Vorticity expansion approximation of the exchange-correlation energy functional in current density functional theory

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We propose the vorticity expansion approximation (VEA) formulas of the exchange and correlation energy functionals of the current density functional theory (CDFT). They have a form of the second-order expansion with respect to the vorticity. Expansion coefficients are determined by requiring them to satisfy exact relations that have been derived from scaling properties of exchange and correlation energy functionals. Resultant VEA formulas satisfy a larger number of exact relations than those of the local-density approximation of the CDFT. Due to the well-behaved forms, the VEA formulas can be in quite good agreement with the exchange and correlation energies of the homogeneous electron liquid under a uniform magnetic field.

I. INTRODUCTION

The density functional theory[1,2] provides the most powerful method to calculate the ground-state electronic structures of atoms, molecules, and solids. Various kinds of extensions have been proposed so far by choosing appropriate physical quantities as basic variables in order to get a more suitable single-particle picture for a system.[3,4] The current-density functional theory (CDFT)[5,6] and its relativistic version, relativistic current- and spin-density functional theory (RCSDFT),[7,8] are examples of these extensions, in which the current density is chosen as a basic variable in addition to the electron density. These theories are useful for describing the ground-state properties of systems such as open-shell atoms and *f*-electron magnetic materials where an orbital current is induced from both the strong spin-orbit interaction and the intra-atomic Coulomb interaction. Also, these theories are applicable to inhomogeneous electronic systems in an external magnetic field, where an orbital current is induced by the external magnetic field.

In order to calculate electronic structures while taking the current density into account, the exchange and correlation energy functionals of the CDFT or RCSDFT must be devised in practicable forms. Many attempts to develop approximate forms of the exchange and correlation energy functionals of the CDFT have been presented so far.[5,6,9–18] Vignale, Rasolt, and Geldart have first proposed the local-density approximation (LDA) of the CDFT.[5,6,9,10] The practical formula[9,10] has been applied to actual calculations.[19–23] Erhard and Gross have derived exact relations that are satisfied with exchange and correlation energy functionals from the virial theorem and uniform scaling properties.[11] By using these exact relations, Liu has proposed local formulas for the exchange and correlation energy functionals under the local and variable-separation assumptions.[12] Capelle and Gross[13] have proposed a method to construct approximate exchange and correlation energy functionals of the CDFT by using those of the SDFT. Lee and Handy[14] have derived a procedure to construct exchange and correlation scalar and vector potentials by ex-

tending the procedure proposed by Zhao, Morrison, and Parr.[24] Recently, Maximoff, Ernzerhof, and Scuseria[15] have developed an empirical form of a current-dependent exchange hole model by using some of the exact relations as constraints. More recently, Zhu and Trickey have investigated analytical solutions of Hook's atom in a magnetic field toward approximate forms of the exchange and correlation energy functionals.[16]

In recent years, we have advanced the development of approximate forms of the exchange and correlation energy functionals on the basis of two strategies.[17,18] One is to start with the coupling-constant expression of the exchange-correlation energy functional of the CDFT.[17] By using this expression, in addition to the LDA, the average-density approximation and weighted-density approximation have been proposed similarly to those in the conventional DFT.[17] Another strategy is to utilize as constraints exact relations that are satisfied with exchange and correlation energy functionals.[17] This strategy is analogous to the generalized gradient approximation (GGA) method[25–27] in developing approximate forms of the exchange and correlation energy functionals of the DFT. To date, a lot of exact relations have been derived[17,18] by means of the virial theorem and nonuniform scaling properties. The set of these exact relations is a complement to those derived by Erhard and Gross.[11]

In this paper, we propose approximate forms of both the exchange and correlation energy functionals of the CDFT along the latter strategy. They have a form of the second-order vorticity expansion, which is hereafter called the vorticity expansion approximation (VEA) formulas. Expansion coefficients of the VEA formulas are determined by requiring them to satisfy a series of exact relations that have been derived from uniform and nonuniform coordinate scaling of electrons.[11,17] We also apply the VEA formulas to exchange and correlation energies of the homogeneous electron liquid under the uniform magnetic field. It is expected that the present VEA formulas make it feasible to perform the actual calculations of the CDFT.

The organization of this paper is as follows. In Sec. II, we shall give the preliminary definitions of various quantities

that will be required in the subsequent discussions. The exchange and correlation energy functionals of the CDFT are also defined there. In Sec. III, it is shown by utilizing the gauge transformation that the exchange and correlation energy functionals are dependent on the paramagnetic current density only through the vorticity. In Sec. IV, the VEA formula of the exchange energy functional is actually proposed by using the scaling behavior of the exchange energy functional as a sum rule. In a similar way to the exchange energy functional, the VEA formula of the correlation energy functional is proposed in Sec. V. In Sec. VI, as a possible example for checking the validity of the VEA formulas plus the practical purpose, the present VEA formulas are fitted to the exchange and correlation energies of the homogeneous electron liquid under the uniform magnetic field. Finally, concluding remarks are given in Sec. VII.

II. PRELIMINARY DEFINITIONS IN THE CDFT

The system we wish to consider consists of N electrons moving in the external electromagnetic fields, $v_{ext}(\mathbf{r})$ and $\mathbf{A}_{ext}(\mathbf{r})$. The Hamiltonian of the system is generally given by

$$\hat{H} = \sum_{i=1}^{N} \frac{1}{2m} \left\{ \mathbf{p}_i + \frac{e}{c} \mathbf{A}_{ext}(\mathbf{r}_i) \right\}^2 + \sum_{i=1}^{N} v_{ext}(\mathbf{r}_i) + \sum_{i>j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (1)$$

where $\mathbf{r}_i$ and $\mathbf{p}_i$ stand for the position and momentum of the ith electron, respectively. The operators of the electron density and paramagnetic current density are defined by

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) \quad (2)$$

and

$$\hat{\mathbf{j}}_p(\mathbf{r}) = \frac{1}{2m} \sum_{i=1}^{N} \{ \mathbf{p}_i \delta(\mathbf{r} - \mathbf{r}_i) + \delta(\mathbf{r} - \mathbf{r}_i) \mathbf{p}_i \}, \quad (3)$$

respectively. Using these operators and neglecting the surface integral at infinity, the Hamiltonian (1) is approximately rewritten as

$$\hat{H}^{CDFT} = \hat{T} + \hat{W} + \frac{e}{c} \int \mathbf{A}_{ext}(\mathbf{r}) \cdot \hat{\mathbf{j}}_p(\mathbf{r}) d\mathbf{r}$$
$$+ \int \hat{\rho}(\mathbf{r}) \left\{ v_{ext}(\mathbf{r}) + \frac{e^2}{2mc^2} \mathbf{A}_{ext}(\mathbf{r})^2 \right\} d\mathbf{r}, \quad (4)$$

where $\hat{T}$ and $\hat{W}$ are operators of the kinetic energy and the electron-electron interaction, respectively, which are given by

$$\hat{T} = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \quad (5)$$

and

$$\hat{W} = \sum_{i>j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (6)$$

This is the starting Hamiltonian of the CDFT. Hereafter, we shall discuss on the basis of Eq. (4).

The exchange-correlation energy functional of the CDFT is formally defined as[5,6]

$$E_{xc}[\rho, \mathbf{j}_p] = F[\rho, \mathbf{j}_p] - T_s[\rho, \mathbf{j}_p] - U[\rho], \quad (7)$$

where according to the constrained-search approach

$$F[\rho, \mathbf{j}_p] = \underset{\Psi \to (\rho, \mathbf{j}_p)}{\text{Min}} \langle \Psi | \hat{T} + \hat{W} | \Psi \rangle$$
$$=: \langle \Psi[\rho, \mathbf{j}_p] | \hat{T} + \hat{W} | \Psi[\rho, \mathbf{j}_p] \rangle, \quad (8)$$

$$T_s[\rho, \mathbf{j}_p] = \underset{\Phi \to (\rho, \mathbf{j}_p)}{\text{Min}} \langle \Phi | \hat{T} | \Phi \rangle$$
$$=: \langle \Phi[\rho, \mathbf{j}_p] | \hat{T} | \Phi[\rho, \mathbf{j}_p] \rangle, \quad (9)$$

$$U[\rho] = \frac{e^2}{2} \int \int \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}', \quad (10)$$

where $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$ are expectation values of Eqs. (2) and (3) with respect to the wave function, respectively. In Eq. (8), the minimizing is performed among antisymmetric wave functions Ψ that yield the prescribed $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$, and $\Psi[\rho, \mathbf{j}_p]$ means the minimizing wave function. Similarly, the minimizing in Eq. (9) is done among the single Slater determinants Φ that yield the prescribed $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$. $\Phi[\rho, \mathbf{j}_p]$ means the minimizing single Slater determinant. Substituting Eqs. (8) and (9) into Eq. (7), we have

$$E_{xc}[\rho, \mathbf{j}_p] = \langle \Phi[\rho, \mathbf{j}_p] | \hat{W} | \Phi[\rho, \mathbf{j}_p] \rangle - U[\rho]$$
$$+ \langle \Psi[\rho, \mathbf{j}_p] | \hat{W} | \Psi[\rho, \mathbf{j}_p] \rangle - \langle \Phi[\rho, \mathbf{j}_p] | \hat{W} | \Phi[\rho, \mathbf{j}_p] \rangle$$
$$+ \langle \Psi[\rho, \mathbf{j}_p] | \hat{T} | \Psi[\rho, \mathbf{j}_p] \rangle$$
$$- \langle \Phi[\rho, \mathbf{j}_p] | \hat{T} | \Phi[\rho, \mathbf{j}_p] \rangle. \quad (11)$$

Let us define the exchange energy functional $E_x[\rho, \mathbf{j}_p]$ as the first two terms on the right-hand side of Eq. (11), and the correlation energy functional $E_c[\rho, \mathbf{j}_p]$ as the remaining four terms, i.e.,

$$E_x[\rho, \mathbf{j}_p] \equiv \langle \Phi[\rho, \mathbf{j}_p] | \hat{W} | \Phi[\rho, \mathbf{j}_p] \rangle - U[\rho], \quad (12)$$

$$E_c[\rho, \mathbf{j}_p] \equiv \langle \Psi[\rho, \mathbf{j}_p] | \hat{W} | \Psi[\rho, \mathbf{j}_p] \rangle - \langle \Phi[\rho, \mathbf{j}_p] | \hat{W} | \Phi[\rho, \mathbf{j}_p] \rangle$$
$$+ \langle \Psi[\rho, \mathbf{j}_p] | \hat{T} | \Psi[\rho, \mathbf{j}_p] \rangle - \langle \Phi[\rho, \mathbf{j}_p] | \hat{T} | \Phi[\rho, \mathbf{j}_p] \rangle. \quad (13)$$

These definitions are the same as those previously given by Erhard and Gross.[11]

III. VORTICITY DEPENDENCE OF $E_x[\rho, \mathbf{j}_p]$ AND $E_c[\rho, \mathbf{j}_p]$

In this section, we shall show that $E_x[\rho, \mathbf{j}_p]$ and $E_c[\rho, \mathbf{j}_p]$ are dependent on $\mathbf{j}_p(\mathbf{r})$ only via the vorticity $\boldsymbol{\nu}(\mathbf{r}) = \nabla \times \{\mathbf{j}_p(\mathbf{r})/\rho(\mathbf{r})\}$. This proof is slightly different from the previous one in that the vorticity dependence will be shown for each of $E_x[\rho, \mathbf{j}_p]$ and $E_c[\rho, \mathbf{j}_p]$ without the restriction of the v representability, while previous work gave such dependence

for $E_{xc}[\rho,\mathbf{j}_p]$ within the v-representable CDFT.[5,6]

First of all, we shall show the following relation:

$$\Psi\left[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\,\boldsymbol{\nabla}\,\chi\right] = e^{-i(e/c\hbar)\sum_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi[\rho,\mathbf{j}_p], \quad (14)$$

where $\chi(\mathbf{r})$ is an arbitrary scalar function. Since it is the minimizing wave function defined in Eq. (8), $\Psi[\rho,\mathbf{j}_p]$ satisfies

$$\left\{\hat{T}+\hat{W}+\int \lambda[\rho,\mathbf{j}_p](\mathbf{r})\hat{\rho}(\mathbf{r})d\mathbf{r} \right.$$
$$\left. +\int \boldsymbol{\mu}[\rho,\mathbf{j}_p](\mathbf{r})\cdot\hat{\mathbf{j}}_p(\mathbf{r})d\mathbf{r}\right\}\Psi[\rho,\mathbf{j}_p] = E\Psi[\rho,\mathbf{j}_p], \quad (15)$$

where $\lambda[\rho,\mathbf{j}_p](\mathbf{r})$ and $\boldsymbol{\mu}[\rho,\mathbf{j}_p](\mathbf{r})$ are the Lagrange multiplier functions that correspond to the constraints $\rho(\mathbf{r}) = \langle\Psi|\hat{\rho}(\mathbf{r})|\Psi\rangle$ and $\mathbf{j}_p(\mathbf{r}) = \langle\Psi|\hat{\mathbf{j}}_p(\mathbf{r})|\Psi\rangle$, respectively, and where E is the Lagrange multiplier coefficient to the constraint $\langle\Psi|\Psi\rangle = 1$. Here note that the Lagrange multiplier functions are explicitly written as the functional of both $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$ because they are determined corresponding to the prescribed values of $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$. If we define

$$\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r}) \equiv \frac{c}{e}\boldsymbol{\mu}[\rho,\mathbf{j}_p](\mathbf{r}) \quad (16)$$

and

$$v[\rho,\mathbf{j}_p](\mathbf{r}) \equiv \lambda[\rho,\mathbf{j}_p](\mathbf{r}) - \frac{1}{2m}\boldsymbol{\mu}[\rho,\mathbf{j}_p](\mathbf{r})^2, \quad (17)$$

then Eq. (15) is formally rewritten as

$$\left[\hat{T}+\hat{W}+\int\left\{v[\rho,\mathbf{j}_p](\mathbf{r})+\frac{e^2}{2mc^2}\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})^2\right\}\hat{\rho}(\mathbf{r})d\mathbf{r}\right.$$
$$\left.+\frac{e}{c}\int \mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})\cdot\hat{\mathbf{j}}_p(\mathbf{r})d\mathbf{r}\right]\Psi[\rho,\mathbf{j}_p] = E\Psi[\rho,\mathbf{j}_p]. \quad (18)$$

Since the left-hand side of Eq. (18) is the same as Eq. (4), the gauge transformation such as $\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r}) \rightarrow \mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r}) + \boldsymbol{\nabla}\chi(\mathbf{r})$ leads to[28]

$$\left[\hat{T}+\hat{W}+\int\left\{v[\rho,\mathbf{j}_p](\mathbf{r})+\frac{e^2}{2mc^2}[\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})\right.\right.$$
$$\left.+\boldsymbol{\nabla}\chi(\mathbf{r})]^2\right\}\hat{\rho}(\mathbf{r})d\mathbf{r}+\frac{e}{c}\int\{\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})$$
$$\left.+\boldsymbol{\nabla}\chi(\mathbf{r})\}\cdot\hat{\mathbf{j}}_p(\mathbf{r})d\mathbf{r}\right]e^{-i(e/c\hbar)\sum_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi[\rho,\mathbf{j}_p]$$
$$= Ee^{-i(e/c\hbar)\sum_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi[\rho,\mathbf{j}_p]. \quad (19)$$

As shown in Ref. 28, solutions of Eq. (19) yield $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r}) - \frac{e}{mc}\rho(\mathbf{r})\boldsymbol{\nabla}\chi(\mathbf{r})$. If we recall the fact that the Lagrange multiplier functions, $\lambda[\rho,\mathbf{j}_p]$ and $\boldsymbol{\mu}[\rho,\mathbf{j}_p]$, are uniquely determined by $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$, then the potentials in Eq. (19),

$v[\rho,\mathbf{j}_p](\mathbf{r}) + \frac{e^2}{2mc^2}[\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})+\boldsymbol{\nabla}\chi(\mathbf{r})]^2$ and $e/c\{\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r}) + \boldsymbol{\nabla}\chi(\mathbf{r})\}$, can be regarded as the Lagrange multiplier functions that reproduce $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r}) - (e/mc)\rho(\mathbf{r})\boldsymbol{\nabla}\chi(\mathbf{r})$. We thus obtain

$$\lambda\left[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\,\boldsymbol{\nabla}\,\chi\right](\mathbf{r}) = v[\rho,\mathbf{j}_p](\mathbf{r}) + \frac{e^2}{2mc^2}[\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})$$
$$+\boldsymbol{\nabla}\chi(\mathbf{r})]^2, \quad (20)$$

$$\boldsymbol{\mu}\left[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\,\boldsymbol{\nabla}\,\chi\right](\mathbf{r}) = \frac{e}{c}\{\mathbf{A}[\rho,\mathbf{j}_p](\mathbf{r})+\boldsymbol{\nabla}\chi(\mathbf{r})\}. \quad (21)$$

Correspondingly, $\Psi[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\boldsymbol{\nabla}\chi]$ is given by Eq. (14).

It should be noted that substitution of Eqs. (16) and (17) into Eqs. (20) and (21) leads to the relation between the Lagrange multiplier functions. Namely, the Lagrange multiplier functions that yield $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r}) - \frac{e}{mc}\rho(\mathbf{r})\boldsymbol{\nabla}\chi(\mathbf{r})$ are related to those that yield $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$. These relations result in the relation (14) between $\Psi[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\boldsymbol{\nabla}\chi]$ and $\Psi[\rho,\mathbf{j}_p]$.

A similar result is available for $\Phi[\rho,\mathbf{j}_p]$ if we consider the case such that $\hat{W}\rightarrow 0$,

$$\Phi\left[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\,\boldsymbol{\nabla}\,\chi\right] = e^{-i(e/c\hbar)\sum_{i=1}^{N}\chi(\mathbf{r}_i)}\Phi[\rho,\mathbf{j}_p]. \quad (22)$$

Using Eqs. (14) and (22), the exchange and correlation energy functionals that are defined by Eqs. (12) and (13) have the following relations:

$$E_x\left[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\,\boldsymbol{\nabla}\,\chi\right] = E_x[\rho,\mathbf{j}_p], \quad (23)$$

$$E_c\left[\rho,\mathbf{j}_p - \frac{e}{mc}\rho\,\boldsymbol{\nabla}\,\chi\right] = E_c[\rho,\mathbf{j}_p]. \quad (24)$$

In order to satisfy Eqs. (23) and (24) for the arbitrary scalar function $\chi(\mathbf{r})$, both energy functionals, $E_x[\rho,\mathbf{j}_p]$ and $E_c[\rho,\mathbf{j}_p]$, are dependent on $\mathbf{j}_p(\mathbf{r})$ via the form of vorticity $\boldsymbol{\nu}(\mathbf{r})$. Hereafter, we shall write the exchange and correlation energy functionals as

$$\bar{E}_x[\rho,\boldsymbol{\nu}] := E_x[\rho,\mathbf{j}_p] \quad (25)$$

and

$$\bar{E}_c[\rho,\boldsymbol{\nu}] := E_c[\rho,\mathbf{j}_p], \quad (26)$$

respectively.

IV. VORTICITY EXPANSION APPROXIMATION OF THE EXCHANGE ENERGY FUNCTIONAL

In this section, we shall propose the practical form of the exchange energy functional on the basis of the VEA. The expansion coefficient is determined by requiring it to satisfy the exact relation that was derived previously.[11] This strategy is similar to that of the GGA of the conventional DFT.[25–27]

With reference to the GGA, the approximate form of $\bar{E}_x[\rho,\boldsymbol{\nu}]$ is assumed to be

$$\bar{E}_x[\rho,\boldsymbol{\nu}] = E_x[\rho] + \int \rho(\mathbf{r}) F_x(\rho,\boldsymbol{\nu})\big|_{\substack{\rho=\rho(\mathbf{r}) \\ \boldsymbol{\nu}=\boldsymbol{\nu}(\mathbf{r})}} d\mathbf{r}, \qquad (27)$$

where $E_x[\rho]$ is the exchange energy functional of the conventional DFT, and where $F_x(\rho,\boldsymbol{\nu})$ is an energy density that should be determined by the exact relation. Here we consider the case in which $\boldsymbol{\nu}$ is small. Then, the Taylor expansion of $F_x(\rho,\boldsymbol{\nu})$ around $\boldsymbol{\nu}=\mathbf{0}$ may be truncated at second order of $\boldsymbol{\nu}$,

$$\begin{aligned} F_x(\rho,\boldsymbol{\nu}) &= F_x(\rho,0) + \boldsymbol{\nu} \cdot \mathbf{D}^{(1)}(\rho) + D_{xx}^{(2)}(\rho)\nu_x^2 + D_{yy}^{(2)}(\rho)\nu_y^2 \\ &+ D_{zz}^{(2)}(\rho)\nu_z^2 + D_{xy}^{(2)}(\rho)\nu_x\nu_y + D_{yz}^{(2)}(\rho)\nu_y\nu_z \\ &+ D_{xz}^{(2)}(\rho)\nu_x\nu_z, \end{aligned} \qquad (28)$$

where $\mathbf{D}^{(1)}(\rho)$ and $D_{ij}^{(2)}(\rho)$ are the expansion coefficients, which are given by

$$\mathbf{D}^{(1)}(\rho) = \boldsymbol{\nabla}_{\boldsymbol{\nu}} F_x(\rho,\boldsymbol{\nu})\big|_{\boldsymbol{\nu}=\mathbf{0}}, \qquad (29)$$

$$D_{ij}^{(2)}(\rho) = \frac{1}{2} \left. \frac{\partial^2 F_x(\rho,\boldsymbol{\nu})}{\partial \nu_i \partial \nu_j} \right|_{\boldsymbol{\nu}=\mathbf{0}}, \quad i,j = x,y,z. \qquad (30)$$

Since $\bar{E}_x[\rho,\boldsymbol{\nu}]\big|_{\boldsymbol{\nu}=\mathbf{0}}$ should coincide with the exchange energy functional of the DFT, we can obtain $F_x(\rho,0)=0$. In addition, if $F_x(\rho,\boldsymbol{\nu})$ is assumed to be spherical with respect to $\boldsymbol{\nu}$, then the first order of $\boldsymbol{\nu}$ becomes zero and the terms of the second order can be rewritten as $D(\rho)|\boldsymbol{\nu}|^2$, where $D(\rho)$ $:= D_{xx}^{(2)}(\rho)=D_{yy}^{(2)}(\rho)=D_{zz}^{(2)}(\rho)$. Consequently, Eq. (28) becomes

$$F_x(\rho,\boldsymbol{\nu}) = D(\rho)|\boldsymbol{\nu}|^2. \qquad (31)$$

Next let us consider the properties of $D(\rho)$ by utilizing the exact relation for the exchange energy functional. The scaling behavior of the exchange energy functional was given by[11]

$$\bar{E}_x[\rho_\lambda,\boldsymbol{\nu}_\lambda] = \lambda \bar{E}_x[\rho,\boldsymbol{\nu}] \qquad (32)$$

with

$$\boldsymbol{\nu}_\lambda(\mathbf{r}) = \boldsymbol{\nabla} \times \left(\frac{\mathbf{j}_p^\lambda(\mathbf{r})}{\rho_\lambda(\mathbf{r})} \right), \qquad (33)$$

where λ is the scaling factor of the electron coordinates, and where $\rho_\lambda(\mathbf{r})$ and $\mathbf{j}_p^\lambda(\mathbf{r})$ are, respectively, electron density and paramagnetic current density, which are calculated from the uniformly scaled wave function.[11] They are related to $\rho(\mathbf{r})$ and $\boldsymbol{\nu}(\mathbf{r})$ by

$$\rho_\lambda(\mathbf{r}) = \lambda^3 \rho(\lambda\mathbf{r}), \qquad (34)$$

$$\boldsymbol{\nu}_\lambda(\mathbf{r}) = \lambda^2 \boldsymbol{\nu}(\lambda\mathbf{r}). \qquad (35)$$

Substituting Eq. (27) into Eq. (32), we get

$$\int \rho(\mathbf{r}) F_x(\rho,\boldsymbol{\nu})\big|_{\substack{\rho=\rho_\lambda(\mathbf{r}) \\ \boldsymbol{\nu}=\boldsymbol{\nu}_\lambda(\mathbf{r})}} d\mathbf{r} = \lambda \int \rho(\mathbf{r}) F_x(\rho,\boldsymbol{\nu})\big|_{\substack{\rho=\rho(\mathbf{r}) \\ \boldsymbol{\nu}=\boldsymbol{\nu}(\mathbf{r})}} d\mathbf{r}, \qquad (36)$$

where the relation $E_x[\rho_\lambda]=\lambda E_x[\rho]$ for the conventional DFT is used.[29] Substitution of Eq. (31) into Eq. (36) yields

$$\int \rho(\mathbf{r})|\boldsymbol{\nu}(\mathbf{r})|^2 \{\lambda^3 D(\rho)\big|_{\rho=\lambda^3\rho(\mathbf{r})} - D(\rho)\big|_{\rho=\rho(\mathbf{r})}\} d\mathbf{r} = 0. \qquad (37)$$

As a sufficient condition for the above, we can obtain $\lambda^3 D(\lambda^3\rho)=D(\rho)$. If $D(\rho)$ is assumed to be expressed as the power of ρ, i.e., $D(\rho)=D_x\rho^\alpha$, then $\alpha=-1$ can be obtained from the sufficient condition. Accordingly, we get the VEA formula

$$\bar{E}_x[\rho,\boldsymbol{\nu}] = E_x[\rho] + D_x \int |\boldsymbol{\nu}(\mathbf{r})|^2 d\mathbf{r}, \qquad (38)$$

where D_x is the constant. By using the dimensionless constant $\bar{D}_x$, Eq. (38) is further rewritten as

$$\bar{E}_x[\rho,\boldsymbol{\nu}] = E_x[\rho] + \bar{D}_x \frac{\hbar^2}{a_H^3 \varepsilon_H} \int |\boldsymbol{\nu}(\mathbf{r})|^2 d\mathbf{r}, \qquad (39)$$

where a_H and ε_H stand for the Bohr radius and Rydberg constant, respectively.

V. VORTICITY EXPANSION APPROXIMATION OF THE CORRELATION ENERGY FUNCTIONAL

A. Vorticity expansion of the correlation energy functional

In the same way as the exchange energy functional, let us consider the following approximate form of $\bar{E}_c[\rho,\boldsymbol{\nu}]$:

$$\bar{E}_c[\rho,\boldsymbol{\nu}] = E_c[\rho] + \int \rho(\mathbf{r}) F_c(\rho,\boldsymbol{\nu})\big|_{\substack{\rho=\rho(\mathbf{r}) \\ \boldsymbol{\nu}=\boldsymbol{\nu}(\mathbf{r})}} d\mathbf{r}, \qquad (40)$$

where $E_c[\rho]$ denotes the correlation energy functional of the conventional DFT, and where $F_c(\rho,\boldsymbol{\nu})$ stands for an energy density that is a function of ρ and $\boldsymbol{\nu}$. Similarly to $F_x(\rho,\boldsymbol{\nu})$, we assume that $F_c(\rho,\boldsymbol{\nu})$ is spherical with respect to $\boldsymbol{\nu}$. Truncating the third- and higher-order terms of the expansion, we get

$$F_c(\rho,\boldsymbol{\nu}) = C(\rho)|\boldsymbol{\nu}|^2, \qquad (41)$$

where $C(\rho)$ is a function of ρ. Substituting Eq. (41) into Eq. (40), we obtain the VEA formula for $\bar{E}_c[\rho,\boldsymbol{\nu}]$

$$\bar{E}_c[\rho,\boldsymbol{\nu}] = E_c[\rho] + \int \rho(\mathbf{r}) C(\rho(\mathbf{r}))|\boldsymbol{\nu}(\mathbf{r})|^2 d\mathbf{r}. \qquad (42)$$

The expansion coefficient $C(\rho)$ is determined by requiring $\bar{E}_c[\rho,\boldsymbol{\nu}]$ to satisfy exact relations.[11,17]

B. Conditions to be satisfied with the expansion coefficient $C(\rho)$

In this subsection, the exact relations for $\bar{E}_c[\rho,\boldsymbol{\nu}]$, which have been derived by means of the uniform and nonuniform scaling techniques,[11,17] are rewritten as conditions for $C(\rho)$. Then, we propose an approximate form of $C(\rho)$ that satisfies their conditions.

The uniform scaling of coordinates of electrons leads to the following exact relations:[11]

$$\bar{E}_c[\rho_\lambda, \boldsymbol{\nu}_\lambda] - \lambda \bar{E}_c[\rho, \boldsymbol{\nu}] \geq 0 \text{ for } \lambda \geq 1, \tag{43}$$

$$\bar{E}_c[\rho_\lambda, \boldsymbol{\nu}_\lambda] - \lambda \bar{E}_c[\rho, \boldsymbol{\nu}] \leq 0 \text{ for } \lambda \leq 1. \tag{44}$$

By using Eq. (42), the left-hand side of Eqs. (43) and (44) is given by

$$\bar{E}_c[\rho_\lambda, \boldsymbol{\nu}_\lambda] - \lambda \bar{E}_c[\rho, \boldsymbol{\nu}] = E_c[\rho_\lambda] - \lambda E_c[\rho]$$
$$+ \lambda \int \rho(\mathbf{r})\{\lambda^3 C(\lambda^3 \rho(\mathbf{r}))$$
$$- C(\rho(\mathbf{r}))\}|\boldsymbol{\nu}(\mathbf{r})|^2 d\mathbf{r}. \tag{45}$$

Since $E_c[\rho]$ satisfies exact relations that are similar to Eqs. (43) and (44),[29] Eqs. (43) and (44) can be rewritten as conditions for $C(\rho)$. We have

$$\lambda^3 C(\lambda^3 \rho) \geq C(\rho) \text{ for } \lambda \geq 1, \tag{46}$$

$$\lambda^3 C(\lambda^3 \rho) \leq C(\rho) \text{ for } \lambda \leq 1. \tag{47}$$

Note that Eqs. (43) and (44) always hold if $C(\rho)$ satisfies the above conditions. Namely, Eqs. (46) and (47) can be recognized as sufficient conditions for Eqs. (43) and (44), respectively.

The nonuniform scaling of coordinates of electrons leads to a lot of exact relations. These have been systematically derived and summarized in Ref. 17. If we scale the x coordinate with λ, the scaled electronic density and vorticity are given by

$$\rho_\lambda^x(\mathbf{r}) = \lambda \rho(\lambda x, y, z), \tag{48}$$

$$\boldsymbol{\nu}_\lambda^x(\mathbf{r}) \equiv \nabla \times \left(\frac{\mathbf{j}_{p\lambda}^x(\mathbf{r})}{\rho_\lambda^x(\mathbf{r})} \right)$$
$$= (\nu_x(\lambda x, y, z), \lambda \nu_y(\lambda x, y, z), \lambda \nu_z(\lambda x, y, z)), \tag{49}$$

respectively, where $\rho_\lambda^x(\mathbf{r})$ and $\mathbf{j}_{p\lambda}^x(\mathbf{r})$ are calculated from the wave function, which is scaled by λ only in the x axis. According to our previous work,[17] the following exact relations hold for $\rho_\lambda^x(\mathbf{r})$ and $\boldsymbol{\nu}_\lambda^x(\mathbf{r})$:

$$\lim_{\lambda \to \infty} \bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x] = 0, \tag{50}$$

$$\lim_{\lambda \to \infty} \lambda \bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x] = \text{const}, \tag{51}$$

$$\lim_{\lambda \to 0} \bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x] = 0, \tag{52}$$

$$\lim_{\lambda \to 0} \lambda^{-1} \bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x] = 0, \tag{53}$$

$$\lim_{\lambda \to 0} \lambda^{-2} \bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x] = \text{const}. \tag{54}$$

By using Eqs. (42), (48), and (49), $\bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x]$ is given by

$$\bar{E}_c[\rho_\lambda^x, \boldsymbol{\nu}_\lambda^x] = E_c[\rho_\lambda^x] + \int \rho(\mathbf{r})\lambda^2 C(\lambda \rho(\mathbf{r}))$$
$$\times \left\{ \frac{\nu_x(\mathbf{r})^2}{\lambda^2} + \nu_y(\mathbf{r})^2 + \nu_z(\mathbf{r})^2 \right\} d\mathbf{r}. \tag{55}$$

Substituting Eq. (55) into Eqs. (50)–(54), and using the exact relations of $E_c[\rho]$,[30] we obtain conditions for $C(\rho)$ that correspond to sufficient conditions for Eqs. (50)–(54),

$$\lim_{\lambda \to \infty} \lambda^2 C(\lambda \rho) = 0, \tag{56}$$

$$\lim_{\lambda \to \infty} \lambda^3 C(\lambda \rho) = 0 \text{ or } \{\text{a positive power of } \rho\}, \tag{57}$$

$$\lim_{\lambda \to 0} C(\lambda \rho) = 0, \tag{58}$$

$$\lim_{\lambda \to 0} \lambda^{-1} C(\lambda \rho) = 0, \tag{59}$$

$$\lim_{\lambda \to 0} \lambda^{-2} C(\lambda \rho) = 0 \text{ or } \{\text{a positive power of } \rho\}. \tag{60}$$

In a similar way to the above discussion, we can obtain conditions for $C(\rho)$ from the other kinds of exact relations of $\bar{E}_c[\rho, \boldsymbol{\nu}]$, which have been derived in Ref. 17. They are summarized as follows:

$$\lim_{\lambda \to \infty} \lambda^4 C(\lambda \rho) = 0, \tag{61}$$

$$\lim_{\lambda \to \infty} \lambda^5 C(\lambda \rho) = 0, \tag{62}$$

$$\lim_{\lambda \to \infty} \lambda^6 C(\lambda \rho) = 0 \text{ or } \{\text{a positive power of } \rho\}, \tag{63}$$

$$\lim_{\lambda \to \infty} \lambda^4 C(\lambda^2 \rho) = 0, \tag{64}$$

$$\lim_{\lambda \to \infty} \lambda^5 C(\lambda^2 \rho) = 0 \text{ or } \{\text{a positive power of } \rho\}, \tag{65}$$

$$\lim_{\lambda \to 0} \lambda^2 C(\lambda^2 \rho) = 0, \tag{66}$$

$$\lim_{\lambda \to 0} \lambda C(\lambda^2 \rho) = 0, \tag{67}$$

$$\lim_{\lambda \to 0} C(\lambda^2 \rho) = 0 \text{ or } \{\text{a positive power of } \rho\}. \tag{68}$$

It should be noted that the exact relations (3.11a)–(3.11e), (3.14a)–(3.14e), and (3.20a)–(3.20f) of Ref. 17 necessarily hold if $C(\rho)$ satisfies the equations from Eqs. (56)–(68). Hereafter, we propose an approximate form of $C(\rho)$ that satisfies the above conditions.

Let us suppose that $C(\rho)$ is given by

$$C(\rho) = \bar{C}_0 \frac{\hbar^2}{a_H^3 \varepsilon_H} \frac{e^{-\bar{\alpha} a_H^3 \rho} \rho^2}{(\rho - \bar{\delta}/a_H^3)^3}, \quad (69)$$

where $\bar{C}_0$, $\bar{\alpha}$, and $\bar{\delta}$ are dimensionless constants. It is easily confirmed that Eq. (69) is satisfied with conditions from Eqs. (56)–(68) if $\bar{\alpha}$ and $\bar{\delta}$ are positive values. Also, Eqs. (46) and (47) hold when we choose $\bar{C}_0$ negative and $\bar{\delta}$ small enough. If $\bar{\delta}/a_H^3$ is much smaller than ρ of interest, and if $\bar{C}_0$ is negative, then the condition (46) holds. Additionally, the condition (47) is satisfied if the scaling factor λ is larger than $(\bar{\delta}/\rho)^{1/3}$ and if $\bar{C}_0$ is negative. Substituting Eq. (69) into Eq. (42), we get the resultant VEA formula of $\bar{E}_c[\rho, \boldsymbol{\nu}]$,

$$\bar{E}_c[\rho, \boldsymbol{\nu}] = E_c[\rho] + \frac{\bar{C}_0 \hbar^2}{a_H^3 \varepsilon_H} \int \frac{e^{-\bar{\alpha} a_H^3 \rho(\mathbf{r})} \rho(\mathbf{r})^3}{\{\rho(\mathbf{r}) - \bar{\delta}/a_H^3\}^3} |\boldsymbol{\nu}(\mathbf{r})|^2 d\mathbf{r}. \quad (70)$$

The comparison of the present VEA and the CDFT-LDA[17] is summarized in Table I from the viewpoint of exact relations fulfilled. The VEA formulas satisfy more "sum rules" than those of the CDFT-LDA.[17] It should be noted that even though an approximate functional is satisfied with more sum rules than another one, it would not always give the quantitatively better results than the functional that is not satisfied with fewer sum rules. The sum rule does not always guarantee to make a good functional. However, to say the least, the sum rule may well get rid of the difficulties that lead to nonphysical results, from the approximate functional. In this sense, it can be expected that the present VEA formulas may lead to more reasonable results than the CDFT-LDA.

At the end of this subsection, we would like to comment on the VEA formulas. The present form includes three constants. In order to satisfy Eqs. (46), (47), and (56)–(68), as mentioned above, the values of $\bar{C}_0$, $\bar{\alpha}$, and $\bar{\delta}$ should be chosen as

$$\bar{C}_0 < 0, \quad \bar{\alpha} > 0, \quad 0 < \bar{\delta} \ll a_H^3 \rho, \quad (71)$$

respectively. It is striking that no matter how we give values of their constants according to Eq. (71), Eq. (70) satisfies all exact relations as shown in Table I.

VI. FITTING TO THE EXCHANGE AND CORRELATION ENERGIES OF THE HOMOGENEOUS ELECTRON LIQUID UNDER THE UNIFORM MAGNETIC FIELD

In this section, the VEA formulas are fitted to the exchange and correlation energies of the homogeneous electron liquid under the uniform magnetic field. These fits are meaningful not only from a practical viewpoint but also for checking the validity of the VEA formulas.

A. Exchange energy

The exchange energy of the homogeneous electron liquid under the uniform magnetic field has already been studied by

TABLE I. Comparison of the VEA and the CDFT-LDA defined in Ref. 17.

	CDFT-LDA	VEA
$E_x[\rho_\lambda, \mathbf{j}_p^\lambda] = \lambda E_x[\rho, \mathbf{j}_p]$	Yes	Yes
$E_c[\rho_\lambda, \mathbf{j}_p^\lambda] \geqslant \lambda E_c[\rho, \mathbf{j}_p], \lambda \geqslant 1$	Yes	Yes
$E_c[\rho_\lambda, \mathbf{j}_p^\lambda] \leqslant \lambda E_c[\rho, \mathbf{j}_p], \lambda \leqslant 1$	Yes	Yes
$\lim_{\lambda \to \infty} E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] = 0$		Yes
$\lim_{\lambda \to \infty} \lambda E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] = \text{const}$		Yes
$\lim_{\lambda \to 0} E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] = 0$	Yes	Yes
$\lim_{\lambda \to 0} \lambda^{-1} E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] = 0$	No	Yes
$\lim_{\lambda \to 0} \lambda^{-2} E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] = \text{const}$	No	Yes
$\lim_{\lambda \to \infty} E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}] = 0$		Yes
$\lim_{\lambda \to \infty} \lambda E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}] = \text{const}$		Yes
$\lim_{\lambda \to 0} E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}] = 0$		Yes
$\lim_{\lambda \to 0} \lambda^{-1} E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}] = 0$	Yes	Yes
$\lim_{\lambda \to 0} \lambda^{-2} E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}] = \text{const}$	No	Yes
$\lim_{\lambda \to \infty} E_c[\rho_{\lambda\lambda\lambda^{-1}}^{xyz}, \mathbf{j}_{p\lambda\lambda\lambda^{-1}}^{xyz}] = 0$		Yes
$\lim_{\lambda \to \infty} \lambda E_c[\rho_{\lambda\lambda\lambda^{-1}}^{xyz}, \mathbf{j}_{p\lambda\lambda\lambda^{-1}}^{xyz}] = 0$		Yes
$\lim_{\lambda \to \infty} \lambda^2 E_c[\rho_{\lambda\lambda\lambda^{-1}}^{xyz}, \mathbf{j}_{p\lambda\lambda\lambda^{-1}}^{xyz}] = \text{const}$	Yes	Yes
$\lim_{\lambda \to 0} E_c[\rho_{\lambda\lambda\lambda^{-1}}^{xyz}, \mathbf{j}_{p\lambda\lambda\lambda^{-1}}^{xyz}] = 0$	No	Yes
$\lim_{\lambda \to 0} \lambda^{-1} E_c[\rho_{\lambda\lambda\lambda^{-1}}^{xyz}, \mathbf{j}_{p\lambda\lambda\lambda^{-1}}^{xyz}] = 0$	No	Yes
$\lim_{\lambda \to 0} \lambda^{-2} E_c[\rho_{\lambda\lambda\lambda^{-1}}^{xyz}, \mathbf{j}_{p\lambda\lambda\lambda^{-1}}^{xyz}] = \text{const}$	No	Yes

some workers.[31,32] If the electron liquid under the uniform magnetic field is at rest, then the vorticity is constant and can be written as

$$\boldsymbol{\nu} = -\frac{e}{mc} \mathbf{B}_{\text{ext}}, \quad (72)$$

where $\mathbf{B}_{\text{ext}} = \boldsymbol{\nabla} \times \mathbf{A}_{\text{ext}}(\mathbf{r})$. Substituting Eq. (72) into Eq. (39), we get

$$\bar{E}_x^{\text{homo}}(\rho, \bar{B}_{\text{ext}}) = E_x^{\text{homo}}(\rho) + \bar{D}_x \frac{\hbar^2 \Omega}{a_H^3 \varepsilon_H} \left(\frac{me^4}{2\hbar^3} \right)^2 \bar{B}_{\text{ext}}^2 \quad (73)$$

with

$$\bar{B}_{\text{ext}} = \frac{\hbar \omega_c}{\varepsilon_H} = \frac{2\hbar^3}{m^2 c e^3} |\mathbf{B}_{\text{ext}}|, \quad (74)$$

where Ω, ω_c, and $\bar{B}_{\text{ext}}$ are the volume of the system, the cyclotron frequency, and the dimensionless magnetic field,
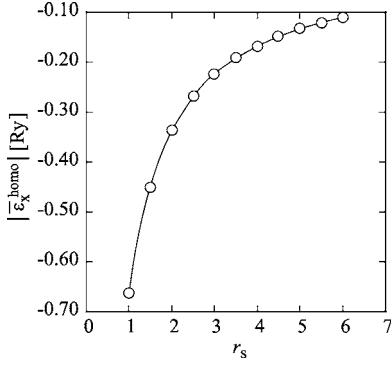
FIG. 1. Dependence of $\bar{\varepsilon}_x^{\text{homo}}$ on r_s. Solid curve and open circles denote the present VEA of Eq. (76) and the calculation results of Ref. 32, respectively, where the ratio (l/r_0) of the magnetic length (l) to the mean interparticle distance (r_0) is fixed at 0.4.
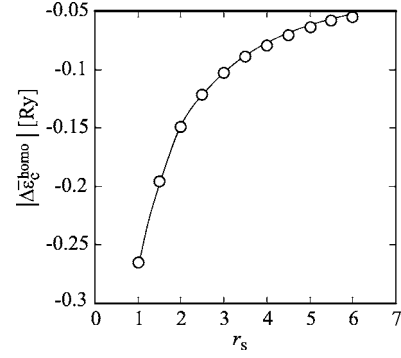

FIG. 2. Dependence of $\Delta\bar{\varepsilon}_c^{\text{homo}}$ on r_s. Solid curve denotes the present VEA of Eq. (78), while open circles denote the calculation results of Ref. 32, where the ratio (l/r_0) of the magnetic length (l) to the mean interparticle distance (r_0) is fixed at 0.4.

respectively. The exchange energy per particle is thus given by

$$\bar{\varepsilon}_x^{\text{homo}}(\rho, \bar{B}_{\text{ext}}) = \frac{E_x^{\text{homo}}(\rho)}{N} + \bar{D}_x \frac{\hbar^2}{a_H^3 \varepsilon_H \rho} \left(\frac{me^4}{2\hbar^3}\right)^2 \bar{B}_{\text{ext}}^2, \quad (75)$$

where N is the number of electrons. Hereafter we shall use atomic units. Using the fact that $E_x^{\text{homo}}[\rho]/N = -0.9163/r_s$ (Ry),[33] Eq. (75) can be rewritten as

$$\bar{\varepsilon}_x^{\text{homo}}(\rho, \bar{B}_{\text{ext}}) = -\frac{0.9163}{r_s} + \bar{D}_x \frac{4\pi}{3} r_s^3 \bar{B}_{\text{ext}}^2 \text{ (Ry)}, \quad (76)$$

where r_s is the usual density parameter that is defined by $r_s = (3/4\pi\rho)^{1/3}$. Fitting Eq. (76) to the results of Takada and Goto,[32] we obtain $\bar{D}_x = 3.76 \times 10^{-4}$. Figure 1 shows the dependence of $\bar{\varepsilon}_x^{\text{homo}}$ on r_s, where the ratio (l/r_0) of the magnetic length $(l = \sqrt{\hbar c/eB_{\text{ext}}})$ to the mean interparticle distance $(r_0 = a_H r_s)$ is fixed at 0.4. As can be seen in Fig. 1, the present formula is in good agreement with the result of Takada and Goto.[32] This means the validity of the VEA formula for the exchange energy functional.

B. Correlation energy

From Eq. (70), the correlation energy $\bar{\varepsilon}_c^{\text{homo}}$ in Ry per particle is given by

$$\bar{\varepsilon}_c^{\text{homo}} = \varepsilon_c^{\text{homo}}(B_{\text{ext}} = 0) + \Delta\bar{\varepsilon}_c^{\text{homo}}, \quad (77)$$

with

$$\Delta\bar{\varepsilon}_c^{\text{homo}} = \bar{C}_0 \frac{\exp\left(-\frac{3\bar{\alpha}}{4\pi} r_s^{-3}\right)\left(\frac{3}{4\pi} r_s^{-3}\right)^2}{\left\{\frac{3}{4\pi} r_s^{-3} - \bar{\delta}\right\}^3} \bar{B}_{\text{ext}}^2, \quad (78)$$

where $\varepsilon_c^{\text{homo}}(B_{\text{ext}} = 0)$ and $\Delta\bar{\varepsilon}_c^{\text{homo}}$ are the correlation energy (in Ry) per particle of the homogeneous electron liquid without magnetic field and the difference from $\bar{\varepsilon}_c^{\text{homo}}$ to $\varepsilon_c^{\text{homo}}(B_{\text{ext}} = 0)$, respectively. The values of constants are determined by fitting calculation results of Eq. (77) to the cor-

relation energy per particle of the homogeneous electron liquid under uniform magnetic fields.[32] As a result, we get $\bar{C}_0 = -4.669 \times 10^{-4}$, $\bar{\alpha} = 0.653$, and $\bar{\delta} = 1.0 \times 10^{-30}$, respectively. Note that these values are consistent with the conditions (71). Figure 2 shows the dependence of $\Delta\bar{\varepsilon}_c^{\text{homo}}$ on r_s. The resultant $\Delta\bar{\varepsilon}_c^{\text{homo}}$ is in good agreement with those of Ref. 32. This means the validity of the VEA formula for the correlation energy functional.

Next, we give a comment on the value of $\bar{\delta}$. As mentioned in Sec. V B, the value of $\bar{\delta}/a_H^3$ should be much smaller than ρ of interest so that the approximate form (70) satisfies all exact relations. The condition $\rho \gg \bar{\delta}/a_H^3$ can be rewritten as $r_s \ll 6.2 \times 10^9$ if $\bar{\delta} = 1.0 \times 10^{-30}$. The r_s parameters that are physically meaningful are up to about six in metals.[33] Therefore, it can be concluded that the approximate form (70) is satisfied with all exact relations for ρ of interest.

At the end of this section, we give a brief comment on the fitting formulas obtained in this section. Judging from the fact that the LDA of the conventional DFT has been successfully applied to various inhomogeneous systems, it is expected that these fitting formulas may be applied not only to the homogeneous electron liquid under the uniform magnetic field, but also to various kinds of inhomogeneous systems.

VII. CONCLUDING REMARKS

In this paper, we present the practical forms of the exchange and correlation energy functionals of the CDFT on the basis of the VEA. The expansion coefficients are determined to satisfy exact relations that have been derived previously.[11,17] These VEA formulas have the following features.

(i) They coincide with exchange and correlation energy functionals of the conventional DFT, respectively, in the limit of vanishing vorticity. (ii) Although each expansion is truncated at second order of ν, the effects of third- and higher-order terms are in principle taken into account by an imposition of the exact relations on the expansion. Due to this fact, the fits of the present expansions to the results of Takada and Goto are quite good, as shown in Figs. 1 and 2.

This is also similar to the fact that the GGA is generally better than the simple gradient approximation.[25–27] (iii) The VEA formulas with fixed constants, which are determined in Sec. VI, have no parameters and are expected to be applicable to various systems if we remember the success of the LDA.

Finally, we give a brief comment on exact relations fulfilled by the VEA formulas. There is an exact relation that is not utilized in Sec. V but is utilized in the development of the PBE functional.[27] The exact relation is such that the correlation energy functional for the uniformly scaled basic variables approaches a constant in the limit of infinite scaling factor.[34] Also in the CDFT, it can be shown that the exact relation of that type holds for the correlation energy functional.[35] Then, it can be confirmed that the VEA formula is satisfied with such an exact relation in addition to the exact relations listed in Table I, while the CDFT-LDA is not satisfied with it. This also indicates the validity of the VEA formulas. The proof and details will be published elsewhere.[35]

The next step is to perform the actual calculations by means of the present VEA formulas.

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[28] If the wave function Ψ is the eigenfunction of the Hamiltonian (4), then $e^{-i(e/c\hbar)\Sigma_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi$ corresponds to the wave function after gauge transformation $\mathbf{A}_{\text{ext}}(\mathbf{r}) \to \mathbf{A}_{\text{ext}}(\mathbf{r}) + \nabla\chi(\mathbf{r})$, where $\chi(\mathbf{r})$ is an arbitrary scalar function. This is easily confirmed by neglecting the surface integral at infinity. Using Eqs. (2) and (3), we have

$$\left\langle e^{-i(e/c\hbar)\Sigma_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi \left| \hat{\rho}(\mathbf{r}) \right| e^{-i(e/c\hbar)\Sigma_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi \right\rangle = \rho(\mathbf{r}),$$

$$\left\langle e^{-i(e/c\hbar)\Sigma_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi \left| \hat{\mathbf{j}}_p(\mathbf{r}) \right| e^{-i(e/c\hbar)\Sigma_{i=1}^{N}\chi(\mathbf{r}_i)}\Psi \right\rangle$$

$$= \mathbf{j}_p(\mathbf{r}) - \frac{e}{mc}\rho(\mathbf{r})\nabla\chi(\mathbf{r}).$$

Thus, the gauge-transformed wave function yields $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r}) - \frac{e}{mc}\rho(\mathbf{r})\nabla\chi(\mathbf{r})$.

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