Sum rules and bounds on the exchange and correlation energy functional of current-density functional theory

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The exact expression for the exchange-correlation energy functional $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ of the current-density functional theory (CDFT) is derived by means of the coupling-constant integration technique. It contains the coupling-constant-averaged pair correlation function, which is a functional of the electron density $\rho(\mathbf{r})$ and paramagnetic current density $\mathbf{j}_p(\mathbf{r})$. On the basis of this expression, the local density approximation and its modifications for $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ are proposed within the CDFT. In addition, we present sum rules and bounds on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ by considering the behaviors of the basic variables and $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ under the various types of the nonuniform coordinate scaling of electrons. They are useful in estimating the validity of the approximate forms of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ proposed.

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I. INTRODUCTION

The current-density functional theory (CDFT)[1,2] and its relativistic version, relativistic current- and spin-density functional theory (RCSDFT),[3–5] have been extensively studied as useful methods for describing the ground state of the systems such as (i) strongly correlated electron systems where the orbital current is induced from the strong spin-orbit interaction, (ii) inhomogeneous electronic systems in an external magnetic field including a two-dimensional electron gas in the quantum Hall regime, and (iii) open-shell atoms and ions where the spontaneous orbital current exists. In order to calculate the electronic structures within the CDFT or RCSDFT, it is imperative that the exchange-correlation energy functional is developed in an applicable form. That is, in the field of the CDFT it is one of the central subjects to develop the approximate form of the exchange-correlation energy functional.

There already exist a few attempts to devise the approximate form of the exchange-correlation energy functional $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$. Here $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$, respectively, show the electron density and paramagnetic current density, which are recognized in the CDFT as the basic variables that uniquely determine the ground state properties of the system. Vignale and co-workers have proposed the local density approximation (LDA) of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ by borrowing the knowledge of the exchange-correlation energy from the homogeneous electron liquid in a uniform magnetic field.[1,2,6–8] This LDA scheme has also been applied to several systems including molecules,[9,10] electron-hole liquids[11,12] and quantum dots[13] in a magnetic field. In another attempt, Cappelle and Gross have suggested the possibility of deriving the exchange-correlation energy functional of the CDFT from that of the spin-density functional theory, though any practical formulas have not been presented, unfortunately.[14]

In this paper, we elaborate two strategies as the first step toward deriving an approximate form of $E_{\mathrm{xe}}[\rho,\mathbf{j}_p]$. One is to derive the coupling-constant expression for $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ via the Hellmann-Feynman theorem, another to derive the exact conditions fulfilled by $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$.

As for the former strategy, the coupling-constant expression is a good starting point to develop the various approximate forms of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$. Once the coupling-constant expression is obtained, we can easily define the CDFT version of the LDA and nonlocal density schemes which correspond to the average-density approximation (ADA)[15–18] and the weighted-density approximation (WDA)[16–20] of the conventional density functional theory (DFT). It is expected that these approximate schemes are applicable to actual energy-band calculations by means of only the knowledge of the homogeneous electron liquid in the uniform magnetic field.

Concerning the latter strategy, the exact conditions on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ can be utilized as sum rules and bounds which should be satisfied by the approximate forms. This strategy is analogous to the generalized gradient approximation (GGA) method of the DFT in developing the approximate form of the exchange-correlation energy functional.[21–23] Erhard and Gross have derived the exact conditions on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ from the viral theorem and the uniform coordinate scaling of electrons.[24] Liu *et al.* have also presented the local formulas for the exchange and correlation energy functionals under the local and variable-separation assumptions.[25] The formalism employed parallels the one used in the conventional DFT.[26–30] In addition, the gauge invariance of the system imposes the additional condition on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$.[2,31,32] It guarantees that the basic variables are reproduced in the fictitious system for any gauges. With reference to these achievements, in this paper we present the exact conditions on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ through the nonuniform coordinate scaling of electrons. They can be regarded as new kinds of sum rules and bounds on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$. Our result and previous ones mentioned above are complementary to each other for the purpose of developing the approximate form of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$.

The organization of this paper is as follows. In Sec. II, the

coupling-constant expression for $E_{\rm xc}[\rho,\mathbf{j}_p]$ is presented. The LDA and its modifications such as the ADA and WDA are proposed on the basis of this expression. In Sec. III, we derive sum rules and bounds on $E_{\rm xc}[\rho,\mathbf{j}_p]$ by using the nonuniform coordinate scaling of electrons. Finally in Sec IV, we summarize the results and discuss the properties of the proposed approximations by means of the sum rules derived.

II. EXCHANGE-CORRELATION ENERGY FUNCTIONAL $E_{\rm xc}[\rho,\mathbf{j}_p]$

In this section we present the exact expression for $E_{\rm xc}[\rho,\mathbf{j}_p]$ with the aid of the coupling-constant integration technique. The exact expression enables us to define the LDA scheme for $E_{\rm xc}[\rho,\mathbf{j}_p]$ within the CDFT. On the basis of the LDA expression, we further propose the nonlocal density schemes which correspond to the ADA and WDA of the conventional DFT.[17–20]

A. Coupling-constant expression for $E_{\rm xc}[\rho,\mathbf{j}_p]$

Let us first consider the exact expression for $E_{\rm xc}[\rho,\mathbf{j}_p]$. The exact expression for $E_{\rm xc}[\rho]$ in the DFT was derived successfully by using the coupling-constant integration technique.[33–35] It is possible to apply the same technique to the CDFT. The starting point is the Hamiltonian,

$$\hat{H}^{\xi}=\hat{T}+\xi\hat{W}+\int\hat{\rho}(\mathbf{r})\,\nu_{\rm ext}^{\xi}(\mathbf{r})d\mathbf{r}+\frac{e}{c}\int\hat{\mathbf{j}}_p(\mathbf{r})\cdot\mathbf{A}_{\rm ext}^{\xi}(\mathbf{r})d\mathbf{r}+\frac{e^2}{2mc}\int\hat{\rho}(\mathbf{r})\mathbf{A}_{\rm ext}^{\xi}(\mathbf{r})^2d\mathbf{r},\tag{2.1}$$

where $\hat{T}$, $\hat{W}$, $\hat{\rho}(\mathbf{r})$, and $\hat{\mathbf{j}}_p(\mathbf{r})$ are the operators of the kinetic energy, electron-electron interaction, electron density, and paramagnetic current density, respectively, and ξ is a parameter characterizing the strength of the electron-electron interaction. The external potentials $\nu_{\rm ext}^{\xi}(\mathbf{r})$ and $\mathbf{A}_{\rm ext}^{\xi}(\mathbf{r})$ are chosen so that the ground-state densities of the system are identical with those of the real many-body system, i.e.,

$$\langle\Psi^{\xi}|\hat{\rho}(\mathbf{r})|\Psi^{\xi}\rangle=\rho(\mathbf{r}),\tag{2.2a}$$

$$\langle\Psi^{\xi}|\hat{\mathbf{j}}_p(\mathbf{r})|\Psi^{\xi}\rangle=\mathbf{j}_p(\mathbf{r}),\tag{2.2b}$$

where Ψ^{ξ} is the ground-state wave function for Hamiltonian (2.1). Assuming that there exist such external potentials for each ξ, the Hohenberg-Kohn theorem guarantees one-to-one correspondences among $\{\nu_{\rm ext}^{\xi}(\mathbf{r}),\mathbf{A}_{\rm ext}^{\xi}(\mathbf{r})\}$, $\{\rho(\mathbf{r}),\mathbf{j}_p(\mathbf{r})\}$ and Ψ^{ξ}.

The system characterized by the Hamiltonian with $\xi=1$ is identical to the real many-body system. The ground-state energy of the system ($\xi=1$) is given by

$$E^1=T_s[\rho,\mathbf{j}_p]+U[\rho]+E_{\rm xc}[\rho,\mathbf{j}_p]+\int\rho(\mathbf{r})\,\nu_{\rm ext}(\mathbf{r})d\mathbf{r}+\frac{e^2}{2mc^2}\int\rho(\mathbf{r})\mathbf{A}_{\rm ext}(\mathbf{r})^2d\mathbf{r}+\frac{e}{c}\int\mathbf{j}_p(\mathbf{r})\cdot\mathbf{A}_{\rm ext}(\mathbf{r})d\mathbf{r},\tag{2.3}$$

where $T_s[\rho,\mathbf{j}_p]$ and $U[\rho]$ denote the kinetic energy of the noninteracting fictitious system and the Hartree energy, respectively. In the case of $\xi=0$, the system is recognized as a noninteracting fictitious system. Using the Kohn-Sham potentials $\nu_{\rm eff}(\mathbf{r})$ and $\mathbf{A}_{\rm eff}(\mathbf{r})$,[2] the ground-state energy of the system ($\xi=0$) is given by

$$E^0=T_s[\rho,\mathbf{j}_p]+\int\rho(\mathbf{r})\,\nu_{\rm eff}(\mathbf{r})d\mathbf{r}+\frac{e^2}{2mc^2}\int\rho(\mathbf{r})\mathbf{A}_{\rm eff}(\mathbf{r})^2d\mathbf{r}+\frac{e}{c}\int\mathbf{j}_p(\mathbf{r})\cdot\mathbf{A}_{\rm eff}(\mathbf{r})d\mathbf{r}.\tag{2.4}$$

On the other hand, from the Hellmann-Feynman theorem, we have

$$E^1-E^0=\int_0^1 d\xi\left\langle\Psi^{\xi}\left|\frac{d\hat{H}^{\xi}}{d\xi}\right|\Psi^{\xi}\right\rangle.\tag{2.5}$$

Substituting Eqs. (2.3) and (2.4) into Eq. (2.5), the exact expression for $E_{\rm xc}[\rho,\mathbf{j}_p]$ is written as

$$E_{\rm xc}[\rho,\mathbf{j}_p]=\frac{e^2}{2}\int\int\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\{\overline{g}(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])-1\}d\mathbf{r}\,d\mathbf{r}',\tag{2.6}$$

where $\overline{g}(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])$ is a coupling-constant-averaged pair correlation function, which is defined by

$$\overline{g}(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])\equiv\int_0^1 g_{\xi}(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])d\xi,\tag{2.7a}$$

$$g_{\xi}(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])\equiv\{\langle\Psi^{\xi}[\rho,\mathbf{j}_p]|\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')|\Psi^{\xi}[\rho,\mathbf{j}_p]\rangle-\delta(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r})\}/\rho(\mathbf{r})\rho(\mathbf{r}').\tag{2.7b}$$

The exact expression (2.6) is quite similar to that of the DFT. The different point is that the coupling-constant-averaged pair correlation function is the functional of $\rho(\mathbf{r})$ in the DFT,[36] while it is the functional of both $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$ in the CDFT.

It should be noted that the exchange-correlation energy functional $E_{\rm xc}[\rho,\mathbf{j}_p]$ of the Kohn-Sham scheme (2.6) is different from the real exchange-correlation energy $\mathcal{E}'_{\rm xc}$ of the many-body system. $\mathcal{E}'_{\rm xc}$ is expressed by leaving out the coupling-constant integration of Eq. (2.6). We have

$$\mathcal{E}'_{\rm xc}[\rho,\mathbf{j}_p]=\frac{e^2}{2}\int\int\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\{g(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])-1\}d\mathbf{r}\,d\mathbf{r}',\tag{2.8a}$$

$$g(\mathbf{r},\mathbf{r}';[\rho,\mathbf{j}_p])\equiv\{\langle\Psi_G[\rho,\mathbf{j}_p]|\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')|\Psi_G[\rho,\mathbf{j}_p]\rangle-\delta(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r})\}/\rho(\mathbf{r})\rho(\mathbf{r}').\tag{2.8b}$$

The difference between $E_{\rm xc}[\rho,\mathbf{j}_p]$ and $\mathcal{E}'_{\rm xc}$ is given by

$$E_{\rm xc}[\rho,\mathbf{j}_p]-\mathcal{E}'_{\rm xc}[\rho,\mathbf{j}_p]=T[\rho,\mathbf{j}_p]-T_s[\rho,\mathbf{j}_p].\tag{2.9}$$

$E_{\rm xc}[\rho,\mathbf{j}_p]$ contains the difference between the real kinetic energy and the kinetic energy of the fictitious system through the coupling-constant integration. In the framework of the

DFT, the difference between $T[\rho]$ and $T_s[\rho]$ cannot be ignored, since its magnitude is comparable to the correlation energy, e.g., just a few electron volts for most atomic and molecular systems.[37] The difference (2.9) may not be negligible either in the case of the CDFT on the analogy of the DFT.

B. Local density approximation and its modifications

In the conventional DFT, the approximation schemes such as the LDA, ADA, and WDA have been developed on the basis of the coupling-constant expression for $E_{\rm xc}[\rho]$.[15–20] Also in the CDFT, the exact expression (2.6) is a good starting point to develop the various approximate forms of $E_{\rm xc}[\rho,\mathbf{j}_p]$. Introducing the exchange-correlation hole $\rho_{\rm xc}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\mathbf{j}_p(\mathbf{r})])$, Eq. (2.6) is rewritten as

$$E_{\rm xc}[\rho,\mathbf{j}_p]=\frac{e^2}{2}\int\int\frac{\rho(\mathbf{r})\rho_{\rm xc}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\mathbf{j}_p(\mathbf{r})])}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}\,d\mathbf{r}' \tag{2.10}$$

with

$$\rho_{\rm xc}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\mathbf{j}_p(\mathbf{r})])=\rho(\mathbf{r}')\{\overline{g}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\mathbf{j}_p(\mathbf{r})])-1\}. \tag{2.11}$$

Here we shall give notes on Eqs. (2.10) and (2.11). As mentioned in Sec. I, the gauge invariance causes the additional condition on $E_{\rm xc}[\rho,\mathbf{j}_p]$.[2,31,32] Using this condition, it is easily shown that $E_{\rm xc}[\rho,\mathbf{j}_p]$ depends on $\mathbf{j}_p(\mathbf{r})$ only through the vorticity $\boldsymbol{\nu}(\mathbf{r})$, defined by

$$\boldsymbol{\nu}(\mathbf{r})\equiv\nabla\times\left\{\frac{\mathbf{j}_p(\mathbf{r})}{\rho(\mathbf{r})}\right\}. \tag{2.12}$$

Therefore, the exchange-correlation energy functional and hole, i.e., Eqs. (2.10) and (2.11), can also be referred to as the functional of $\rho(\mathbf{r})$ and $\boldsymbol{\nu}(\mathbf{r})$.[2]

In a similar way to the DFT, the approximation schemes can be devised by modeling the exchange-correlation hole [Eq. (2.11)]. We will borrow the knowledge of $\rho_{\rm xc}$ or $\overline{g}$ from the homogeneous electron liquid. We first consider the local density approximation. The LDA scheme is obtained if the exchange-correlation hole is replaced by the corresponding homogeneous electron liquid expression and evaluated at the local densities $\rho(\mathbf{r})$ and $\boldsymbol{\nu}(\mathbf{r})$, i.e.,

$$\rho_{\rm xc}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r})])\rightarrow\rho(\mathbf{r})\{\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))-1\}, \tag{2.13}$$

where $\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))$ is the coupling-constant-averaged pair correlation function of the homogeneous electron liquid. Substituting Eq. (2.13) into Eq. (2.10), we have

$$\begin{aligned}E_{\rm xc}^{\rm LDA}[\rho,\mathbf{j}_p]&=E_{\rm xc}'^{\rm LDA}[\rho,\boldsymbol{\nu}]\\&=\frac{e^2}{2}\int\int\frac{\rho(\mathbf{r})^2}{|\mathbf{r}-\mathbf{r}'|}\\&\quad\times\{\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))-1\}d\mathbf{r}\,d\mathbf{r}'.\end{aligned} \tag{2.14}$$

This is just the LDA expression for the exchange-correlation energy functional of the CDFT. This expression is equivalent to the previous result which was discussed in Refs. 7 and 8. In Eq. (2.14), $\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))$ can be obtained from the Fourier transform of the coupling-constant-averaged static structure factor $\overline{S}^{\rm hom}(\mathbf{q})$ of the homogeneous electron liquid. Vignale and co-workers have evaluated $\overline{S}^{\rm hom}(\mathbf{q})$ with respect to the ground-state of the homogeneous electron liquid in a uniform magnetic field.[6,38] Note that a state of uniform density and vorticity can be identified as a state of uniform density in a uniform magnetic field via $\mathbf{B}=-mc\boldsymbol{\nu}/e$.[7] Skudlarski and Vignale have further investigated the behaviors of the exchange-correlation hole for several sets of ρ and $\boldsymbol{\nu}$ through numerical calculations.[6] Thus it is possible to perform energy-band calculations within the LDA by utilizing the knowledge of the homogeneous electron liquid in the uniform magnetic field.

Next, as modifications to the LDA we propose the nonlocal density schemes which can be regarded as the CDFT version of the ADA and WDA. In the ADA, $\overline{g}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r})])$ is borrowed from the homogeneous electron liquid and evaluated at the averaged densities $\overline{\rho}(\mathbf{r})$ and $\overline{\boldsymbol{\nu}}(\mathbf{r})$. Furthermore the prefactor $\rho(\mathbf{r}')$ in Eq. (2.11) is replaced by the averaged density $\overline{\rho}(\mathbf{r})$,

$$\rho_{\rm xc}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r})])\rightarrow\overline{\rho}(\mathbf{r})\{\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}(\mathbf{r}),\overline{\boldsymbol{\nu}}(\mathbf{r}))-1\}, \tag{2.15}$$

with

$$\overline{\rho}(\mathbf{r})=\int d\mathbf{r}'\,w(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}(\mathbf{r}'),\overline{\boldsymbol{\nu}}(\mathbf{r}'))\rho(\mathbf{r}'), \tag{2.16a}$$

$$\overline{\boldsymbol{\nu}}(\mathbf{r})=\int d\mathbf{r}'\,w(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}(\mathbf{r}'),\overline{\boldsymbol{\nu}}(\mathbf{r}'))\boldsymbol{\nu}(\mathbf{r}'), \tag{2.16b}$$

where $w(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}(\mathbf{r}'),\overline{\boldsymbol{\nu}}(\mathbf{r}'))$ is the weight function to be determined. We are led to the exchange-correlation energy functional in the ADA as

$$\begin{aligned}E_{\rm xc}^{\rm ADA}[\rho,\mathbf{j}_p]&=E_{\rm xc}'^{\rm ADA}[\rho,\boldsymbol{\nu}]\\&=\frac{e^2}{2}\int\int\frac{\rho(\mathbf{r})\overline{\rho}(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}\\&\quad\times\{\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}(\mathbf{r}),\overline{\boldsymbol{\nu}}(\mathbf{r}))-1\}d\mathbf{r}\,d\mathbf{r}'.\end{aligned} \tag{2.17}$$

In the WDA, one also replaces the pair correlation function $\overline{g}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r})])$ with that of the homogeneous electron liquid, but the prefactor is kept at the exact density $\rho(\mathbf{r}')$:

$$\begin{aligned}&\rho_{\rm xc}(\mathbf{r},\mathbf{r}';[\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r})])\\&\quad\rightarrow\rho(\mathbf{r}')\{\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\tilde{\rho}(\mathbf{r}),\tilde{\boldsymbol{\nu}}(\mathbf{r}))-1\}.\end{aligned} \tag{2.18}$$

The density arguments of $\overline{g}^{\rm hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))$ are replaced by the weighted densities $\tilde{\rho}(\mathbf{r})$ and $\tilde{\boldsymbol{\nu}}(\mathbf{r})$, which are determined by requiring the following sum rule to be satisfied for each $\mathbf{r}$:

$$\int d\mathbf{r}'(\mathbf{r}')\{\bar{g}^{\hom}(|\mathbf{r}-\mathbf{r}'|,\tilde{\rho}(\mathbf{r}),\tilde{\boldsymbol{\nu}}(\mathbf{r}))-1\}=-1. \tag{2.19}$$

The WDA expression for the exchange-correlation energy functional is given by

$$E_{\rm xc}^{\rm WDA}[\rho,\mathbf{j}_p]=E'^{\rm WDA}_{\rm xc}[\rho,\boldsymbol{\nu}] =\frac{e^2}{2}\int\int\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \times\{\bar{g}^{\hom}(|\mathbf{r}-\mathbf{r}'|,\tilde{\rho}(\mathbf{r}),\tilde{\boldsymbol{\nu}}(\mathbf{r}))-1\}d\mathbf{r}\,d\mathbf{r}'. \tag{2.20}$$

In a way similar to the LDA calculations,[9–13] the actual energy-band calculations are feasible in the ADA and WDA because the knowledge of $\bar{g}^{\hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))$ can also be employed from the homogeneous electron liquid in the uniform magnetic field.[6,38] So far, the available form of $\bar{g}^{\hom}(|\mathbf{r}-\mathbf{r}'|,\rho(\mathbf{r}),\boldsymbol{\nu}(\mathbf{r}))$ has been restricted to the random phase approximation (RPA).[6,38] In cases where the paramagnetic current or magnetic field does not exist, a more sophisticated theory which includes the higher-order short-range correlations and the exchange terms beyond the RPA has been developed by Singwi *et al.*[39] It is so-called STLS theory. This scheme utilizes the generalized RPA expression for the dielectric function and approximates the exchange-correlation contribution by the local field factor. It is possible to introduce the STLS theory into the present expression of the CDFT in a similar way to the conventional DFT.[40]

At the end of this section, we will emphasize that modifications to the LDA, such as ADA and WDA, cannot be defined until the exchange-correlation energy functional $E_{\rm xc}[\rho,\mathbf{j}_p]$ is given in an exact form [Eq. (2.16)].

III. EXACT CONDITIONS ON $E_{\rm xc}[\rho,\mathbf{j}_p]$ FROM NONUNIFORM COORDINATE SCALINGS

A. Behavior of $E_c[\rho,\mathbf{j}_p]$ for scaling parameter going to zero or infinity

On the basis of the method developed by Görling and Levy in the DFT,[41] we shall investigate the exact conditions on the correlation energy functional $E_c[\rho,\mathbf{j}_p]$ of the CDFT. The systematic analysis enables us to derive the kinds of conditions on $E_c[\rho,\mathbf{j}_p]$, some of which are never obtained by simple analogy with the conventional DFT.[41]

Let us first consider a nonuniform coordinate scaling such that the x coordinates of electrons are scaled with λ, where λ is the scaling factor and takes a positive value. The scaled ground-state wave function

$$\Psi_G[\rho,\mathbf{j}_p]^x_\lambda(\mathbf{r}_1,\ldots,\mathbf{r}_N) \equiv\lambda^{N/2}\Psi_G[\rho,\mathbf{j}_p](\lambda x_1,\ldots,\lambda x_N,y_1,\ldots,y_N,z_1,\ldots,z_N) \tag{3.1}$$

is normalized to unity, and leads to the scaled basic variables

$$\rho^x_\lambda(\mathbf{r})\equiv\lambda\rho(\lambda x,y,z), \tag{3.2}$$

$$\mathbf{j}_{p\lambda}{}^x(\mathbf{r})\equiv(\lambda^2 j_p(\lambda x,y,z)_x,\lambda j_p(\lambda x,y,z)_y,\lambda j_p(\lambda x,y,z)_z). \tag{3.3}$$

The correlation energy functional corresponding to the scaled basic variables is given by

$$E_c[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]=\langle\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]|\hat{T}|\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]\rangle +\langle\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]|\hat{W}|\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]\rangle -\langle\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]|\hat{T}|\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]\rangle -\langle\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]|\hat{W}|\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]\rangle. \tag{3.4}$$

Here $\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]$ and $\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]$ denote the ground-state wave function of the real many-body system and the noninteracting fictitious system, respectively, both of which have the ground-state densities $\rho^x_\lambda(\mathbf{r})$ and $\mathbf{j}_{p\lambda}{}^x(\mathbf{r})$. The constrained-search formulation for $\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]$ leads to a simple and important condition:

$$E_c[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]\leqslant 0. \tag{3.5}$$

The transformation of the integration variables in Eq. (3.4) from $(x_1,\ldots,x_N,y_1,\ldots,y_N,z_1,\ldots,z_N)$ into $(\lambda^{-1}x_1,\ldots,\lambda^{-1}x_N,y_1,\ldots,y_N,z_1,\ldots,z_N)$ yields the following form:

$$E_c[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]=\int\cdots\int\Psi^*_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]^x_{\lambda^{-1}}\sum_{i=1}^N-\frac{\hbar^2}{2m}\left(\lambda^2\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right)\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]^x_{\lambda^{-1}}d\mathbf{r}_1\cdots d\mathbf{r}_N +\int\cdots\int\frac{e^2}{2}\sum_{i\neq j}\sum_{j=1}^N\frac{|\Psi_G[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]^x_{\lambda^{-1}}|^2}{\sqrt{\lambda^{-2}(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}}d\mathbf{r}_1\cdots d\mathbf{r}_N -\int\cdots\int\Phi^*_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]^x_{\lambda^{-1}}\sum_{i=1}^N-\frac{\hbar^2}{2m}\left(\lambda^2\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right)\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]^x_{\lambda^{-1}}d\mathbf{r}_1\cdots d\mathbf{r}_N -\int\cdots\int\frac{e^2}{2}\sum_{i\neq j}\sum_{j=1}^N\frac{|\Phi_s[\rho^x_\lambda,\mathbf{j}_{p\lambda}{}^x]^x_{\lambda^{-1}}|^2}{\sqrt{\lambda^{-2}(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}}d\mathbf{r}_1\cdots d\mathbf{r}_N. \tag{3.6}$$

From the constrained-search formulation for $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$, the function $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ in Eq. (3.6) yields $\rho(\mathbf{r})$ and $\mathbf{j_p}(\mathbf{r})$, and minimizes the expectation value of

$$\sum_{i=1}^{N} -\frac{\hbar^2}{2m}\left(\lambda^2\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right)+\sum_{i\neq j}\sum_{j=1}^{N}\frac{e^2/2}{\sqrt{\lambda^{-2}(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}} \tag{3.7}$$

among the inversely scaled functions $X_{\lambda^{-1}}^x(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ defined by

$$X_{\lambda^{-1}}^x(\mathbf{r}_1,\ldots,\mathbf{r}_N)\equiv\lambda^{-N/2}X(\lambda^{-1}x_1,\lambda^{-1}x_2,\ldots,\lambda^{-1}x_N,y_1,y_2,\ldots,y_N,z_1,z_2,\ldots,z_N). \tag{3.8}$$

Here $X(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the arbitrary N-particle wave function which yields $\rho_\lambda^x(\mathbf{r})$ and $\mathbf{j}_{p\lambda}^x(\mathbf{r})$. With the aid of the constrained-search formulation for $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$, the function $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ yields $\rho(\mathbf{r})$ and $\mathbf{j_p}(\mathbf{r})$, and minimizes the expectation value of

$$\sum_{i=1}^{N} -\frac{\hbar^2}{2m}\left(\lambda^2\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right) \tag{3.9}$$

among the set of functions (3.8). This property of $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ leads to the fact that the kinetic-energy part (the first and third terms) of Eq. (3.6) is positive or zero.

In the following discussions, both $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ and $\Phi_S[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ are assumed to approach the limit values when λ goes to infinity. Since Eqs. (3.7) and (3.9) approach the same operators in the limit $\lambda\to\infty$, the limits of $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ and $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ are equal to each other:

$$\lim_{\lambda\to\infty}\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x=\lim_{\lambda\to\infty}\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x. \tag{3.10}$$

The integrand of the second term in Eq. (3.6) is equal to that of the fourth term in the limit $\lambda\to\infty$ because of Eq. (3.10). Therefore, the electron-electron interaction energy part (the second and fourth terms) of Eq. (3.6) goes to zero as $\lambda\to\infty$. Since the kinetic-energy part of Eq. (3.6) is positive or zero, one obtains $\lim_{\lambda\to\infty}E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]\geqslant 0$. Accordingly, with Eq. (3.5) in mind, we obtain

$$\lim_{\lambda\to\infty}E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]=0. \tag{3.11a}$$

In addition, if both $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ and $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ are expanded in powers of λ^{-1} for large values of λ, then we obtain tighter condition than Eq. (3.11a):

$$\lim_{\lambda\to\infty}\lambda E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]=\text{const.} \tag{3.11b}$$

The other exact conditions concerning the x coordinate scaling can be obtained under the assumption that $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ and $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ become the limit values for $\lambda\to 0$. We have

$$\lim_{\lambda\to 0}E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]=0, \tag{3.11c}$$

$$\lim_{\lambda\to 0}\lambda^{-1}E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]=0, \tag{3.11d}$$

$$\lim_{\lambda\to 0}\lambda^{-2}E_c[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]=\text{const.} \tag{3.11e}$$

Here conditions (3.11d) and (3.11e) are derived under the assumption that both $\Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ and $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]_{\lambda^{-1}}^x$ are expanded in powers of λ for small values of λ.

Further exact conditions on $E_c[\rho, \mathbf{j}_p]$ can be derived from other types of a nonuniform coordinate scaling of electrons. If we scale two coordinates with λ and leave the third one unchanged, the scaled basic variables are given by

$$\rho_{\lambda\lambda}^{xy}(\mathbf{r})\equiv\lambda^2\rho(\lambda x,\lambda y,z), \tag{3.12}$$

$$\mathbf{j}_{p\lambda\lambda}^{xy}(\mathbf{r})\equiv(\lambda^3 j_p(\lambda x,\lambda y,z)_x,\ \lambda^3 j_p(\lambda x,\lambda y,z)_y,\lambda^2 j_p(\lambda x,\lambda y,z)_z). \tag{3.13}$$

In a similar way to the above discussions, the exact conditions for Eqs. (3.12) and (3.13) are given by

$$\lim_{\lambda\to\infty}E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}]=0, \tag{3.14a}$$

$$\lim_{\lambda\to\infty}\lambda E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}]=\text{const}, \tag{3.14b}$$

$$\lim_{\lambda\to 0}E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}]=0, \tag{3.14c}$$

$$\lim_{\lambda\to 0}\lambda^{-1}E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}]=0, \tag{3.14d}$$

$$\lim_{\lambda\to 0}\lambda^{-2}E_c[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}]=\text{const.} \tag{3.14e}$$

In the case of the scaling such that two coordinates are scaled with λ and λ^{-1}, respectively, and the third one is left unchanged, the scaled basic variables are given by

$$\rho_{\lambda\ 1/\lambda}^{x\ y}(\mathbf{r})\equiv\rho(\lambda x,\lambda^{-1}y,z), \tag{3.15}$$

$$\mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}(\mathbf{r}) \equiv (\lambda j_p(\lambda x,\lambda^{-1}y,z)_x, \lambda^{-1} j_p(\lambda x,\lambda^{-1}y,z)_y, j_p(\lambda x,\lambda^{-1}y,z)_z). \tag{3.16}$$

The corresponding exact conditions on $E_c[\rho,\mathbf{j}_p]$ are obtained as follows:

$$\lim_{\lambda\to\infty} E_c[\rho_\lambda^{x\ y}{}_{1/\lambda}, \mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}] = 0, \tag{3.17a}$$

$$\lim_{\lambda\to\infty} \lambda E_c[\rho_\lambda^{x\ y}{}_{1/\lambda}, \mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}] = 0, \tag{3.17b}$$

$$\lim_{\lambda\to\infty} \lambda^2 E_c[\rho_\lambda^{x\ y}{}_{1/\lambda}, \mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}] = \text{const}, \tag{3.17c}$$

$$\lim_{\lambda\to 0} E_c[\rho_\lambda^{x\ y}{}_{1/\lambda}, \mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}] = 0, \tag{3.17d}$$

$$\lim_{\lambda\to 0} \lambda^{-1} E_c[\rho_\lambda^{x\ y}{}_{1/\lambda}, \mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}] = 0, \tag{3.17e}$$

$$\lim_{\lambda\to 0} \lambda^{-2} E_c[\rho_\lambda^{x\ y}{}_{1/\lambda}, \mathbf{j}_{p\lambda}^{x\ y}{}_{1/\lambda}] = \text{const}. \tag{3.17f}$$

Finally, in the case of the scaling such that two coordinates are scaled with λ and the third one with λ^{-1}, the scaled basic variables are given by

$$\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}(\mathbf{r}) \equiv \lambda\rho(\lambda x,\lambda y,\lambda^{-1}z), \tag{3.18}$$

$$\mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}(\mathbf{r}) \equiv (\lambda^2 j_p(\lambda x,\lambda y,\lambda^{-1}z)_x, \lambda^2 j_p(\lambda x,\lambda y,\lambda^{-1}z)_y, j_p(\lambda x,\lambda y,\lambda^{-1}z)_z). \tag{3.19}$$

The corresponding exact conditions are as follows:

$$\lim_{\lambda\to\infty} E_c[\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}, \mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}] = 0, \tag{3.20a}$$

$$\lim_{\lambda\to\infty} \lambda E_c[\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}, \mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}] = 0, \tag{3.20b}$$

$$\lim_{\lambda\to\infty} \lambda^2 E_c[\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}, \mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}] = \text{const} \tag{3.20c}$$

$$\lim_{\lambda\to 0} E_c[\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}, \mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}] = 0, \tag{3.20d}$$

$$\lim_{\lambda\to 0} \lambda^{-1} E_c[\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}, \mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}] = 0, \tag{3.20e}$$

$$\lim_{\lambda\to 0} \lambda^{-2} E_c[\rho_{\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}, \mathbf{j}_{p\lambda\lambda\ \ 1/\lambda}^{xy\ \ z}] = \text{const}. \tag{3.20f}$$

In the GGA method of the conventional DFT, the approximate form of $E_c[\rho]$ has been devised so that it satisfies some of the exact conditions which are derived from the nonuniform coordinate scalings.[22,23] Therefore, the present exact conditions derived can be regarded as new sum rules on $E_c[\rho,\mathbf{j}_p]$ which provide the useful guidelines for developing and testing the approximate forms of $E_c[\rho,\mathbf{j}_p]$. It should be noted that exact conditions (3.11e), (3.14b), (3.17c), (3.17f), (3.20b), and (3.20c) are not only tighter than those of the DFT which were previously derived by Görling and Levy,[41] but also are never obtained by simple analogy with their results.

B. Upper and lower bounds on $E_{xc}[\rho,\mathbf{j}_p]$

In this subsection, we derive the upper and lower bounds on $E_{xc}[\rho,\mathbf{j}_p]$ by means of a different method than in Sec. III A. We first consider a nonuniform coordinate scaling such that the x coordinates of electrons are scaled with λ. From the constrained-search formulation of the CDFT, $\Psi_G[\rho_\lambda^x,\mathbf{j}_{p\lambda}^x]$, minimizes the expectation value of $\hat{T}+\hat{W}$ among the arbitrary N-particle wave functions that yield $\rho_\lambda^x(\mathbf{r})$ and $\mathbf{j}_{p\lambda}^x(\mathbf{r})$. The constrained-search formulation also guarantees that $\Psi_G[\rho,\mathbf{j}_p]_\lambda^x$ minimizes the expectation value of

$$\sum_{i=1}^{N} -\frac{\hbar^2}{2m}\left(\lambda^{-2}\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right) + \sum_{i\neq j}\sum_{j=1}^{N} \frac{e^2/2}{\sqrt{\lambda^2(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}}. \tag{3.21}$$

among the scaled functions $Y_\lambda^x(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ defined by

$$Y_\lambda^x(\mathbf{r}_1,\ldots,\mathbf{r}_N) \equiv \lambda^{N/2} Y(\lambda x_1,\lambda x_2,\ldots,\lambda x_N, y_1,y_2,\ldots,y_N,z_1,z_2,\ldots z_N). \tag{3.22}$$

Here $Y(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is an arbitrary N-particle wave function that yields $\rho(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$. Since $\Psi_G[\rho,\mathbf{j}_p]_\lambda^x$ and $\Psi_G[\rho_\lambda^x,\mathbf{j}_{p\lambda}^x]$ obey different equations, respectively, they are different from each other, i.e.,

$$\Psi_G[\rho_\lambda^x,\mathbf{j}_{p\lambda}^x] \neq \Psi_G[\rho,\mathbf{j}_p]_\lambda^x. \tag{3.23}$$

This leads to the following two kinds of inequalities after the changes of variables:

$$\langle \Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] | \sum_{i=1}^N \frac{-\hbar^2}{2m} \left(\lambda^{-2} \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right) + \sum_{i=1}^N \sum_{j \neq i} \frac{e^2/2}{\sqrt{\lambda^2 (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}} | \Psi_G[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \rangle$$
$$\geqslant T[\rho, \mathbf{j}_p] + W[\rho, \mathbf{j}_p], \tag{3.24}$$

and

$$T[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] + W[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \leqslant \langle \Psi_G[\rho, \mathbf{j}_p] | \sum_{i=1}^N \frac{-\hbar^2}{2m} \left(\lambda^2 \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right)$$
$$+ \sum_{i=1}^N \sum_{j \neq i} \frac{e^2/2}{\sqrt{\lambda^{-2} (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}} | \Psi_G[\rho, \mathbf{j}_p] \rangle. \tag{3.25}$$

Similarly, the scaled function $\Phi_s[\rho, \mathbf{j}_p]_\lambda^x$ is different from $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$ because they obey the respective equations. We have

$$\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \neq \Phi_s[\rho, \mathbf{j}_p]_\lambda^x. \tag{3.26}$$

Since $\Phi_s[\rho, \mathbf{j}_p]_\lambda^x$ minimizes the expectation value of

$$\sum_{i=1}^N - \frac{\hbar^2}{2m} \left(\lambda^{-2} \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right)$$

among the set of functions (3.22), we obtain the inequality.

$$\langle \Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \left| \sum_{i=1}^N \frac{-\hbar^2}{2m} \left(\lambda^{-2} \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right) \right| \Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \rangle$$
$$\geqslant T_s[\rho, \mathbf{j}_p]. \tag{3.27}$$

Because of inequality (3.26), the constrained-search formulation for $\Phi_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$ leads to

$$T_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \leqslant \langle \Phi_s[\rho, \mathbf{j}_p] \left| \sum_{i=1}^N \frac{-\hbar^2}{2m} \left(\lambda^2 \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} \right. \right.$$
$$\left. \left. + \frac{\partial^2}{\partial z_i^2} \right) \right| \Phi_s[\rho, \mathbf{j}_p] \rangle. \tag{3.28}$$

If $\lambda \geqslant 1$, then inequalities (3.24), (3.25), (3.27), and (3.28) are turned to

$$T[\rho, \mathbf{j}_p] + W[\rho, \mathbf{j}_p] \leqslant T[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] + W[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$$
$$\leqslant \lambda^2 T[\rho, \mathbf{j}_p] + \lambda W[\rho, \mathbf{j}_p], \tag{3.29}$$

and

$$T_s[\rho, \mathbf{j}_p] \leqslant T_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \leqslant \lambda^2 T_s[\rho, \mathbf{j}_p]. \tag{3.30}$$

Likewise, if $\lambda \leqslant 1$, we obtain the following inequalities:

$$T[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] + W[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \leqslant T[\rho, \mathbf{j}_p] + W[\rho, \mathbf{j}_p]$$
$$\leqslant \lambda^{-2} T[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] + \lambda^{-1} W[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x], \tag{3.31}$$

and

$$\lambda^2 T_s[\rho, \mathbf{j}_p] \leqslant T_s[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x] \leqslant T_s[\rho, \mathbf{j}_p]. \tag{3.32}$$

On the other hand, the Hartree term $U[\rho_\lambda^x]$ can be written through the changes of variables as

$$U[\rho_\lambda^x] = \frac{e^2}{2} \int \int \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{\sqrt{\lambda^{-2} (x - x')^2 + (y - y')^2 + (z - z')^2}} d\mathbf{r}\, d\mathbf{r}'.$$

Using this expression, we have the inequalities for the Hartree term. The results are

$$U[\rho] \leqslant U[\rho_\lambda^x] \leqslant \lambda U[\rho] \leqslant \lambda^2 U[\rho] \quad \text{for } \lambda \geqslant 1, \tag{3.33}$$

$$\lambda^2 U[\rho] \leqslant \lambda U[\rho] \leqslant U[\rho_\lambda^x] \leqslant U[\rho] \quad \text{for } \lambda \leqslant 1. \tag{3.34}$$

From inequalities (3.29)–(3.34), we finally arrive at the following exact conditions:

$$-(\lambda^2 - 1)(T_s[\rho, \mathbf{j}_p] + U[\rho]) + E_{xc}[\rho, \mathbf{j}_p]$$
$$\leqslant E_{xc}[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$$
$$\leqslant (\lambda^2 - 1)(T_s[\rho, \mathbf{j}_p] + U[\rho]) + \lambda^2 E_{xc}[\rho, \mathbf{j}_p] \quad \text{for } \lambda \geqslant 1, \tag{3.35}$$

$$-(1 - \lambda^2)(T_s[\rho, \mathbf{j}_p] + U[\rho]) + \lambda^2 E_{xc}[\rho, \mathbf{j}_p]$$
$$\leqslant E_{xc}[\rho_\lambda^x, \mathbf{j}_{p\lambda}^x]$$
$$\leqslant (1 - \lambda^2)(T_s[\rho, \mathbf{j}_p] + U[\rho]) + E_{xc}[\rho, \mathbf{j}_p] \quad \text{for } \lambda \leqslant 1. \tag{3.36}$$

Next let us consider another kind of the nonuniform coordinate scaling which is given by Eqs. (3.12) and (3.13). It gives a different type of exact conditions than Eqs. (3.35) and (3.36). About $T[\rho, \mathbf{j}_p]$ and $W[\rho, \mathbf{j}_p]$, we obtain the relations

$$T[\rho, \mathbf{j}_p] + W[\rho, \mathbf{j}_p] \leqslant T[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}] + W[\rho_{\lambda\lambda}^{xy}, \mathbf{j}_{p\lambda\lambda}^{xy}]$$
$$\leqslant \lambda^2 T[\rho, \mathbf{j}_p] + \lambda W[\rho, \mathbf{j}_p] \quad \text{for } \lambda \geqslant 1, \tag{3.37}$$

$$T[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}]+W[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}] \leqslant T[\rho,\mathbf{j}_p]+W[\rho,\mathbf{j}_p] \leqslant \lambda^{-2}T[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}]+\lambda^{-1}W[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}] \quad \text{for } \lambda \leqslant 1, \tag{3.38}$$

Similarly, the functional $T_s[\rho,\mathbf{j}_p]$ satisfies

$$T_s[\rho,\mathbf{j}_p] \leqslant T_s[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}] \leqslant \lambda^2 T_s[\rho,\mathbf{j}_p] \quad \text{for } \lambda \geqslant 1, \tag{3.39}$$

$$\lambda^2 T_s[\rho,\mathbf{j}_p] \leqslant T_s[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}] \leqslant T_s[\rho,\mathbf{j}_p] \quad \text{for } \lambda \leqslant 1. \tag{3.40}$$

Using Eqs. (3.37)–(3.40), we finally obtain

$$-(\lambda^2-1)(T_s[\rho,\mathbf{j}_p]+U[\rho])+E_{xc}[\rho,\mathbf{j}_p] \leqslant E_{xc}[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}] \leqslant (\lambda^2-1)(T_s[\rho,\mathbf{j}_p]+U[\rho])+\lambda^2 E_{xc}[\rho,\mathbf{j}_p] \quad \text{for } \lambda \geqslant 1, \tag{3.41}$$

$$-(1-\lambda^2)(T_s[\rho,\mathbf{j}_p]+U[\rho])+\lambda^2 E_{xc}[\rho,\mathbf{j}_p] \leqslant E_{xc}[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}] \leqslant (1-\lambda^2)(T_s[\rho,\mathbf{j}_p]+U[\rho])+E_{xc}[\rho,\mathbf{j}_p] \quad \text{for } \lambda \leqslant 1. \tag{3.42}$$

The present exact conditions (3.35), (3.36), (3.41), and (3.42) provide both upper and lower bounds on the exchange-correlation energy functional for the scaled basic variables. Both upper and lower bounds explicitly depend on $\mathbf{j}_p(\mathbf{r})$ because $T_s[\rho,\mathbf{j}_p]+U[\rho]$ is rewritten by

$$T_s[\rho,\mathbf{j}_p]+U[\rho] = \sum_k^{occ.} \varepsilon_k - \frac{e}{c}\int \mathbf{j}_p(\mathbf{r})\cdot\mathbf{A}_{\mathrm{eff}}(\mathbf{r})d\mathbf{r} - \int \rho(\mathbf{r}) \times \left\{ \nu_{\mathrm{eff}}(\mathbf{r}) - \frac{e^2}{2}\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \frac{e^2}{2mc^2}\mathbf{A}_{\mathrm{eff}}(\mathbf{r})^2 \right\} d\mathbf{r}, \tag{3.43}$$

with the aid of the Kohn-Sham equation.[2] Assuming that we obtain an approximate form of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$, then $T_s[\rho,\mathbf{j}_p]+U[\rho]$ is calculated from Eq. (3.43). Substituting the value of $T_s[\rho,\mathbf{j}_p]+U[\rho]$ thus calculated into Eqs. (3.35), (3.36), (3.41), and (3.42), we can evaluate the validity of the approximate form of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$.

Conditions (3.30), (3.32), (3.35), (3.36), and (3.39)–(3.42) should be recognized as the requirements in the approximate functionals of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ and $T_s[\rho,\mathbf{j}_p]$. Vignale, Skudlarski, and Rasolt have calculated the surface properties of an electron-hole droplet by means of the approximate expressions for $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ and $T_s[\rho,\mathbf{j}_p]$.[11] In their paper, $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ was replaced with the LDA expression while $T_s[\rho,\mathbf{j}_p]$ was approximated in the spirit of Thomas-Fermi theory plus second-order gradient expansion. The present conditions mentioned above can be used as the upper and lower bounds on the approximate forms of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ and $T_s[\rho,\mathbf{j}_p]$.

IV. SUMMARY AND DISCUSSIONS

In the first half of this paper, we have derived the exact expression for the exchange-correlation energy functional of the CDFT by means of the coupling-constant integration technique. On the basis of the coupling-constant expression, we have also proposed three kinds of the approximation schemes, which should be called the CDFT versions of the LDA, ADA, and WDA. It is shown that the LDA, ADA, and WDA schemes are applicable to actual energy-band calculations by borrowing the knowledge of the exchange-correlation hole from the homogeneous electron liquid in the uniform magnetic field.

In the second half of this paper, the exact conditions fulfilled by $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ have been derived from the various types of nonuniform coordinate scaling of electrons. After a systematic analysis, we have obtained about 30 kinds of conditions on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$. The set of these exact conditions is a complement to the previous results derived from the gauge invariance,[2,31,32] the virial theorem, and uniform coordinate scaling of electrons.[24] All of them can be utilized as sum rules and bounds on $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$ when we develop and check the approximate form of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$.

Thus, we have obtained the new kinds of sum rules and bounds as well as the proposal of the approximate functionals of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$. On the basis of these results, let us discuss which of the sum rules derived are satisfied by the approximate functionals proposed. First, we shall discuss the case of the LDA expression of $E_{\mathrm{xc}}[\rho,\mathbf{j}_p]$. Like the conventional DFT[42] the LDA of the CDFT violates most of sum rules derived from the nonuniform coordinate scalings. Suppose that the external magnetic field is parallel to the x axis, and $\bar{g}^{\mathrm{hom}}(|\mathbf{r}-\mathbf{r}'|,\rho,\boldsymbol{\nu})$ is calculated within the RPA.[6] In this case, the LDA obeys the sum rules (3.11c), (3.14c), and (3.20d), because $E_c^{\mathrm{LDA}}[\rho^x_\lambda,\mathbf{j}_p^x{}_\lambda]$, $E_c^{\mathrm{LDA}}[\rho^{xy}_{\lambda\lambda},\mathbf{j}_p^{xy}_{\lambda\lambda}]$, and $E_c^{\mathrm{LDA}}[\rho^{xyz}_{\lambda\lambda 1/\lambda},\mathbf{j}_p^{xyz}_{\lambda\lambda 1/\lambda}]$ are proportional to $-\lambda^{1/2}$, $-\lambda^{1/4}$, and $-\lambda^{1/2}$, respectively, when $\lambda\to 0$. The same is true for the sum rules which are derived from a uniform coordinate scaling. However, the LDA expression does not obey the sum rules (3.11d), (3.11e), (3.14d), (3.14e), (3.17b), (3.17c), (3.17e), (3.17f), (3.20e), and (3.20f) because they become $-\infty$ for each limit. Sum rules (3.17a) and (3.17d) are not satisfied by the LDA expression either, because they approach constants for each limit. With respect to the other sum rules, we cannot conclude whether they are satisfied by the LDA expression or not. These ambiguities will be removed by studying at greater lengths the homogeneous electron liquid under the weak magnetic field, especially in the cases of high- and low-density limits.[6] Here it should be noted that we may obtain the different results if the magnetic field is parallel to the z axis. In this case, the sum rules derived from a uniform coordinate scaling are also satisfied by the LDA expression, while the sum rules (3.11a), (3.11b), (3.14a), (3.14b), (3.17a)–(3.17f), and (3.20a)–(3.20c) are not satisfied. About the other sum rules, there remain the ambiguities

similarly to the previous case. In this way, the sum rules satisfied by the LDA expression strongly depend on the direction of the magnetic field.

Next let us consider the ADA and WDA expressions defined in Sec. II. The difference between the LDA and ADA is that an exchange-correlation hole of the ADA expression is evaluated at certain averaged densities. Here the densities mean the electron density and vorticity. In order to estimate how the exchange-correlation energy functional varies with λ, one has to investigate how the averaged scaled densities change with λ. Suppose that the weight function is determined independently of λ, and thus the resultant averaged scaled-densities change with λ just as the scaled densities do. Under this assumption, the ADA expression obeys the same sum rules as the LDA. In addition, the ADA has the possibility of satisfying more exact conditions than the LDA by choosing the weight function appropriately. The same is true for the WDA expression. In the WDA, a coupling-constant-averaged pair correlation function is replaced by $\bar{g}^{\mathrm{hom}}(|\mathbf{r}-\mathbf{r}'|,\tilde{\rho}(\mathbf{r}),\tilde{\boldsymbol{\nu}}(\mathbf{r}))$, as shown in Sec. II. The weighted densities $\tilde{\rho}(\mathbf{r})$ and $\tilde{\boldsymbol{\nu}}(\mathbf{r})$ are one of the solutions of the integral equation (2.19) which is the sum rule on the exchange-correlation hole. If the weighted scaled densities are determined by the requirement that they vary with λ similarly to the scaled densities, the WDA expression also obeys the same sum rules as the LDA.

Consequently, the LDA expression violates most of sum rules derived from the nonuniform coordinate scalings, though it obeys sum rules from the uniform coordinate scaling. Thus it seems reasonable to expect that the sum rules derived from the nonuniform coordinate scalings play an important role as a constraint when we construct more accurate approximations than the LDA. As mentioned above, the ADA and WDA expressions potentially satisfy more sum rules than the LDA if the averaged densities and the weighted densities are determined appropriately. Judging from not only the nonlocality of the exchange-correlation hole but also the sum rules satisfied, we may expect that the ADA and WDA improve on the LDA with respect to the accuracy.

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