

Construction of energy density functional for arbitrary spin polarization using functional renormalization group

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We show an application of the functional-renormalization-group aided density functional theory to the homogeneous electron gas with arbitrary spin polarization, which gives an energy density functional in the local spin density approximation. The correlation energy per particle is calculated at arbitrary Wigner–Seitz radius r_s and spin polarization ζ . In the high-density region, our result shows good agreement with Monte Carlo (MC) data. The agreement with MC data is better in the case of small spin polarization, while the discrepancy increases as the spin polarization increases. The magnetic properties given by our numerical results are also discussed.

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I. INTRODUCTION

Density functional theory [1–3] is a powerful framework for many-body systems employed in various fields, including condensed matter physics, quantum chemistry, and nuclear physics. The accuracy of DFT depends on an energy density functional (EDF) [4], which returns the ground-state energy as a functional of the ground-state density. Although the Hohenberg–Kohn theorem [1] guarantees the existence of the *exact* EDF, it does not provide a microscopic way to derive EDF; hence its development is a long-standing problem.

A useful framework for the construction of EDF is the effective action formalism [5–8]. In this formalism, Polonyi, Sailer, and Schwenk [9,10] put forward an approach inspired by the functional renormalization group (FRG) [11–14]. We refer to this approach as the functional-renormalization-group aided density functional theory (FRG-DFT). This approach is based on a functional differential equation, called flow equation, in a closed form of the effective action, which corresponds to the free-energy density functional multiplied by the temperature [5–7]. For such a closed form of equation, some systematic approximation methods were proposed [9,15–17]. The FRG-DFT has been numerically applied to low-dimensional toy models [15–21] including a mimic of the nuclear systems [18–20], and, recently, applied to electronic systems [22,23], where we achieved the first application to the two- and three-dimensional cases in the study of the homogeneous electron gas (HEG) and EDFs for electrons are constructed in the local density approximation.

In the previous works of the FRG-DFT [9,10,15–23], the EDF of the total particle-number density has been studied. The Hohenberg–Kohn theorem guarantees that the ground-

state properties are determined by the total particle-number density. However, the Kohn–Sham scheme [2], which is a commonly used method in DFT, has limited power when formulated based on the EDF of total particle number: Although it is suitable for accurate analysis of the ground-state energy and density, the calculations of other quantities are not always straightforward [24]. A way to extend the Kohn–Sham scheme is introducing EDF depending on additional densities [25]; one of such generalizations is taking into account the particle-number densities of each spin component to describe the magnetic properties [26]. Such a formulation of EDF for multicomponent systems can also be directly applied to analyses of nuclear matter, which is an infinite system of nucleons composed of various components such as protons, neutrons, and hyperons [27–37]. In the context of the FRG-DFT, the EDF depending on the pairing density in addition to the particle-number density to describe superfluid systems was discussed in Ref. [38].

As for electron systems, a simple EDF of the particle-number densities of each spin component is that in the local spin density approximation (LSDA), in which the exchange-correlation part of the EDF $E_{xc}[\rho_\uparrow, \rho_\downarrow]$ is approximated as

$$E_{xc}[\rho_\uparrow, \rho_\downarrow] \approx \int d\mathbf{x} (\rho_\uparrow(\mathbf{x}) + \rho_\downarrow(\mathbf{x})) \epsilon_{xc}(\rho_\uparrow(\mathbf{x}), \rho_\downarrow(\mathbf{x})), \quad (1)$$

where $\epsilon_{xc}(\rho_\uparrow, \rho_\downarrow)$ is the exchange-correlation energy per particle, i.e., energy density, of the HEG of densities of particles with up spin ρ_\uparrow and down spin ρ_\downarrow . At some values of ρ_\uparrow and ρ_\downarrow , $\epsilon_{xc}(\rho_\uparrow, \rho_\downarrow)$ has been obtained by the quantum Monte Carlo (QMC) calculations [39]. The QMC results are of significance not only for the construction of EDF [40–42] but also for the discussion of the properties of the HEG itself: In three dimensions, the existence of the phase transitions from paramagnetic phase to partially polarized or ferromagnetic phase and from ferromagnetic phase to Wigner crystal is predicted [40,43–50], although the predicted values of the

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transition densities are not always similar among these works. In two dimensions, the existence of the ferromagnetic phase is indicated by Refs. [51–56], while it is suggested in Ref. [57] that the ferromagnetic phase is never stable compared to the paramagnetic one.

Since the QMC results are available only at a few values of the densities due to the numerical cost, an empirical fitting function for the data is needed to obtain the value of EDF at arbitrary densities. In our previous work [23], we applied the FRG-DFT for the calculation of the correlation energy per particle in the spin-unpolarized (paramagnetic) case. We obtained the values at many values of density, namely 65 536 points in the Wigner–Seitz radii $r_s \in [10^{-6} \text{ a.u.}, 100 \text{ a.u.}]$, which enables us to determine EDF almost without the dependence on the fitting function.

In this paper, we extend our works [22,23] to the case of arbitrary spin polarization $\zeta = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow)$. We give a formulation of the FRG-DFT with arbitrary spin polarization and dimensions. In the vertex expansion, which is a functional Taylor expansion around densities of interest, we give the flow equations for the density correlation functions at arbitrary order. The correlation energy per particle $\epsilon_c(r_s, \zeta)$ is calculated at various r_s and ζ in the three- and two-dimensional cases. In the high-density region, our result shows good agreement with QMC data as a result of the fact that our correlation energy reproduces the exact behavior at high density given by the Gell-Mann–Brueckner (GB) resummation [58,59]. The agreement with QMC data is better in the case of small spin polarization, while the discrepancy increases as the spin polarization increases, which causes the absence of the magnetic phase transition predicted by the QMC calculations.

We also discuss the interpolation function $f_c(r_s, \zeta)$ defined by

$$f_c(r_s, \zeta) = \frac{\epsilon_c(r_s, \zeta) - \epsilon_c(r_s, 0)}{\epsilon_c(r_s, 1) - \epsilon_c(r_s, 0)}, \quad (2)$$

which characterizes the ζ dependence of EDF. Since ϵ_c at only a few values of ζ and r_s are available in QMC calculation, interpolation with respect to ζ is demanded to obtain ϵ_c for arbitrary ζ to perform LSDA calculations, as similar to the interpolation with respect to r_s . A popular approach to determine $\epsilon_c(r_s, \zeta)$ [24,26] is the approximation $f_c(r_s, \zeta) \approx f_x(\zeta)$ with the interpolation function for the exchange part $f_x(\zeta)$ given analytically. We find the deviation of $f_c(r_s, \zeta)$ from $f_x(\zeta)$ at small r_s , where the FRG-DFT gives accurate results.

This paper is organized as follows: In Sec. II, we show an FRG-DFT formalism with arbitrary spin polarization and dimensions. The flow equations for the density correlation functions at arbitrary order are given. The expression for the correlation energy density is given in the case of the second-order truncation. It is analytically shown that the expression reproduces the GB resummation at high density. Our numerical results are presented in Sec. III. We show the result of the r_s and ζ dependencies of the correlation energy and discuss the magnetic properties given by our calculation. Section IV is devoted to the conclusion. In the Appendix, we give the derivation of Eqs. (15) and (16).

II. FORMALISM

We consider the HEG with the homogeneous density $\bar{\rho}$ and the inverse temperature β neutralized by the background ions with the same density. In order to apply our formalism to the three- and two-dimensional cases, we present the formulation in a general spatial dimension D . The action in the imaginary-time formalism is given by

$$S[\psi, \psi^*] = S_{\text{el}}[\psi, \psi^*] + S_{\text{int}}[\psi, \psi^*], \quad (3a)$$

$$S_{\text{el}}[\psi, \psi^*] = \sum_s \int_X \psi_s^*(X_\epsilon) \left(\partial_\tau - \frac{1}{2} \nabla^2 \right) \psi_s(X),$$

$$S_{\text{int}}[\psi, \psi^*] = \frac{1}{2} \iint_{X, X'} U_{2b}(X, X') \hat{\rho}_\Delta(X) \hat{\rho}_\Delta(X'). \quad (3b)$$

Here, we have introduced the following notations: $X = (\tau, \mathbf{x})$ with the imaginary time τ and spatial coordinate \mathbf{x} , the coordinate integral $\int_X = \int_0^\beta d\tau \int d\mathbf{x}$, $\hat{\rho}_\Delta(X) = \sum_s \hat{\rho}_s(X) - \bar{\rho}$ with the electron field $\psi_s(X)$ having spin s and the electron density operator $\hat{\rho}_s(X) = \psi_s^*(X_\epsilon) \psi_s(X)$, and the simultaneous Coulomb interaction,

$$U_{2b}(X, X') = \frac{1}{|\mathbf{x} - \mathbf{x}'|} \delta(\tau - \tau'). \quad (4)$$

The interaction term S_{int} contains not only the electron-electron interaction term but also the electron-ion and ion-ion ones, which cancel each other, and consequently avoid the divergence from the Hartree term in the infinite system [22]. Additionally, $X_\epsilon = (\tau + \epsilon, \mathbf{x})$ with a positive infinitesimal ϵ has been introduced so that the corresponding Hamiltonian is normal ordered.

A. FRG-DFT flow equation

Following Refs. [9,10], we analyze the evolution of the system with respect to the gradual change of the strength of the two-body Coulomb interaction [Eq. (4)]. For this purpose, the evolution parameter $\lambda \in [0, 1]$ is attached to the interaction term $S_{\text{int}}[\psi, \psi^*]$ as follows:

$$S_\lambda[\psi, \psi^*] = S_{\text{el}}[\psi, \psi^*] + \lambda S_{\text{int}}[\psi, \psi^*]. \quad (5)$$

This action becomes that for a noninteracting system at $\lambda = 0$ and Eq. (3a) at $\lambda = 1$.

Our previous works [22,23] were focused on EDFs of the total density. In the present study, we extend our analysis to the case of EDFs for spin-polarized systems. For this purpose, we introduce the generating functional for the correlation functions for $\hat{\rho}_{\uparrow, \downarrow}(X)$:

$$Z_\lambda[J_\uparrow, J_\downarrow] = \iint \mathcal{D}\psi \mathcal{D}\psi^* e^{-S_\lambda[\psi, \psi^*] + \sum_s \int_X \hat{\rho}_s(X) J_s(X)}. \quad (6)$$

The Legendre transformation of the generating functional for connected correlation functions $W_\lambda[J_\uparrow, J_\downarrow] = \ln Z_\lambda[J_\uparrow, J_\downarrow]$ gives the effective action:

$$\begin{aligned} \Gamma_\lambda[\rho_\uparrow, \rho_\downarrow] &= \sup_{J_\uparrow, J_\downarrow} \left(\sum_s \int_X \rho_s(X) J_s(X) - W_\lambda[J_\uparrow, J_\downarrow] \right) \\ &= \sum_s \int_X \rho_s(X) J_{\text{sup}, \lambda, s}[\rho_\uparrow, \rho_\downarrow](X) \\ &\quad - W_\lambda[J_{\text{sup}, \lambda, \uparrow}[\rho_\uparrow, \rho_\downarrow], J_{\text{sup}, \lambda, \downarrow}[\rho_\uparrow, \rho_\downarrow]]. \quad (7) \end{aligned}$$

Here, the external field $J_{\text{sup}, \lambda, s}[\rho_{\uparrow}, \rho_{\downarrow}]$, which gives the supremum of the first line of Eq. (7), satisfies

$$\frac{\delta W_{\lambda}[J_{\text{sup}, \lambda, \uparrow}[\rho_{\uparrow}, \rho_{\downarrow}], J_{\text{sup}, \lambda, \downarrow}[\rho_{\uparrow}, \rho_{\downarrow}]]}{\delta J_s(X)} = \rho_s(X). \quad (8)$$

The equilibrium densities $\rho_{\text{eq}, s}(X)$ are determined through

$$\frac{\delta \Gamma_{\lambda}[\rho_{\text{eq}, \uparrow}, \rho_{\text{eq}, \downarrow}]}{\delta \rho_s(X)} = \mu_s, \quad (9)$$

where μ_s is the chemical potential of the electrons with the spin component s . In this case, Eq. (7) becomes

$$\Gamma_{\lambda}[\rho_{\text{eq}, \uparrow}, \rho_{\text{eq}, \downarrow}] = \sum_s \mu_s \int_X \rho_{\text{eq}, s}(X) - W_{\lambda}[\mu_{\uparrow}, \mu_{\downarrow}], \quad (10)$$

because of $J_{\text{sup}, \lambda, s}[\rho_{\text{eq}, \uparrow}, \rho_{\text{eq}, \downarrow}](X) = \mu_s$, which is obtained by the relation,

$$\frac{\delta \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]}{\delta \rho_s(X)} = J_{\text{sup}, \lambda, s}[\rho_{\uparrow}, \rho_{\downarrow}](X). \quad (11)$$

Since $W_{\lambda}[\mu_{\uparrow}, \mu_{\downarrow}]/\beta$ is the grand potential, $\Gamma_{\lambda}[\rho_{\text{eq}, \uparrow}, \rho_{\text{eq}, \downarrow}]$ gives the free energy multiplied by β . At zero temperature, $\rho_{\text{eq}, s}(X)$ and $\beta^{-1}\Gamma_{\lambda}[\rho_{\text{eq}, \uparrow}, \rho_{\text{eq}, \downarrow}]$ are reduced to the ground-state density and energy, respectively. Therefore, the EDF of densities with each spin component is given as follows [15]:

$$E_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}] = \lim_{\beta \rightarrow \infty} \beta^{-1} \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}], \quad (12)$$

which is a natural extension of the relation between EDF of total density and the effective action [5,7].

The evolution of $\Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]$ can be described by a functional differential equation. This equation is derived in the same manner as EDFs for total density [10,15,18,19,22] and reads

$$\partial_{\lambda} \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}] = \frac{1}{2} \iint_{X, X'} U_{2b}(X - X') \left[\rho_{\Delta}(X) \rho_{\Delta}(X') + \sum_{s, s'} \Gamma_{\lambda, ss'}^{(2)-1}[\rho_{\uparrow}, \rho_{\downarrow}](X_{e'}, X') - \sum_s \rho_s(X) \delta(\mathbf{x} - \mathbf{x}') \right]. \quad (13)$$

Here, we have introduced $\rho_{\Delta}(X) = \sum_s \rho_s(X) - \bar{\rho}$ and the inverse of the second derivative of the effective action $\Gamma_{\lambda, ss'}^{(2)-1}[\rho_{\uparrow}, \rho_{\downarrow}](X, X')$ defined through the following relation:

$$\sum_{s''} \int_{X''} \Gamma_{\lambda, ss''}^{(2)-1}[\rho_{\uparrow}, \rho_{\downarrow}](X, X'') \frac{\delta^2 \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]}{\delta \rho_{s''}(X'') \delta \rho_s(X')} = \delta_{ss'} \delta(X - X'), \quad (14)$$

where $\delta(X - X') = \delta(\tau - \tau') \delta(\mathbf{x} - \mathbf{x}')$ with $X = (\tau, \mathbf{x})$ and $X' = (\tau', \mathbf{x}')$.

B. Vertex expansion

In principle, $\Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]$ is obtained by solving Eq. (13) with using the noninteracting system as the initial condition. In practice, however, some approximation for $\Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]$ is needed to solve Eq. (13) due to difficulty of direct numerical treatment of functional differential equations. Following Refs. [9,10], we introduce the vertex expansion scheme, where a functional Taylor expansion at some densities of interest is applied and the differential equations for the Taylor coefficients of $\Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]$ are truncated at some order. As derived in the Appendix, these differential equations up to an arbitrary order read in terms of the density correlation functions as follows:

$$\partial_{\lambda} \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}] = \frac{1}{2} \iint_{X, X'} U_{2b}(X - X') \left[\rho_{\Delta}(X) \rho_{\Delta}(X') + \sum_{s, s'} G_{\lambda, ss'}^{(2)}(X_{e'}, X') - \sum_s \rho_s(X) \delta(\mathbf{x} - \mathbf{x}') \right], \quad (15)$$

$$\begin{aligned} \partial_{\lambda} G_{\lambda, s_1 \dots s_m}^{(m)}(X_1, \dots, X_m) &= \sum_s \int_X G_{\lambda, s, s_1 \dots s_m}^{(m+1)}(X, X_1, \dots, X_m) \partial_{\lambda} J_{\text{sup}, \lambda, s}[\rho_{\uparrow}, \rho_{\downarrow}](X) \\ &\quad - \frac{1}{2} \sum_s \iint_{X, X'} U_{2b}(X, X') (\rho_{\Delta}(X) G_{\lambda, ss_1 \dots s_m}^{(m+1)}(X', X_1, \dots, X_m) + \rho_{\Delta}(X') G_{\lambda, ss_1 \dots s_m}^{(m+1)}(X, X_1, \dots, X_m)) \\ &\quad - \frac{1}{2} \sum_{s, s'} \iint_{X, X'} U_{2b}(X, X') \left(G_{\lambda, ss' s_1 \dots s_m}^{(m+2)}(X_{e'}, X', X_1, \dots, X_m) - G_{\lambda, ss_1 \dots s_m}^{(m+1)}(X, X_1, \dots, X_m) \delta_{ss'} \delta(\mathbf{x} - \mathbf{x}') \right. \\ &\quad \left. + \sum_{k=1}^{m-1} \frac{1}{k! (m-k)!} \sum_{\sigma \in \mathcal{S}_m} G_{\lambda, ss_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(m)}}^{(m-k+1)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(m)}) \right), \end{aligned} \quad (16)$$

(a) $\partial_\lambda \Gamma_\lambda = \frac{1}{2} \text{diagram} + \frac{1}{2} \text{diagram} - \frac{1}{2} \text{diagram}$

(b) $\partial_\lambda G_{\lambda, s_1 \dots s_m}^{(m)}(X_1, \dots, X_m) = \text{diagram} - \text{diagram} - \frac{1}{2} \text{diagram} + \frac{1}{2} \text{diagram} - \frac{1}{2} \sum_{k=1}^{m-1} \frac{1}{k!(m-k)!} \sum_{\sigma \in S_m} \text{diagram}$

FIG. 1. Diagrammatic representation of Eqs. (15) and (16). The wavy lines represent the two-body interaction $U_{2b}(X - X')$. The numbers 1, 2, ..., m attached to the diagrams of the correlation functions $G_\lambda^{(2)}$, $G_\lambda^{(3)}$, ..., $G_\lambda^{(m+2)}$ stand for the sets of the coordinate and spin (X_1, s_1) , (X_2, s_2) , ..., (X_m, s_m) , respectively.

where $m \geq 1$ is an integer, S_m stands for the symmetry group of order m , and the m -point density correlation function is defined by

$$G_{\lambda, s_1 \dots s_m}^{(m)}(X_1, \dots, X_m) = \frac{\delta^m W_\lambda[J_{\text{sup}, \lambda, \uparrow}[\rho_\uparrow, \rho_\downarrow], J_{\text{sup}, \lambda, \downarrow}[\rho_\uparrow, \rho_\downarrow]]}{\delta J_{s_1}(X_1) \dots \delta J_{s_m}(X_m)}. \quad (17)$$

The diagrammatic representation of Eqs. (15) and (16) is given in Fig. 1. Note that Eq. (16) at $m = 1$ should be regarded as an equation describing the evolution of $J_{\text{sup}, \lambda, s}[\rho_\uparrow, \rho_\downarrow](X)$ since the left-hand side is already determined by $\partial_\lambda G_{\lambda, s_1}^{(1)}(X_1) = \partial_\lambda \rho_{s_1}(X_1) = 0$ as obtained from Eq. (8).

C. Application to LSDA

Our purpose is the application to the LSDA EDF, which is described in terms of the effective action by

$$\Gamma_{\text{xc}, \lambda}[\rho_\uparrow, \rho_\downarrow] \approx \int_X (\rho_\uparrow(X) + \rho_\downarrow(X)) \epsilon_{\text{xc}, \lambda}(\rho_\uparrow(X), \rho_\downarrow(X)). \quad (18)$$

Here, $\Gamma_{\text{xc}, \lambda}[\rho_\uparrow, \rho_\downarrow]$ is given by the exchange-correlation part of the effective action,

$$\Gamma_{\text{xc}, \lambda}[\rho_\uparrow, \rho_\downarrow] = \Gamma_\lambda[\rho_\uparrow, \rho_\downarrow] - \Gamma_{\lambda=0}[\rho_\uparrow, \rho_\downarrow] - \frac{1}{2} \iint_{X, X'} \lambda U_{2b}(X - X') \rho_\Delta(X) \rho_\Delta(X'),$$

with the second and third terms of the right-hand side corresponding to the kinetic and Hartree terms, respectively, and $\epsilon_{\text{xc}, \lambda}(\rho_\uparrow, \rho_\downarrow)$ is the exchange-correlation energy per particle obtained in the homogeneous case with densities ρ_\uparrow and ρ_\downarrow . Actually, Eq. (18) is reduced to the conventional definition of LSDA for EDF Eq. (1) as obtained from Eq. (12) with the density independent of the imaginary time $\rho_s(X) = \rho_s(\mathbf{x})$. By putting Eq. (18) into Eq. (15), we have an equation to determine $\epsilon_{\text{xc}, \lambda}(\rho_\uparrow, \rho_\downarrow)$:

$$\int_X (\rho_\uparrow(X) + \rho_\downarrow(X)) \partial_\lambda \epsilon_{\text{xc}, \lambda}(\rho_\uparrow(X), \rho_\downarrow(X)) \approx \frac{1}{2} \iint_{X, X'} U_{2b}(X - X') \left[\sum_{s, s'} G_{\lambda, ss'}^{(2)}(X_{\epsilon'}, X') - \sum_s \rho_s(X) \delta(\mathbf{x} - \mathbf{x}') \right]. \quad (19)$$

Particularly, Eq. (19) becomes exact at the homogeneous limit [60]. Given the homogeneous densities $\bar{\rho}_s$ satisfying $\bar{\rho}_\uparrow + \bar{\rho}_\downarrow = \bar{\rho}$, Eq. (19) is reduced to

$$\partial_\lambda \epsilon_{\text{xc}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{1}{2\bar{\rho}} \int_X U_{2b}(X) \left[\sum_{s, s'} G_{\lambda, ss'}^{(2)}(X_{\epsilon'}, 0) - \bar{\rho} \delta(\mathbf{x}) \right]. \quad (20)$$

Here, we have used $G_{\lambda, ss'}^{(2)}(X_{\epsilon'}, X') = G_{\lambda, ss'}^{(2)}(X_{\epsilon'} - X', 0)$, which follows from the translational symmetry. Equation (20) is further reduced to the equation for the correlation part $\epsilon_{\text{c}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \epsilon_{\text{xc}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) - \epsilon_{\text{x}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow)$:

$$\partial_\lambda \epsilon_{\text{c}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{1}{2\bar{\rho}} \sum_{s, s'} \int_X U_{2b}(X) [G_{\lambda, ss'}^{(2)}(X_{\epsilon'}, 0) - G_{\lambda=0, ss'}^{(2)}(X_{\epsilon'}, 0)], \quad (21)$$

which is obtained by use of the expression for the exchange part $\epsilon_{\text{x}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow)$:

$$\epsilon_{\text{x}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{\lambda}{2\bar{\rho}} \int_X U_{2b}(X) \left[\sum_{s, s'} G_{\lambda=0, ss'}^{(2)}(X_{\epsilon'}, 0) - \bar{\rho} \delta(\mathbf{x}) \right]. \quad (22)$$

The analytic result of $\epsilon_{\text{x}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow)$ is known as follows [61,62]:

$$\epsilon_{\text{x}, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = -\frac{\lambda a_D}{r_s} [1 + (2^{1/D} - 1) f_\lambda(\zeta)]. \quad (23)$$

Here, $\zeta = (\bar{\rho}_\uparrow - \bar{\rho}_\downarrow)/\bar{\rho}$ is the spin polarization and r_s is the Wigner–Seitz radius given by $r_s = (V_D \bar{\rho})^{-1/D}$ with $V_{D=2} = \pi$ and $V_{D=3} = 4\pi/3$ being the volume of a D -dimensional unit sphere. The interpolation function $f_\chi(\zeta)$ is defined by

$$f_\chi(\zeta) = \frac{(1 + \zeta)^{(D+1)/D} + (1 - \zeta)^{(D+1)/D} - 2}{2^{(D+1)/D} - 2}. \quad (24)$$

The coefficient a_D is given by $a_2 = 4\sqrt{2}/(3\pi)$ and $a_3 = 3[3/(16\pi)]^{2/3}$. The momentum representation is a convenient choice for the homogeneous case. Then, Eqs. (16) and (21) are written as follows:

$$\partial_\lambda \epsilon_{c, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{1}{2\bar{\rho}} \sum_{s, s'} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) e^{iP^0 \epsilon'} [\tilde{G}_{\lambda, ss'}^{(2)}(P) - \tilde{G}_{\lambda=0, ss'}^{(2)}(P)], \quad (25)$$

$$\begin{aligned} \partial_\lambda \tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1}) &= \sum_s \tilde{G}_{\lambda, ss_1 \dots s_m}^{(m+1)}(0, P_1, \dots, P_{m-1}) \partial_\lambda J_{\text{sup}, \lambda, s}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) \\ &\quad - \frac{1}{2} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(\int_{P^0} e^{iP^0 \epsilon'} \sum_{s, s'} \tilde{G}_{\lambda, ss' s_1 \dots s_m}^{(m+2)}(P, -P, P_1, \dots, P_{m-1}) - \sum_s \tilde{G}_{\lambda, ss_1 \dots s_m}^{(m+1)}(0, P_1, \dots, P_{m-1}) \right) \\ &\quad - \frac{1}{2} \sum_{k=1}^{m-1} \frac{1}{k! (m-k)!} \sum_{\sigma \in \mathcal{S}_m} \tilde{U} \left(\sum_{i=1}^k p_{\sigma(i)} \right) \sum_s \tilde{G}_{\lambda, ss_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)} \left(- \sum_{i=1}^k P_{\sigma(i)}, P_{\sigma(1)}, \dots, P_{\sigma(k-1)} \right) \\ &\quad \times \sum_{s'} \tilde{G}_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(m)}}^{(m-k+1)} \left(- \sum_{i=1}^k P_{\sigma(i)}, P_{\sigma(k+1)}, \dots, P_{\sigma(m-1)} \right). \end{aligned} \quad (26)$$

Here, we have introduced the four-vector $P = (P^0, \mathbf{p})$ with the imaginary frequency P^0 and the spatial momentum \mathbf{p} and $\int_{\mathbf{p}} = \int dP^0/(2\pi) \int d\mathbf{p}/(2\pi)^D$. The Fourier components $\tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1})$ and $\tilde{U}(\mathbf{p})$ are defined as follows:

$$\begin{aligned} (2\pi)^4 \delta \left(\sum_{i=1}^m P_i \right) \tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1}) &= \int_{X_1, \dots, X_m} e^{i \sum_{i=1}^m P_i \cdot X_i} G_{\lambda, s_1 \dots s_m}^{(m)}(X_1, \dots, X_m), \\ \tilde{U}(\mathbf{p}) = \int_X e^{i\mathbf{p} \cdot X} U_{2b}(X) &= \begin{cases} 2\pi/|\mathbf{p}| & (D=2), \\ 4\pi/|\mathbf{p}|^2 & (D=3). \end{cases} \end{aligned} \quad (27)$$

In Eq. (26), one of $P_{\sigma(1)}, \dots, P_{\sigma(m)}$ becomes P_m , which stands for $P_m = -\sum_{i=1}^{m-1} P_i$.

In this paper, we consider the vertex expansion up to the second order. The first and second order of Eq. (26) read

$$\begin{aligned} 0 &= \sum_s \tilde{G}_{\lambda, ss_1}^{(2)}(0) \partial_\lambda J_{\text{sup}, \lambda, s}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) - \frac{1}{2} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(\int_{P^0} e^{iP^0 \epsilon'} \sum_{s, s'} \tilde{G}_{\lambda, ss' s_1}^{(3)}(P, -P) - \sum_s \tilde{G}_{\lambda, ss_1}^{(2)}(0) \right), \\ \partial_\lambda \tilde{G}_{\lambda, s_1 s_2}^{(2)}(P_1) &= \sum_s \tilde{G}_{\lambda, ss_1 s_2}^{(3)}(0, P_1) \partial_\lambda J_{\text{sup}, \lambda, s}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) - \tilde{U}(\mathbf{p}_1) \sum_{s, s'} \tilde{G}_{\lambda, ss_1}^{(2)}(-P_1) \tilde{G}_{\lambda, s' s_2}^{(2)}(P_1) \\ &\quad - \frac{1}{2} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(\int_{P^0} e^{iP^0 \epsilon'} \sum_{s, s'} \tilde{G}_{\lambda, ss' s_1 s_2}^{(4)}(P, -P, P_1) - \sum_s \tilde{G}_{\lambda, ss_1 s_2}^{(3)}(0, P_1) \right). \end{aligned} \quad (28)$$

By canceling $\partial_\lambda J_{\text{sup}, \lambda, s}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow)$ in these equations, we have

$$\partial_\lambda \tilde{G}_{\lambda, s_1 s_2}^{(2)}(P_1) = -\tilde{U}(\mathbf{p}_1) \sum_{s, s'} \tilde{G}_{\lambda, ss_1}^{(2)}(-P_1) \tilde{G}_{\lambda, s' s_2}^{(2)}(P_1) + C_{\lambda, s_1 s_2}(P_1), \quad (30)$$

$$C_{\lambda, s_1 s_2}(P_1) = -\frac{1}{2} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \int_{P^0} e^{iP^0 \epsilon'} \sum_{s, s'} \left(\tilde{G}_{\lambda, ss' s_1 s_2}^{(4)}(P, -P, P_1) - \sum_{t, t'} \tilde{G}_{\lambda, ts_1 s_2}^{(3)}(0, P_1) [\tilde{G}_\lambda^{(2)}(0)]_{tt'}^{-1} \tilde{G}_{\lambda, ss' t'}^{(3)}(P, -P) \right), \quad (31)$$

where $[\tilde{G}_\lambda^{(2)}(0)]_{tt'}^{-1}$ is the inverse of $\tilde{G}_{\lambda, tt'}^{(2)}(0)$ with respect to the spin indices t and t' . As shown in Eq. (31), $C_{\lambda, s_1 s_2}(P_1)$ is composed of higher-order correlation functions.

As in our previous works [22,23], we ignore the λ dependence of $C_{\lambda, s_1 s_2}(P_1)$ as

$$C_{\lambda, s_1 s_2}(P_1) \approx C_{\lambda=0, s_1 s_2}(P_1). \quad (32)$$

Applying this approximation and summing up the spin indices, Eqs. (25) and (30) are rewritten as follows:

$$\partial_\lambda \epsilon_{c, \lambda}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{1}{2\bar{\rho}} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) e^{iP^0 \epsilon'} [\tilde{G}_\lambda^{(2)}(P) - \tilde{G}_{\lambda=0}^{(2)}(P)], \quad (33)$$

$$\partial_\lambda \tilde{G}_\lambda^{(2)}(P_1) \approx -\tilde{U}(\mathbf{p}_1) [\tilde{G}_\lambda^{(2)}(P_1)]^2 + C_{\lambda=0}(P_1), \quad (34)$$

where we have introduced the total density correlation functions:

$$\tilde{G}_\lambda^{(m)}(P_1, \dots, P_{m-1}) = \sum_{s_1, \dots, s_m} \tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1}), \quad (35)$$

and

$$C_{\lambda=0}(P_1) = \sum_{s, s'} C_{\lambda=0, ss'}(P_1). \quad (36)$$

The solution of Eq. (34), which has the form of the Riccati equation, can be obtained analytically with respect to λ . With this solution, the λ integral in Eq. (33) is performed analytically. The solutions read

$$\tilde{G}_{\lambda=1}^{(2)}(P) = \tilde{G}_{\lambda=0}^{(2)}(P) \frac{1 + (B_P/A_P) \tanh B_P}{1 + (A_P/B_P) \tanh B_P}, \quad (37)$$

$$\epsilon_{c, \lambda=1}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{1}{2\bar{\rho}} \int_P \left[\ln \left(\cosh B_P + \frac{A_P}{B_P} \sinh B_P \right) - A_P \right], \quad (38)$$

where

$$A_P = \tilde{U}(\mathbf{p}) \tilde{G}_{\lambda=0}^{(2)}(P), \quad (39a)$$

$$B_P = \sqrt{\tilde{U}(\mathbf{p}) C_{\lambda=0}(P)}. \quad (39b)$$

The quantity $C_{\lambda=0}(P_1)$ is given by the density correlation functions in the noninteracting case $\tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1})$:

$$\begin{aligned} & \tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1}) \\ &= - \sum_{\sigma \in S_{m-1}} \int_{P'} \prod_{k=0}^{m-1} \tilde{G}_{F, s_{\sigma(k)} s_{\sigma(k+1)}} \left(\sum_{i=1}^k P_{\sigma(i)} + P' \right), \end{aligned} \quad (40)$$

where $\tilde{G}_{F, ss'}(P)$ is the propagator of the free fermion defined by

$$\begin{aligned} \tilde{G}_{F, ss'}(P = (\omega, \mathbf{p})) &= \delta_{ss'} \tilde{G}_F(p_{F, s}; P = (\omega, \mathbf{p})) \\ &= \delta_{ss'} \frac{e^{i\omega\epsilon}}{i\omega - \xi_s(\mathbf{p})}, \end{aligned} \quad (41)$$

with $\xi_s(\mathbf{p}) = \mathbf{p}^2/2 - p_{F, s}^2/2$ and the Fermi momentum $p_{F, s} = 2\pi(\bar{\rho}_s/V_D)^{1/D}$. In Eq. (40), $\sigma(0)$ is defined by $\sigma(0) = \sigma(m)$. For efficient numerical calculation of $C_{\lambda=0}(P_1)$, a technique in Refs. [22,23] can be used: It is convenient to describe $C_{\lambda=0}(P_1)$ in terms of the total density correlation function $\tilde{G}_{\lambda=0}^{(m)}(p_F; P_1, \dots, P_{m-1})$ for spin unpolarized systems with the Fermi momentum p_F , which is defined by

$$\begin{aligned} & \tilde{G}_{\lambda=0}^{(m)}(p_F; P_1, \dots, P_{m-1}) \\ &= -2 \sum_{\sigma \in S_{m-1}} \int_{P'} \prod_{k=0}^{m-1} \tilde{G}_F \left(p_F; \sum_{i=1}^k P_{\sigma(i)} + P' \right), \end{aligned} \quad (42)$$

and related to Eq. (40) as

$$\begin{aligned} & \tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1}) \\ &= \frac{1}{2} \left(\prod_{k=1}^{m-1} \delta_{s_k s_{k+1}} \right) \tilde{G}_{\lambda=0}^{(m)}(p_{F, s_1}; P_1, \dots, P_{m-1}). \end{aligned} \quad (43)$$

Then, $C_{\lambda=0, s_1 s_2}(P_1)$ is written as follows:

$$C_{\lambda=0, s_1 s_2}(P_1) = \frac{\delta_{s_1 s_2}}{2} C_{\lambda=0}(p_{F, s_1}; P_1), \quad (44)$$

where

$$\begin{aligned} C_{\lambda=0}(p_F; P_1) &= -\frac{1}{2} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \int_{P_0} e^{iP_0\epsilon'} \left[\tilde{G}_{\lambda=0}^{(4)}(p_F; P, -P, P_1) \right. \\ &\quad \left. - \frac{\tilde{G}_{\lambda=0}^{(3)}(p_F; P, -P) \tilde{G}_{\lambda=0}^{(3)}(p_F; P_1, -P_1)}{\tilde{G}_{\lambda=0}^{(2)}(p_F; 0)} \right]. \end{aligned} \quad (45)$$

As shown in Refs. [22,23], the momentum integrals in Eq. (45) can be reduced to double integrals, which reduces the computational time and enables us to calculate $\epsilon_{c, \lambda=1}$ in a few minutes even on a laptop computer for each set of (r_s, ζ) .

D. Validity of the approximation

We discuss the validity of our approximation described by Eq. (32). First, we show that the resultant $\epsilon_{c, \lambda=1}$ given by Eq. (38) reproduces the exact result at the dense limit given by the GB resummation, which is given by the random phase approximation and the second-order exchange term. To show this, we employ the following scaling rules for $C_{\lambda=0, s_1 s_2}(p_F; P_1)$ and $\tilde{G}_{\lambda=0, s_1 s_2}^{(2)}(p_F; P_1)$:

$$\tilde{G}_{\lambda=0, s_1 s_2}^{(2)}(p_F; P_1) = a^{D-2} \tilde{G}_{\lambda=0, s_1 s_2}^{(2)} \left(\frac{p_F}{a}; \left(\frac{P_1^0}{a^2}, \frac{\mathbf{p}_1}{a} \right) \right), \quad (46a)$$

$$C_{\lambda=0, s_1 s_2}(p_F; P_1) = a^{D-3} C_{\lambda=0, s_1 s_2} \left(\frac{p_F}{a}; \left(\frac{P_1^0}{a^2}, \frac{\mathbf{p}_1}{a} \right) \right), \quad (46b)$$

for an arbitrary number a . By applying these rules to Eqs. (35), (36), (43), and (44) with $a = r_s^{-1}$ and using $r_s p_{F, s} = 2\pi[(1+s\zeta)/(2V_D^2)]^{1/D}$, we obtain

$$\tilde{G}_{\lambda=0}^{(2)}(P_1) = r_s^{2-D} \tilde{G}_{\lambda=0}^{(2)}(\bar{P}_1), \quad (47a)$$

$$C_{\lambda=0}(P_1) = r_s^{3-D} C_{\lambda=0}(\bar{P}_1). \quad (47b)$$

Here, we have introduced $\bar{P}_1 = (r_s^2 P_1^0, r_s \mathbf{p}_1)$ and

$$\tilde{G}_{\lambda=0}^{(2)}(\bar{P}_1) = \frac{1}{2} \sum_s \tilde{G}_{\lambda=0}^{(2)} \left(2\pi \left(\frac{1+s\zeta}{2V_D^2} \right)^{1/D}; \bar{P}_1 \right), \quad (48a)$$

$$C_{\lambda=0}(P_1) = \frac{1}{2} \sum_s C_{\lambda=0} \left(2\pi \left(\frac{1+s\zeta}{2V_D^2} \right)^{1/D}; \bar{P}_1 \right), \quad (48b)$$

which are independent of r_s except for \bar{P}_1 . Using Eqs. (47a) and (47b), and $\tilde{U}(\mathbf{p}) = r_s^{D-1} \tilde{U}(\bar{\mathbf{p}})$ given by Eq. (27), we obtain the scaling for A_P and B_P as follows:

$$A_P = r_s A_{\bar{P}}, \quad (49a)$$

$$B_P = r_s B_{\bar{P}}, \quad (49b)$$

where we have introduced

$$A_{\bar{P}} = \tilde{U}(\bar{\mathbf{p}}) \tilde{G}_{\lambda=0}^{(2)}(\bar{P}), \quad (50a)$$

$$B_{\bar{P}} = \sqrt{\tilde{U}(\bar{\mathbf{p}}) C_{\lambda=0}(\bar{P})}, \quad (50b)$$

which are independent of r_s except for \bar{P} . Changing the integral variable P to \bar{P} in Eq. (38) and using $r_s = (V_D \bar{\rho})^{-1/D}$,

we have

$$\epsilon_{c, \lambda=1}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) = \frac{V_D^{1/D}}{2r_s^2} \int_{\bar{P}} \left(\ln \left[\cosh(r_s \mathcal{B}_{\bar{P}}) + \frac{\mathcal{A}_{\bar{P}}}{\mathcal{B}_{\bar{P}}} \sinh(r_s \mathcal{B}_{\bar{P}}) \right] - r_s \mathcal{A}_{\bar{P}} \right). \quad (51)$$

By expanding this equation with respect to r_s , we obtain

$$\begin{aligned} \epsilon_{c, \lambda=1}(\bar{\rho}_\uparrow, \bar{\rho}_\downarrow) &= \frac{V_D^{1/D}}{2r_s^2} \int_{\bar{P}} \left[\ln(1 + r_s \mathcal{A}_{\bar{P}}) - r_s \mathcal{A}_{\bar{P}} + \frac{(r_s \mathcal{B}_{\bar{P}})^2}{2} \right] + \mathcal{O}(r_s) \\ &= \frac{1}{2\bar{\rho}} \int_P \left[\ln(1 + \tilde{U}(\mathbf{p}) \tilde{G}_{\lambda=0}^{(2)}(P)) - \tilde{U}(\mathbf{p}) \tilde{G}_{\lambda=0}^{(2)}(P) \right] + \frac{1}{4\bar{\rho}} \int_P \tilde{U}(\mathbf{p}) C_{\lambda=0}(P) + \mathcal{O}(r_s). \end{aligned} \quad (52)$$

The first term of the last line is the contribution from the random phase approximation. By performing the frequency integrals, the second term is evaluated as follows:

$$\begin{aligned} \frac{1}{4\bar{\rho}} \int_P \tilde{U}(\mathbf{p}) C_{\lambda=0}(P) &= \frac{1}{2\bar{\rho}} \sum_s \iiint_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \frac{\tilde{U}(\mathbf{p}) \tilde{U}(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')}{\mathbf{p} \cdot (\mathbf{p} + \mathbf{p}' + \mathbf{p}'')} \theta(-\xi_s(\mathbf{p}')) [1 - \theta(-\xi_s(\mathbf{p} + \mathbf{p}'))] \\ &\quad \times \theta(-\xi_s(\mathbf{p}'')) [1 - \theta(-\xi_s(\mathbf{p} + \mathbf{p}''))], \end{aligned} \quad (53)$$

which is identical to the expression for the second-order exchange term [58]. In summary, Eq. (52) is identical to the expression for the GB resummation.

Although our approximation reproduces the exact behavior at $r_s \rightarrow 0$ as shown above, the flow of the higher-order correlation functions becomes important for the accurate calculation as r_s increases. This can be seen from Eq. (26) at arbitrary order roughly: For simplicity, we consider the case of $\lambda = 0$. The following scaling holds:

$$\tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1}) = r_s^{2m-2-D} \tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(\bar{P}_1, \dots, \bar{P}_{m-1}), \quad (54)$$

where $\tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(\bar{P}_1, \dots, \bar{P}_{m-1})$ is a function independent of r_s given by

$$\tilde{G}_{\lambda=0, s_1 \dots s_m}^{(m)}(\bar{P}_1, \dots, \bar{P}_{m-1}) = \frac{1}{2} \left(\prod_{k=1}^{m-1} \delta_{s_k s_{k+1}} \right) \tilde{G}_{\lambda=0}^{(m)} \left(2\pi \left(\frac{1 + s_1 \zeta}{2V_D^2} \right)^{1/D}; \bar{P}_1, \dots, \bar{P}_{m-1} \right). \quad (55)$$

By use of this scaling, we find that the flow represented by Eq. (26) at $\lambda = 0$ behaves as

$$\left. \frac{\partial_\lambda \tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1})}{\tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1})} \right|_{\lambda=0} \sim r_s, \quad (56)$$

which shows that $\tilde{G}_{\lambda, s_1 \dots s_m}^{(m)}(P_1, \dots, P_{m-1})$ rapidly evolves as r_s increases. This result indicates that the evolution of $\tilde{G}_{\lambda, s_1 \dots s_m}^{(m \geq 3)}(P_1, \dots, P_{m-1})$, which is ignored in our approximation given by Eq. (32), becomes important for the accuracy at large r_s .

III. NUMERICAL RESULTS

In this section, we show the numerical results for HEG. Figure 2 shows the FRG-DFT results of $\epsilon_{c, \lambda=1}$ in three dimensions in the paramagnetic ($\zeta = 0$) and ferromagnetic ($\zeta = 1$) states, together with the results by the diffusion Monte Carlo (DMC) simulation and the GB resummation, as functions of the Wigner–Seitz radius r_s .¹ The DMC results are obtained by subtracting the kinetic and exchange energies per particle from the total energy per particle given in Table IV in Ref. [39], which summarizes the results in Refs. [48,50]. For

both cases of $\zeta = 0$ and 1, the FRG-DFT reproduces the results by the GB resummation and the discrepancies between the FRG-DFT and DMC results decrease as r_s becomes close

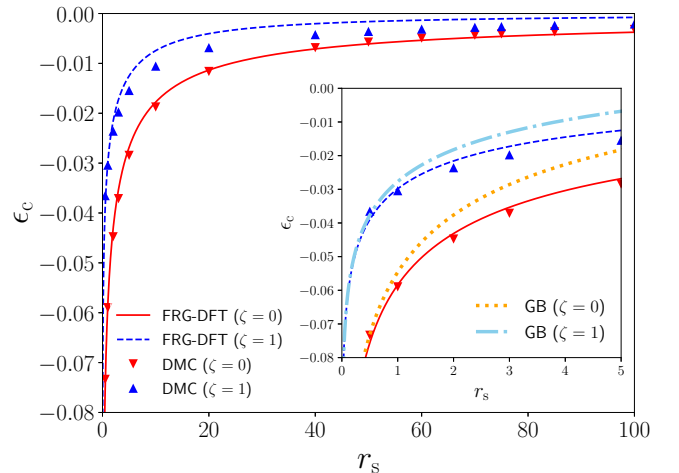


FIG. 2. Correlation energy per particle ϵ_c for three-dimensional ($D = 3$) homogeneous electron gas in the cases of $\zeta = 0$ (paramagnetic) and 1 (ferromagnetic) calculated by using the FRG-DFT (this work) and DMC shown as functions of Wigner–Seitz radius r_s . The data of DMC calculations are obtained from the values in Table IV in Ref. [39], which summarizes the results in Refs. [48,50]. The inset is the enlarged view in $0 \leq r_s \leq 5$, where the results by the GB resummation are also shown.

¹There is a tiny difference between the result of FRG-DFT at $\zeta = 0$ in this work and that in Fig. 1 in Ref. [23]. We find that a coefficient is underestimated in the numerical code to obtain the latter one. The present result is based on a corrected code.

TABLE I. Absolute difference $\Delta\epsilon_c = |\epsilon_c^{\text{FRG}} - \epsilon_c^{\text{DMC}}|$ and relative difference $\Delta\epsilon_c/|\epsilon_c^{\text{DMC}}|$ between the FRG-DFT result ϵ_c^{FRG} (this work) and DMC result ϵ_c^{DMC} [39] at $r_s = 1, 2, 3, 5, 10, 50$, and 100 a.u. and $\zeta = 0$ and 1 .

r_s (a.u.)		1	2	3	5	10	50	100
$\zeta = 0$	$\Delta\epsilon_c \times 10^4$	6.0	16.4	17.9	16.1	9.9	3.6	5.5
	$\Delta\epsilon_c/ \epsilon_c^{\text{DMC}} $ (%)	1.0	3.7	4.8	5.7	5.3	6.2	17.0
$\zeta = 1$	$\Delta\epsilon_c \times 10^4$	5.6	20.1	24.9	29.2	31.1	19.6	13.0
	$\Delta\epsilon_c/ \epsilon_c^{\text{DMC}} $ (%)	1.8	8.5	12.6	18.9	29.5	54.8	62.6

to 0, which is also indicated by the relative differences shown in Table I. On the other hand, the increase of the relative differences at larger r_s is due to the ignorance of the flow of the higher-order correlation functions as discussed in Sec. II D. In the case of $\zeta = 1$, FRG-DFT overestimates ϵ_c compared to DMC. This is a natural result since the truncation up to the second order breaks the Pauli-blocking condition [18,19], which allows two electrons with the same spin to get closer to each other and increases the energy. At $\zeta = 0$ and $r_s \gtrsim 40$ a.u., FRG-DFT underestimates ϵ_c with smaller deviation compared to the case of $\zeta = 1$ as indicated in the absolute and relative differences shown in Table I. This suggests that the correlation between two electrons with the different spins is underestimated and compensates the overestimation coming from the correlation between those with the same spin.

For the purpose of discussing stability of phases, we show the FRG-DFT results of the total energy per particle ϵ_{total} for arbitrary spin polarization at $r_s = 1, 10, 50$, and 100 a.u. in Fig. 3. For comparison, this figure also shows the DMC results and the Hartree–Fock results. The latter are given by

$$\epsilon_{\text{total}}(r_s, \zeta) \approx \epsilon_{\text{kin}}(r_s, \zeta) + \epsilon_{x, \lambda=1}(r_s, \zeta), \quad (57)$$

where the kinetic term ϵ_{kin} and the exchange term ϵ_x are given by

$$\epsilon_{\text{kin}}(r_s, \zeta) = \frac{3}{10} \left(\frac{9\pi}{4} \right)^{2/3} \frac{(1+\zeta)^{5/3} + (1-\zeta)^{5/3}}{2r_s^2}, \quad (58)$$

and Eq. (23), respectively. According to the DMC results [48], a second-order phase transition to spin-polarized states is found at $r_s = 50 \pm 2$ a.u. and the system becomes (partially) spin-polarized states for larger r_s and unpolarized ones for smaller r_s . In contrast to this, the unpolarized state is stable even in $r_s \gtrsim 50$ a.u. in the FRG-DFT result.

Next, we shall discuss the interpolation function $f_c(r_s, \zeta)$ defined in Eq. (2). In Fig. 4(a), the results for $r_s = 1, 5, 10, 50$, and 100 a.u. calculated by using the FRG-DFT are shown as functions of ζ . For comparison, DMC results and the interpolation function for the exchange part $f_x(\zeta)$ defined in Eq. (24) are also shown. Figure 4(b) shows the relative deviation of $f_c(r_s, \zeta)$ from $f_x(\zeta)$: $[f_c(r_s, \zeta) - f_x(\zeta)]/f_x(\zeta)$. A conventional approximation for $f_c(r_s, \zeta)$ [Eq. (2)] is $f_c(r_s, \zeta) \approx f_x(\zeta)$ [24,26]. Actually, the DMC results in Fig. 4 suggest that this approximation is valid for $r_s \gtrsim 10$ a.u. However, the FRG-DFT results show stronger r_s dependence. Particularly, the deviation of the FRG-DFT results from $f_x(\zeta)$ can be seen in small r_s , where the FRG-DFT is accurate, as well as in large r_s . The deviation from $f_x(\zeta)$ also can be seen in the DMC results in $r_s \lesssim 5$ a.u.

Finally, we mention the case of two dimensions. Figure 5 shows the FRG-DFT and DMC results of r_s dependence of ϵ_c at $\zeta = 0$ and 1 . The FRG-DFT result at $\zeta = 0$ is the same as that in Ref. [22]. The DMC results are obtained from the total energies given in Refs. [52,53,57], which are summarized in Table VI in Ref. [39]. In dense cases, reproducing the exact results at $r_s = 0$ a.u. given by the GB resummation, the FRG-DFT results agree with the DMC results. On the other hand, the discrepancy between the FRG-DFT and DMC results increases as the system becomes dilute and the FRG-DFT, respectively, gives underestimated and overestimated results at $\zeta = 0$ and 1 in comparison with DMC. This behavior of ϵ_c

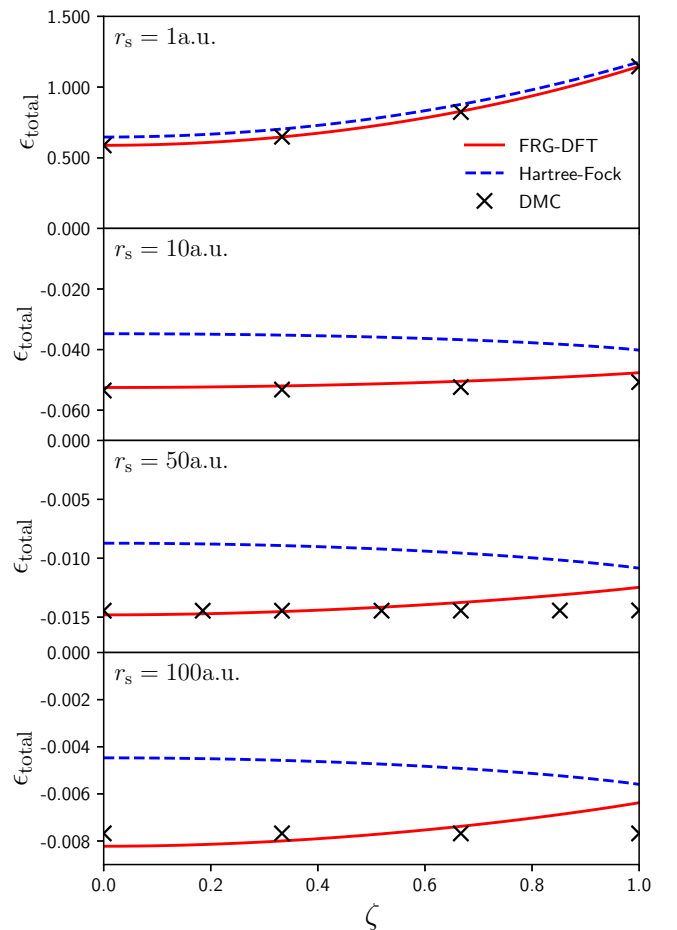


FIG. 3. Total energy per particle ϵ_{total} at $r_s = 1, 10, 50$, and 100 a.u. calculated by using the FRG-DFT shown as functions of ζ . The results from the Hartree–Fock approximation and DMC are also shown. The data of DMC calculations are taken from Table IV in Ref. [39], which summarizes the results in Refs. [48,50].

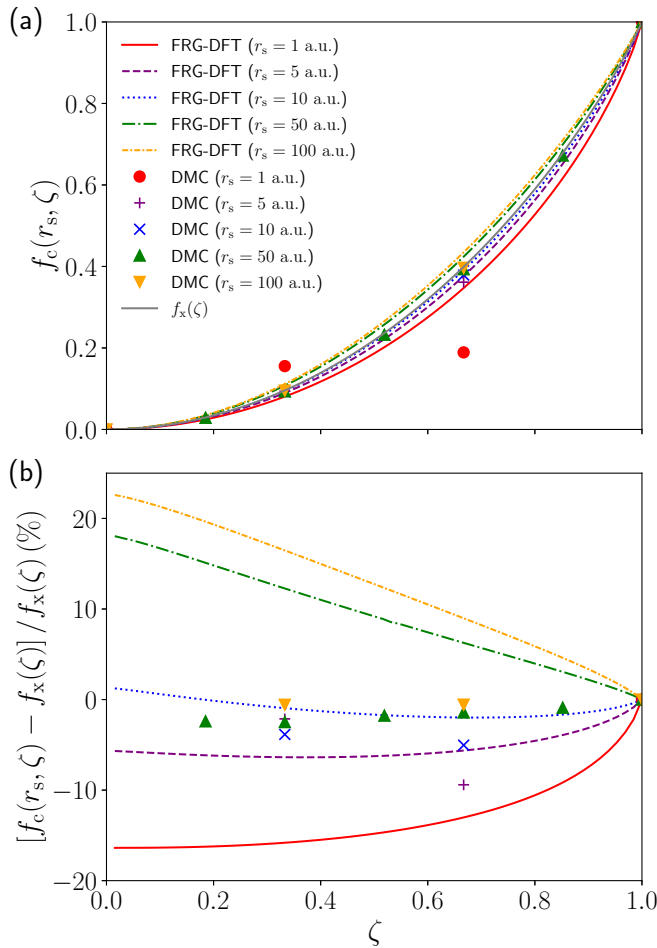


FIG. 4. (a) Interpolation function $f_c(r_s, \zeta)$ for $r_s = 1, 5, 10, 50$, and 100 a.u. calculated by using the FRG-DFT as functions of ζ . For comparison, DMC results [48,50] and $f_x(\zeta)$ [Eq. (24)] are also shown. (b) Relative deviation of $f_c(r_s, \zeta)$ from $f_x(\zeta)$. The data at $\zeta = 0$, where $f_x(\zeta) = 0$, are excluded. The DMC data at $r_s = 1$ a.u. are out of the range of the figure.

favors the paramagnetic phase even if the system is dilute as in the case of three dimensions.

IV. CONCLUSION

We have developed the functional-renormalization-group aided density functional theory (FRG-DFT) for the description of arbitrary spin-polarized systems and achieved numerical derivation of the correlation energy per particle of homogeneous electron gas ϵ_c with arbitrary density and spin polarization, which gives the energy density functional in the local spin density approximation. The hierarchical flow equations for the density correlation functions have been derived up to arbitrary order based on the FRG-DFT flow equation. Our numerical calculation has been performed based on the second-order truncation for the hierarchical equations. Our correlation energy per particle reproduces the exact behavior at the high-density limit given by the Gell-Mann-Brueckner resummation and agrees with the diffusion Monte Carlo (DMC) results in relatively high-density cases. On the other hand, the discrepancy between the FRG-DFT and DMC

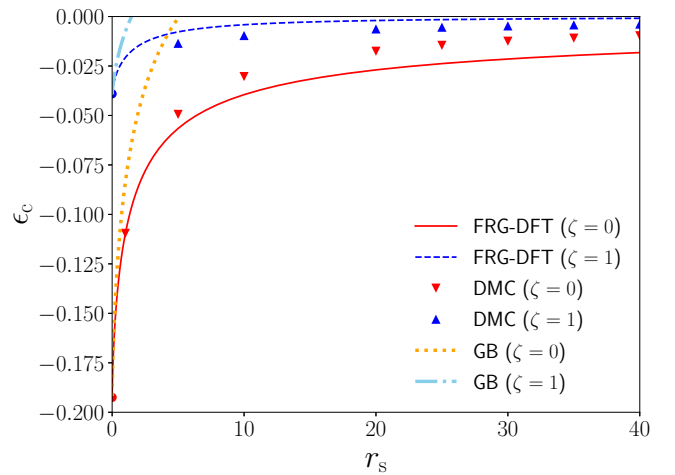


FIG. 5. Correlation energy per particle ϵ_c at $\zeta = 0$ and 1 given by the FRG-DFT, DMC, and GB resummation in the two-dimensional ($D = 2$) case. The data of DMC calculations are obtained from the values in Table VI in Ref. [39], which summarizes the results in Refs. [52,53,57]. The values at $r_s = 0$ given by the FRG-DFT (and the GB resummation), which are finite in contrast to the three-dimensional case, are shown as the red and blue circles for $\zeta = 0$ and 1, respectively.

results becomes significant in the spin-polarized case in comparison with the spin-unpolarized case as the system becomes dilute. In contrast to DMC results, the correlation energy given by FRG-DFT stabilizes the spin-unpolarized state even in dilute cases. We have also discuss the interpolation function $f_c(r_s, \zeta)$, which characterizes the ζ dependence of ϵ_c . We have found the deviation from the interpolation function for the exchange part at small r_s , where the FRG-DFT gives accurate results.

The growth of the discrepancy in the spin-polarized case may be attributed to the effect of the Pauli blocking, which is broken in our approximation. In order to retain the Pauli-blocking effect, one may introduce a correction factor to the four-point density correlation function [18]. When applying this method, it is required to solve the flow equation numerically with respect to the evolution parameter λ . This is in contrast to the fact that the flow equation can be solved analytically in the approximation in this paper. The introduction of another approximation scheme valid even for dilute systems also may change the situation. In Ref. [63], a possibility of using small expansion parameters within some frameworks including the derivative expansion is discussed. As for the application of the derivative expansion in the framework of the functional renormalization group based on density, there is a work for classical liquids [64].

A great goal of studies of the FRG-DFT is systematic inclusion of the gradient effect. In dilute cases, particularly, this is important for the description of the Wigner crystal. One of the ways to realize this in our framework may be the use of the derivative expansion. Methods to describe solid-liquid phase transition developed for the classical DFT [65] are also expected to give hints for the treatment of the Wigner crystal.

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APPENDIX: DERIVATION OF EQS. (15) AND (16)

In this Appendix, we show the derivation of Eqs. (15) and (16). Equation (15) is derived from Eq. (13) and

$$\Gamma_{\lambda, ss'}^{(2)-1}[\rho_{\uparrow}, \rho_{\downarrow}](X, X') = G_{\lambda, ss'}^{(2)}(X, X'). \quad (\text{A1})$$

The derivation of this relation is as follows: Differentiating Eq. (8), we have

$$\sum_t \int_Y \frac{\delta J_{\text{sup}, \lambda, t}[\rho_{\uparrow}, \rho_{\downarrow}](Y)}{\delta \rho_{s'}(X')} \frac{\delta^2 W_{\lambda}[J_{\text{sup}, \lambda, \uparrow}[\rho_{\uparrow}, \rho_{\downarrow}], J_{\text{sup}, \lambda, \downarrow}[\rho_{\uparrow}, \rho_{\downarrow}]]}{\delta J_t(Y) \delta J_s(X)} = \delta_{ss'} \delta(X - X'). \quad (\text{A2})$$

By use of Eqs. (11) and (17), this is rewritten as

$$\sum_t \int_Y \frac{\delta^2 \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]}{\delta \rho_{s'}(X') \delta \rho_t(Y)} G_{\lambda, ts}^{(2)}(Y, X) = \delta_{ss'} \delta(X - X'), \quad (\text{A3})$$

which is equivalent to Eq. (A1).

The following relation is useful for the derivation of Eq. (16):

$$\sum_s \int_X G_{\lambda, s_1 \dots s_m}^{(2)}(X_{m+1}, X) \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_m}^{(m)}(X_1, \dots, X_m) = G_{\lambda, s_1 \dots s_{m+1}}^{(m+1)}(X_1, \dots, X_{m+1}). \quad (\text{A4})$$

This is obtained by differentiating Eqs. (11) and (17):

$$\begin{aligned} \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_m}^{(m)}(X_1, \dots, X_m) &= \frac{\delta}{\delta \rho_s(X)} \frac{\delta^m W_{\lambda}[J_{\text{sup}, \lambda, \uparrow}[\rho_{\uparrow}, \rho_{\downarrow}], J_{\text{sup}, \lambda, \downarrow}[\rho_{\uparrow}, \rho_{\downarrow}]]}{\delta J_{s_1}(X_1) \cdots \delta J_{s_m}(X_m)} \\ &= \sum_{s_{m+1}} \int_{X_{m+1}} \frac{\delta J_{\text{sup}, \lambda, s_{m+1}}[\rho_{\uparrow}, \rho_{\downarrow}](X_{m+1})}{\delta \rho_s(X)} \frac{\delta^{m+1} W_{\lambda}[J_{\text{sup}, \lambda, \uparrow}[\rho_{\uparrow}, \rho_{\downarrow}], J_{\text{sup}, \lambda, \downarrow}[\rho_{\uparrow}, \rho_{\downarrow}]]}{\delta J_{s_1}(X_1) \cdots \delta J_{s_m}(X_m) \delta J_{s_{m+1}}(X_{m+1})} \\ &= \sum_{s_{m+1}} \int_{X_{m+1}} \frac{\delta^2 \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]}{\delta \rho_s(X) \delta \rho_{s_{m+1}}(X_{m+1})} G_{\lambda, s_1 \dots s_{m+1}}^{(m+1)}(X_1, \dots, X_{m+1}). \end{aligned} \quad (\text{A5})$$

Multiplying $\Gamma_{\lambda}^{(2)-1}$ to both sides and using Eq. (A1), we have Eq. (A4).

The derivation of Eq. (16) is based on the mathematical induction. As a first step, we derive the equation for $m = 1$. Differentiating Eq. (13), we have

$$\begin{aligned} \partial_{\lambda} \frac{\delta \Gamma_{\lambda}[\rho_{\uparrow}, \rho_{\downarrow}]}{\delta \rho_{s_1}(X_1)} &= \frac{1}{2} \iint_{X, X'} U_{2b}(X - X') [\rho_{\Delta}(X) \delta(X' - X_1) + \rho_{\Delta}(X') \delta(X - X_1)] \\ &\quad + \frac{1}{2} \iint_{X, X'} U_{2b}(X - X') \left[\sum_{s, s'} \frac{\delta G_{\lambda, ss'}^{(2)}(X_{e'}, X')}{\delta \rho_{s_1}(X_1)} - \delta(X - X_1) \delta(\mathbf{x} - \mathbf{x}') \right]. \end{aligned} \quad (\text{A6})$$

Multiplying $G_{\lambda}^{(2)}$ and using Eqs. (A4) and (11), we obtain

$$\begin{aligned} &\sum_s \int_X G_{\lambda, s_1 s}^{(2)}(X_1, X) \partial_{\lambda} J_{\text{sup}, \lambda, s}[\rho_{\uparrow}, \rho_{\downarrow}](X) \\ &= \frac{1}{2} \sum_s \iint_{X, X'} U_{2b}(X - X') [\rho_{\Delta}(X) G_{\lambda, ss_1}^{(2)}(X', X_1) + \rho_{\Delta}(X') G_{\lambda, ss_1}^{(2)}(X, X_1)] \\ &\quad + \frac{1}{2} \iint_{X, X'} U_{2b}(X - X') \left[\sum_{s, s'} G_{\lambda, ss's_1}^{(3)}(X_{e'}, X', X_1) - \sum_s \delta(\mathbf{x} - \mathbf{x}') G_{\lambda, ss_1}^{(2)}(X, X_1) \right]. \end{aligned} \quad (\text{A7})$$

Remembering $\partial_{\lambda} G_{\lambda, s}^{(1)}(X_1) = \partial_{\lambda} \rho_s(X_1) = 0$, one finds that Eq. (A7) is equivalent to Eq. (16) in the case of $m = 1$.

Next, we assume that Eq. (16) holds for $m = j$ and derive the equation for $m = j + 1$. Differentiating Eq. (16) for $m = j$ with respect to the density, multiplying $G_\lambda^{(2)}$, and using Eq. (A4), we obtain

$$\begin{aligned}
& \sum_s \int_X G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \partial_\lambda \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_j}^{(j)}(X_1, \dots, X_j) \\
&= \sum_{s, s'} \iint_{X, X'} G_{\lambda, s s_1 \dots s_j}^{(j+1)}(X, X_1, \dots, X_j) G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X') \partial_\lambda \frac{\delta J_{\text{sup}, \lambda, s}[\rho_\uparrow, \rho_\downarrow](X)}{\delta \rho_{s'}(X')} \\
&+ \sum_s \int_X G_{\lambda, s s_1 \dots s_{j+1}}^{(j+2)}(X, X_1, \dots, X_{j+1}) \partial_\lambda J_{\text{sup}, \lambda, s}[\rho_\uparrow, \rho_\downarrow](X) \\
&- \frac{1}{2} \sum_{s, s'} \iint_{X, X'} U_{2b}(X, X') (G_{\lambda, s' s_{j+1}}^{(2)}(X, X_{j+1}) G_{\lambda, s s_1 \dots s_j}^{(j+1)}(X', X_1, \dots, X_j) + G_{\lambda, s' s_{j+1}}^{(2)}(X', X_{j+1}) G_{\lambda, s s_1 \dots s_j}^{(j+1)}(X, X_1, \dots, X_j)) \\
&- \frac{1}{2} \sum_s \iint_{X, X'} U_{2b}(X, X') (\rho_\Delta(X) G_{\lambda, s s_1 \dots s_{j+1}}^{(j+2)}(X', X_1, \dots, X_{j+1}) + \rho_\Delta(X') G_{\lambda, s s_1 \dots s_{j+1}}^{(j+2)}(X, X_1, \dots, X_{j+1})) \\
&- \frac{1}{2} \sum_{s, s'} \iint_{X, X'} U_{2b}(X, X') \left(G_{\lambda, s s' s_1 \dots s_{j+1}}^{(j+2)}(X_{e'}, X', X_1, \dots, X_{j+1}) - G_{\lambda, s s_1 \dots s_{j+1}}^{(j+2)}(X, X_1, \dots, X_{j+1}) \delta_{s s'} \delta(\mathbf{x} - \mathbf{x}') \right. \\
&+ \sum_{k=1}^{j-1} \frac{1}{k! (j-k)!} \sum_{\sigma \in S_j} G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)} s_{j+1}}^{(k+2)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}, X_{j+1}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)}}^{(j-k+1)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}) \\
&\left. + G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)} s_{j+1}}^{(j-k+2)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}, X_{j+1}) \right]. \tag{A8}
\end{aligned}$$

The left-hand side is evaluated through the derivative of Eq. (A4) with respect to λ :

$$\begin{aligned}
& \sum_s \int_X G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \partial_\lambda \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_j}^{(j)}(X_1, \dots, X_j) \\
&= \partial_\lambda G_{\lambda, s_1 \dots s_{j+1}}^{(j+1)}(X_1, \dots, X_{j+1}) \sum_s \int_X \partial_\lambda G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_j}^{(j)}(X_1, \dots, X_j). \tag{A9}
\end{aligned}$$

By use of Eq. (A2), this is rewritten as follows:

$$\begin{aligned}
& \sum_s \int_X G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \partial_\lambda \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_j}^{(j)}(X_1, \dots, X_j) \\
&= \partial_\lambda G_{\lambda, s_1 \dots s_{j+1}}^{(j+1)}(X_1, \dots, X_{j+1}) \\
&- \sum_{s, s'} \iint_{X, X'} \partial_\lambda G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \sum_t \int_Y \frac{\delta J_{\text{sup}, \lambda, t}[\rho_\uparrow, \rho_\downarrow](Y)}{\delta \rho_s(X)} G_{\lambda, t s'}^{(2)}(Y, X') \frac{\delta}{\delta \rho_{s'}(X')} G_{\lambda, s_1 \dots s_j}^{(j)}(X_1, \dots, X_j). \tag{A10}
\end{aligned}$$

By differentiating Eq. (A2) with respect to λ , we have

$$\sum_s \int_X \partial_\lambda G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \frac{\delta J_{\text{sup}, \lambda, t}[\rho_\uparrow, \rho_\downarrow](Y)}{\delta \rho_s(X)} = - \sum_s \int_X G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \partial_\lambda \frac{\delta J_{\text{sup}, \lambda, t}[\rho_\uparrow, \rho_\downarrow](Y)}{\delta \rho_s(X)}. \tag{A11}$$

By use of this relation and Eq. (A4), Eq. (A10) is rewritten as follows:

$$\begin{aligned}
& \sum_s \int_X G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \partial_\lambda \frac{\delta}{\delta \rho_s(X)} G_{\lambda, s_1 \dots s_j}^{(j)}(X_1, \dots, X_j) \\
&= \partial_\lambda G_{\lambda, s_1 \dots s_{j+1}}^{(j+1)}(X_1, \dots, X_{j+1}) + \sum_{s, t} \iint_{X, Y} G_{\lambda, t s_1 \dots s_j}^{(j+1)}(Y, X_1, \dots, X_j) G_{\lambda, s_{j+1}^s}^{(2)}(X_{j+1}, X) \partial_\lambda \frac{\delta J_{\text{sup}, \lambda, t}[\rho_\uparrow, \rho_\downarrow](Y)}{\delta \rho_s(X)}. \tag{A12}
\end{aligned}$$

The second term of this equation and the first term in the right-hand side of Eq. (A8) cancel each other. The last term in the right-hand side of Eq. (A8) is deformed as follows:

$$\begin{aligned}
& \sum_{k=1}^{j-1} \frac{1}{k!(j-k)!} \sum_{\sigma \in S_j} \left[G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)} s_{j+1}}^{(k+2)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}, X_{j+1}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)}}^{(j-k+1)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}) \right. \\
& \quad \left. + G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)} s_{j+1}}^{(j-k+2)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}, X_{j+1}) \right] \\
& = \sum_{\sigma \in S_j} \left[\sum_{k=2}^j \frac{1}{(k-1)!(j-k+1)!} G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k-1)} s_{j+1}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k-1)}, X_{j+1}) G_{\lambda, s' s_{\sigma(k)} \dots s_{\sigma(j)}}^{(j-k+2)}(X', X_{\sigma(k)}, \dots, X_{\sigma(j)}) \right. \\
& \quad \left. + \sum_{k=1}^{j-1} \frac{1}{k!(j-k)!} G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)} s_{j+1}}^{(j-k+2)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}, X_{j+1}) \right] \\
& = \sum_{\sigma \in S_j} \frac{1}{k!(j+1-k)!} \left[\sum_{k=2}^j k G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k-1)} s_{j+1}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k-1)}, X_{j+1}) G_{\lambda, s' s_{\sigma(k)} \dots s_{\sigma(j)}}^{(j-k+2)}(X', X_{\sigma(k)}, \dots, X_{\sigma(j)}) \right. \\
& \quad \left. + \sum_{k=1}^{j-1} (j+1-k) G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)} s_{j+1}}^{(j-k+2)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}, X_{j+1}) \right] \\
& = \sum_{\sigma \in S_j} \frac{1}{k!(j+1-k)!} \left[\sum_{k=1}^j k G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k-1)} s_{j+1}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k-1)}, X_{j+1}) G_{\lambda, s' s_{\sigma(k)} \dots s_{\sigma(j)}}^{(j-k+2)}(X', X_{\sigma(k)}, \dots, X_{\sigma(j)}) \right. \\
& \quad \left. + \sum_{k=1}^{j-1} (j+1-k) G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j)} s_{j+1}}^{(j-k+2)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j)}, X_{j+1}) \right] \\
& \quad - \sum_{\sigma \in S_j} \frac{1}{j!} \left[G_{\lambda, s s_{j+1}}^{(2)}(X, X_{j+1}) G_{\lambda, s' s_{\sigma(1)} \dots s_{\sigma(j)}}^{(j+1)}(X', X_{\sigma(1)}, \dots, X_{\sigma(j)}) + G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(j)}}^{(j+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(j)}) G_{\lambda, s' s_{j+1}}^{(2)}(X', X_{j+1}) \right] \\
& = \sum_{\sigma \in S_{j+1}} \sum_{k=1}^j \frac{1}{k!(j+1-k)!} G_{\lambda, s s_{\sigma(1)} \dots s_{\sigma(k)}}^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_{\lambda, s' s_{\sigma(k+1)} \dots s_{\sigma(j+1)}}^{(j-k+2)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(j+1)}) \\
& \quad - G_{\lambda, s s_{j+1}}^{(2)}(X, X_{j+1}) G_{\lambda, s' s_1 \dots s_j}^{(j+1)}(X', X_1, \dots, X_j) - G_{\lambda, s s_1 \dots s_j}^{(j+1)}(X, X_1, \dots, X_j) G_{\lambda, s' s_{j+1}}^{(2)}(X', X_{j+1}). \tag{A13}
\end{aligned}$$

By substituting Eqs. (A12) and (A13) into Eq. (A8), we obtain Eq. (16) for $m = j + 1$. Therefore, Eq. (16) holds for all integers $m \geq 1$.

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