appropriate because short-range correlation in the region of metallic densities is too strong to deal with to the lowest order. In fact, the RPA exaggerates the effect of short-range Coulomb repulsion to such an extent as makes the value of $g^{\uparrow\downarrow}(r)$ negative at short distances for $r_s \gtrsim 1.7$. From the diagrammatic analysis it has been proved that an infinite series of particle-particle ladder interactions make the most important contribution to large momentum-transfer interactions of all perturbation processes;[10] its lowest-order contribution is the second-order direct term. The inclusion of these higher-order particle-particle ladder interactions gives a reasonable description of $g^{\uparrow\downarrow}(r)$ at short distances ($0 \lesssim k_f r \lesssim 3.0$) for any r_s.[11] It is important to notice that these higher-order particle-particle ladder interactions involve the most complete mixing of different wave-number components of the Coulomb interaction, in striking contrast to the RPA series. It is this property of the ladder series that is responsible for the appropriate description of local density fluctuations like the Coulomb hole. Furthermore, it should be stressed that the ladder series fulfills the cusp condition[12] on the many-body wave function that holds rigorously for any systems interacting via the Coulomb interaction. The cusp condition is a direct consequence of the fact that in the short-range limit correlation is essentially reduced to the two-electron problem in the medium. As the electron density is lowered to metallic levels, $g^{\uparrow\downarrow}(r)$ is remarkably reduced from unity at short distances, thus forming the Coulomb hole. The inclusion of higher-order ladder interactions between spin-antiparallel electrons reduces the magnitude of large momentum-transfer interactions, thus correcting such an overestimate in the correlation energy as comes from interactions between spin-antiparallel electrons. The same interactions between spin-parallel electrons, on the other hand, are always accompanied with their exchange counterparts. In their contribution to large momentum-transfer interactions every direct and exchange pair of higher-order ladder interactions cancel each other in the same way as a direct and exchange pair of second-order perturbation terms. The spin-parallel pair correlation function $g^{\uparrow\uparrow}(r)$ vanishes at zero separation because of the Pauli principle. This can be satisfied if one takes direct and exchange perturbation terms in pairs. In the dielectric formulation the requirement of the Pauli principle imposes an extremely complicated self-consistency on the proper polarization function. This is because the dielectric formulation is originally suitable for the description of long-range correlation. We conclude as follows: under the influence of the Coulomb interaction, $g^{\uparrow\uparrow}(r)$ is somewhat depressed on the short-distance side and enhanced beyond unity on the long-distance side compared with $g^{\uparrow\uparrow}_{\mathrm{HF}}(r)$, thus leading to a gain in the potential energy. The above influence of the Coulomb interaction on the Fermi hole is minor compared with the Coulomb hole, but it cannot possibly be neglected for the quantitative evaluation of the correlation energy in the region of metallic densities.

In conclusion, the RPA can thus be improved drastically by including higher-order particle-particle ladder interactions together with the second- and higher-order exchange counterparts. In contrast to the leading term of order $\ln r_s$ in the high-density expansion, the correlation energy in the region of metallic densities comes, for the most part, from correlation between spin-antiparallel electrons. Their contribution occupies about 75% of the total correlation energy at a typical metallic density corresponding to $r_s=4.0$.

A variety of computational techniques and theoretical methods have been devised for investigating strongly correlated features of an electron liquid at metallic densities. These are variational Monte Carlo method, Green's function Monte Carlo method,[1] Fermi hypernetted chain method,[13] coupled-cluster expansion,[14] effective potential expansion,[15] and partial summation of perturbation expansion.[16] The basic idea underlying these theoretical methods is to interpolate between long-range correlation in the RPA and strong short-range correlation between spin-antiparallel electrons, together with the corresponding exchange counterparts. The numerical values of the correlation energy per electron calculated from several different methods, at present, agree within an accuracy of 0.5 mRy throughout the whole region of metallic densities.

IV. AN EXTRAPOLATION

In this section we shall propose a smooth and accurate extrapolation formula for the correlation energy. It is not only reduced rigorously to the r_s expansion [Eq. (8)] correct up to order r_s for high densities, but also is best fitted to the most accurate values of the correlation energy[1,16] throughout the whole region of metallic densities. From a variety of possible extrapolated forms we have chosen a simple but physically motivated form as follows:

$$\epsilon_c(r_s)=\left(0.0622+\frac{0.0184\, r_s}{1+br_s}\right)\ln\left(\frac{r_s}{1+ar_s}\right)$$

$$+\frac{-0.0938}{1-(1/0.0938)\{0.020-0.0622a\}r_s}, \tag{9}$$

$$a=1.13, \quad b=0.202, \tag{10}$$

where we have written so as to make the relation to the original r_s expansion explicit. In the limit $r_s\rightarrow 0$ the formula above can be expanded in a series of $r_s^n \ln r_s$ and r_s^n in the same way as the r_s expansion. Two parameters a, b in Eq. (9) have been determined such that $\epsilon_c(r_s)$ is best fitted to the following numerical values of the correlation energy[1,16] at $r_s=1,2,3,4,5,6$.

$$\epsilon_c(1)=-120.0(-118.9), \quad \epsilon_c(2)=-89.6(-88.7),$$

$$\epsilon_c(3)=-73.8(-73.2), \quad \epsilon_c(4)=-63.6(-63.3),$$

$$\epsilon_c(5)=-56.3(-56.3), \quad \epsilon_c(6)=-50.7(-51.0),$$

where the values in the parentheses are due to Ref. 16. Figure 2 plots the above extrapolation formula as a function of r_s; for comparison the r_s expansion is also drawn there. The deviation from the input value at each r_s above is smaller than 0.5 mRy.

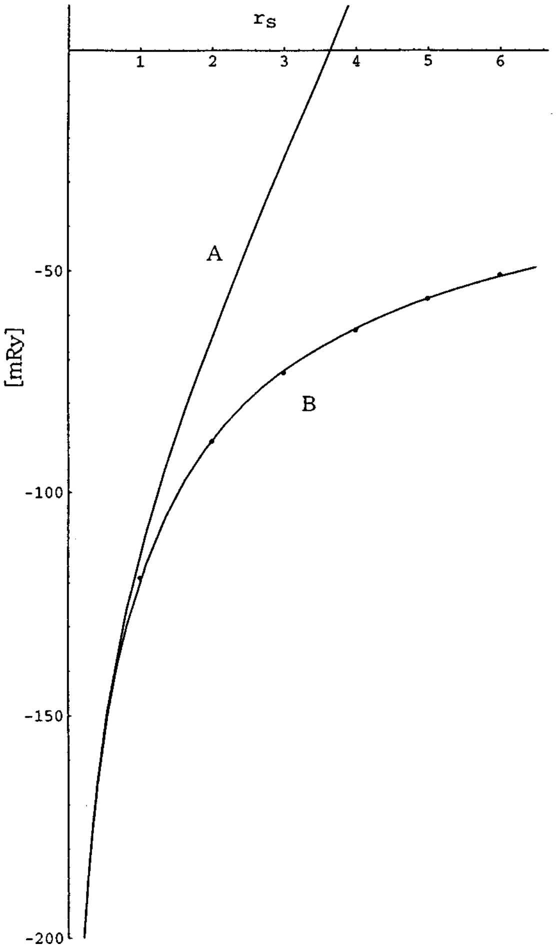

FIG. 2. Correlation energy per electron $\epsilon_c(r_s)$ from the fitting formula in Eq. (9); triangles represent the input values from Ref. 1 and circles those from Ref. 16, (a) high density expansion, (b) present extrapolation formula.

We shall mention the physical implications of the extrapolation formula above. The appearance of logarithmic factors in the r_s expansion is ascribed to the treatment of screening for high densities. Specifically, a summation of the most divergent series amounts to cutting off small wave-number components of one of the two Coulomb interactions entering the second-order direct term E_{24} around the Thomas-Fermi wave number $k_{\mathrm{TF}}[=(4\alpha r_s/\pi)^{1/2}k_f]$ for very small r_s and gives rise to $0.0622\ln r_s$. The screening length, measured in units of the average interparticle distance, is of order $k_f/k_{\mathrm{TF}}=(\pi/4\alpha r_s)^{1/2}$ and is much larger than unity for small r_s. A straightforward extension of this definition to metallic densities, however, leads to the absurdity that it is shorter than the average interparticle distance. Even if the exact dielectric function $\epsilon(\mathbf{q},\omega)$ were available, one could not possibly obtain any reasonable value of the screening length from its static and small wave-number limit; the result would be worse. In the rigorous sense the screening length in the region of the metallic densities should be defined from the $\mathbf{p}'\rightarrow\mathbf{p}$ limit of Landau's quasiparticle interaction $f(\mathbf{p},\mathbf{p}')$, not from the $\mathbf{q}\rightarrow 0$ limit of the effective interaction $v(q)/\epsilon(\mathbf{q},0)$. This is because by definition $f(\mathbf{p},\mathbf{p}')$ involves not only linear but also nonlinear screening. Practically, the replacement of the parameter r_s in two logarithmic factors of the r_s expansion by a factor of $r_s/(1+ar_s)$ in the fitting formula substantially corrects the above underestimate in the screening length. The constant term in the r_s expansion, if directly applied to metallic densities, overestimates its magnitude. We have, therefore, cast the term of order r_s in the form of a denominator of the constant term together with an additional correction due to the replacement $r_s\rightarrow r_s/(1+ar_s)$. A factor of $1/(1+br_s)$ attached to the term of order $r_s \ln r_s$ also corrects the overestimate of its magnitude in the region of metallic densities. A number of interpolation formulas for the correlation energy have been proposed so far.[17–19] However, an extrapolated form of the r_s expansion has not been proposed so far as the authors are aware. We stress that the present formula is a simple and smooth extrapolation of the r_s expansion, sufficiently accurate throughout the whole region of metallic densities.

[1] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980); S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).
[2] L. Cooper, Phys. Rev. **104**, 1189 (1956).
[3] W. Macke, Z. Naturforsch. A **5A**, 192 (1950).
[4] W. J. Carr, Jr. and A. A. Maradudin, Phys. Rev. **133**, A371 (1964).
[5] D. Pines, *The Many-Body Problem* (Benjamin, New York, 1962).
[6] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).
[7] L. Onsager, L. Mittag, and M. J. Stephan, Ann. Phys. (Leipzig) **18**, 71 (1966).
[8] D. F. DuBois, Ann. Phys. (N.Y.) **7**, 174 (1959); **8**, 24 (1959).
[9] L. Hedin and S. Lundqvist, *Solid State Physics* (Academic, New York, 1969), Vol. 23.
[10] H. Yasuhara, Solid State Commun. **11**, 1481 (1972); J. Phys. Soc. Jpn. **36**, 361 (1974); Physica (Amsterdam) **78**, 420 (1974).
[11] Y. Ousaka, H. Suehiro, and H. Yasuhara, J. Phys. C **19**, 4247 (1986); **19**, 4263 (1986); H. Yasuhara, H. Suehiro, and Y. Ousaka, *ibid.* **21**, 4045 (1988).
[12] T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957); J. C. Kimball, Phys. Rev. A **5**, 1648 (1973); A. K. Rajagopal, J. C. Kimball, and Mahadev Banerjee, Phys. Rev. B **18**, 2339 (1978).
[13] L. J. Lantto, Phys. Rev. B **22**, 1380 (1980); J. G. Zabolitzky, *ibid.* **22**, 2353 (1980); E. Krotscheck, Ann. Phys. (N.Y.) **155**, 1 (1984).
[14] K. Emrich and J. G. Zabolitzky, Phys. Rev. B **30**, 2049 (1984).
[15] Y. Takada, Phys. Rev. B **35**, 6923 (1987).
[16] H. Suehiro, Ph.D. thesis, Hokkaido University, 1987.
[17] K. S. Singwi and M. P. Tosi, *Solid State Physics* (Academic, New York, 1981), Vol. 36.
[18] S. Ichimaru, Rev. Mod. Phys. **84**, 1017 (1982).
[19] J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13 244 (1992).