

# Microscopic derivation of density functional theory for superfluid systems based on effective action formalism

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A density-functional theory for superfluid systems is developed in the framework of the functional renormalization group based on the effective action formalism. We introduce the effective action for the particle-number and non-local pairing densities and demonstrate that the Hohenberg–Kohn theorem for superfluid systems is established in terms of the effective action. The flow equation for the effective action is then derived, where the flow parameter runs from 0 to 1, corresponding to the non-interacting and interacting systems. From the flow equation and the variational equation that the equilibrium density satisfies, we obtain the exact expression for the Kohn–Sham potential generalized to include the pairing potentials. The resultant Kohn–Sham potential has a nice feature in that it expresses the microscopic formulae of the external, Hartree, pairing and exchange–correlation terms separately. It is shown that our Kohn–Sham potential gives the ground-state energy of the Hartree–Fock–Bogoliubov theory by neglecting the correlations. An advantage of our exact formalism lies in the fact that it provides ways to improve the correlation part systematically.  
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## 1. Introduction

The purpose of the present paper is to develop a density-functional theory (DFT) for superfluid systems based on the effective action formalism, where the Hohenberg–Kohn theorem is readily established for superfluid systems with the spontaneous symmetry breaking (SSB) being incorporated. Moreover, it will be shown that the exact expression for the Kohn–Sham (KS) potential is derived by making use of the functional renormalization group.

DFT has been widely applied and proven to be an efficient and convenient framework to deal with the many-body problems in various fields including quantum chemistry and atomic, molecular, condensed-matter, and nuclear physics; see Refs. [1–6] for some recent reviews. DFT rests upon the Hohenberg–Kohn theorem [7], which states that the ground state of a quantum many-body system is obtained by minimizing the energy-density functional (EDF) with respect to the particle density only. In a practical implementation of DFT, one usually relies on the KS scheme [8], where the ground-state density of the interacting system is reproduced by just solving the Hartree–Fock-type single-particle Schrödinger equation, called the KS equation, for the non-interacting reference system.

However, it is known to be clumsy for a naive application of the original DFT to describe systems with SSB such as magnetization or superfluidity solely with the particle density. Thus the order

parameter as given by an anomalous density is included explicitly as an additional density to describe such a system with SSB [9–20].

A great challenge in the current study of DFT is to develop a microscopic and systematic framework for constructing the EDF from an inter-particle interaction. The notion of the effective action [21, 22] has brought forth the non-perturbative framework for dealing with the quantum many-body problems, and the concepts and recipes developed and accumulated in the study of quantum-field theory (QFT) can be brought into the study of many-body systems. In particular, the effective action for composite fields [23–25] links DFT and concepts and recipes of QFT. Indeed, the two-particle point-irreducible effective action [26] for the density field is identified with the free-energy density functional containing all the information of not only the ground state but also the excited states [27,28]. Thus a promising strategy to overcome the perennial challenge has come out. In Ref. [29], what they call the inversion method was developed to calculate the ground-state energy non-perturbatively, and it was further extended to the Fermion system with superfluidity [30]. Along with this line of method, the notion of effective field theory is applied to construct the free-energy density functional including superfluidity [31–34].

Although the inversion method is certainly a well-founded and powerful non-perturbative scheme, the notions and techniques developed in QFT may not have been fully utilized. An established method is currently available for the calculation of effective actions, which is called the functional renormalization group (FRG) [35–38]. The FRG provides a non-perturbative and systematic procedure for the analyses of renormalization flows by solving one-parameter functional differential equations in a closed form of effective actions. Recently, the application to the effective action for composite fields aimed at an *ab-initio* construction of DFT, which we call the functional-renormalization-group aided density functional theory (FRG-DFT), has been developed: After the proposal of the formalism in Refs. [39,40], several approximation schemes have been proposed, whose performances were tested in (0+0)- or (0+1)-dimensional toy models [41,42]. The application was extended to (1+1)-dimensional systems composed of nucleons in the canonical formalism [43] and the grand-canonical formalism [44]. The excited states in (1+1)-dimensional systems were also investigated [45]. Furthermore, analyses of more realistic systems such as homogeneous electron gases in (2+1) dimensions [46] and (3+1) dimensions [47] were recently achieved.

The purpose of this paper is to extend the FRG-DFT formalism as developed in Refs. [44,45] so as to be applicable to superfluid systems at finite temperature. To this end, we introduce the effective action for the particle-number and non-local pairing densities, whereby the Hohenberg–Kohn theorem in terms of the Helmholtz free energy is found to be readily established. We then derive the flow equation for the effective action by introducing a flow parameter  $\lambda$  with which the strength of the inter-particle interaction is adiabatically increased as  $\lambda$  is changed from 0 to 1. The differentiation of the effective action with respect to  $\lambda$  gives the coupled flow equations for the particle-number and pairing densities. Together with the variational equation which the equilibrium densities should satisfy, the exact expression for the KS potential generalized to include the pairing potentials is derived. The resultant KS potential has a nice feature in that it expresses the microscopic formulae of the external, Hartree, pairing, and exchange–correlation terms separately. As a demonstration of the validity of our formalism, we show that a lowest-order approximation to our flow equations with respect to the flow parameter reproduces the gap equation, the ground-state energy and pairing density given in the Bardeen Cooper Schrieffer (BCS) theory for the case of short-range interactions in the

weak-coupling limit. Although we show the validity of our microscopic formulation by applying it to simple cases, an advantage of our exact FRG-DFT formalism lies in the fact that it provides ways to systematically improve the correlation part.

This paper is organized as follows: In Sect. 2, we introduce the effective action for the particle-number and pairing densities and derive the flow equation to calculate the effective action. From the flow equation, the exact expression of the KS potential is derived. In Sect. 3, we apply the lowest-order approximation to our formalism and compare our results with those given by the BCS theory. Section 4 is devoted to a brief summary and the conclusions.

## 2. Formalism

In this section, we develop a formalism to describe microscopically the superfluid systems at finite temperature in the framework of FRG-DFT, where the effective action given in the functional-integral form is fully utilized. The formalism starts with construction of the effective action  $\Gamma[\rho, \kappa, \kappa^*]$  for the non-local pairing densities as well as particle-number ones, and then we show that  $\Gamma[\rho, \kappa, \kappa^*]$  can be identified with the free-energy *density functional* for which the Hohenberg–Kohn theorem holds. We then introduce a flow parameter  $\lambda$  with which the inter-particle interaction is switched on gradually as  $\lambda$  is varied from 0 to 1. Differentiating the thus constructed effective action  $\Gamma_\lambda[\rho, \kappa, \kappa^*]$  with respect to  $\lambda$ , we obtain the coupled flow equations for the particle-number and pairing densities. Thus the problem of deriving the governing equation of the superfluid systems in the context of DFT is reduced to solving the flow equations. Inherently in the way of the introduction of the flow parameter, the governing equation thus obtained actually leads to the exact expression of the KS potential. Moreover, because of the very exact nature of the governing equation thus obtained, the resultant equation can be a starting point for an introduction of various systematic approximations.

We consider a system composed of non-relativistic fermions interacting via two-body interactions subject to the external potential at finite temperature  $1/\beta$  with  $\beta$  being the inverse temperature. The action describing the system in the imaginary-time formalism is given as follows:

$$S[\psi, \psi^*] = \int_{\xi} \psi^*(\xi + \epsilon_\tau) \left( \partial_\tau - \frac{\Delta}{2} + \mathcal{V}(\xi) \right) \psi(\xi) + \frac{1}{2} \int_{\xi, \xi'} \mathcal{U}(\xi, \xi') \psi^*(\xi + \epsilon_\tau) \psi^*(\xi' + \epsilon_\tau) \psi(\xi') \psi(\xi). \quad (1)$$

Here, the short-hand notations  $\xi = (\tau, \mathbf{x}, a)$ ,  $\xi' = (\tau', \mathbf{x}', a')$ ,  $\xi' + \epsilon_\tau = (\tau' + \epsilon, \mathbf{x}', a')$  and  $\int_{\xi} = \sum_a \int_0^\beta d\tau \int d\mathbf{x}$  have been introduced, where  $\tau$ ,  $\mathbf{x}$ , and  $a$  represent the imaginary time, spatial coordinate, and index for internal degree of freedoms, respectively, with  $\epsilon$  being an infinitesimal constant. The fermion fields are represented by Grassmann variables  $\psi(\xi)$  and  $\psi^*(\xi)$ . The static external potential and the instantaneous two-body interaction are denoted by  $\mathcal{V}(\xi) = V_a(\mathbf{x})$  and  $\mathcal{U}(\xi, \xi') = \delta(\tau - \tau') U_{aa'}(\mathbf{x} - \mathbf{x}')$ , respectively. The shifted coordinate  $\xi + \epsilon_\tau = (\tau + \epsilon, \mathbf{x}, a)$  is introduced so that the corresponding Hamiltonian becomes normal-ordered [44].

### 2.1. Effective action for superfluid systems

Let us introduce the effective action, which is to be identified with the free-energy density functional for superfluid systems. The construction of the effective action [21,22] starts by defining the generating functional of the correlation functions of density fields. In this work, we generalize the previous works [27,44,45] and introduce the generating functional for the correlation functions of

particle-number and (non-local) pairing densities as

$$\begin{aligned} Z[\vec{J}] &= \int \mathcal{D}\psi \mathcal{D}\psi^* e^{-S[\psi, \psi^*] + \int_{\xi} J^{\rho}(\xi) \psi^*(\xi + \epsilon_{\tau}) \psi(\xi) + \int_{\xi, \xi'} J^{\kappa}(\xi, \xi') \psi(\xi) \psi(\xi') + \int_{\xi, \xi'} J^{\kappa^*}(\xi, \xi') \psi^*(\xi') \psi^*(\xi)} \\ &= \int \mathcal{D}\psi \mathcal{D}\psi^* e^{-S[\psi, \psi^*] + \sum_{i=\rho, \kappa, \kappa^*} \int_{\bar{\xi}^i} J^i(\bar{\xi}^i) \hat{\rho}_i(\bar{\xi}^i)}. \end{aligned} \tag{2}$$

$\vec{J} = (J^{\rho}(\bar{\xi}^{\rho}), J^{\kappa}(\bar{\xi}^{\kappa}), J^{\kappa^*}(\bar{\xi}^{\kappa^*}))$  denotes the external source coupled to the respective density fields:

$$\left\{ \hat{\rho}_i(\bar{\xi}^i) \right\}_{i=\rho, \kappa, \kappa^*} = \{ \psi^*(\xi + \epsilon_{\tau}) \psi(\xi), \psi(\xi) \psi(\xi'), \psi^*(\xi') \psi^*(\xi) \}. \tag{3}$$

with the following abbreviated notations for arguments

$$\bar{\xi}^i \equiv \begin{cases} \xi & = (\tau, \mathbf{x}, a) & ; & i = \rho \\ (\xi, \xi') & = (\tau, \mathbf{x}, a, \tau', \mathbf{x}', a') & ; & i = \kappa^{(*)} \end{cases} \tag{4}$$

We emphasize that the pairing fields are introduced as non-local ones with which the present formalism is applicable for describing not only the conventional spin-singlet pairing but any type of pairings as in Ref. [48]; furthermore the UV divergence, which appears in the case of local interactions and local pairings, can be avoided.

Now we define the generating functional for connected correlation functions  $W[\vec{J}]$  by

$$W[\vec{J}] := \ln Z[\vec{J}]. \tag{5}$$

Then the effective action  $\Gamma[\vec{\rho} = (\rho, \kappa, \kappa^*)]$  for the particle-number density  $\rho(\xi)$  as well as non-local pairing densities  $\kappa^{(*)}(\xi, \xi')$  is given by a Legendre transformation of  $W[\vec{J}]$ :

$$\begin{aligned} \Gamma[\vec{\rho}] &= \sup_{\vec{J}} \left( \sum_i \int_{\bar{\xi}^i} J^i(\bar{\xi}^i) \rho_i(\bar{\xi}^i) - W[\vec{J}] \right) \\ &=: \sum_i \int_{\bar{\xi}^i} J_{\text{sup}}^i[\vec{\rho}](\bar{\xi}^i) \rho_i(\bar{\xi}^i) - W[\vec{J}_{\text{sup}}[\vec{\rho}]]. \end{aligned} \tag{6}$$

Here  $\vec{J}_{\text{sup}}[\vec{\rho}]$  denotes the source that gives the supremum of the quantity in the bracket of the first line and gives the expectation value of the density operator  $\hat{\rho}^i$

$$\left. \frac{\delta W[\vec{J}]}{\delta J^i(\bar{\xi}^i)} \right|_{\vec{J}=\vec{J}_{\text{sup}}[\vec{\rho}]} = \rho_i(\bar{\xi}^i) \tag{7}$$

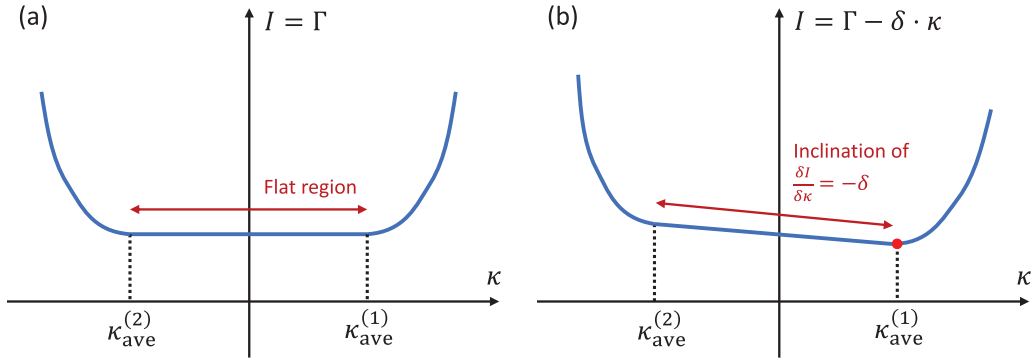
on account of Eqs. (2) and (5).

## 2.2. The Hohenberg–Kohn theorem for superfluid systems

Having defined the effective action by Eq. (6) for superfluid systems in a rather natural way, we are in a position to show one of the most important points in this article, i.e., a proof of the Hohenberg–Kohn theorem for superfluid systems with non-zero temperature [11] on the basis of the effective action without recourse to any heuristic arguments.

### ◦ Variational principle for Eq. (6).

For a proper description of the superfluidity where the SSB is accompanied, it is most convenient to introduce a  $\tau$ -independent artificial external potential  $\mu^{\kappa^{(*)}}(\bar{\xi}^{\kappa^{(*)}})$  coupled to the pairing



**Fig. 1.** Schematic pictures of the  $\kappa$ -dependence of  $I$  in the case of (a) no external potential and (b) small non-zero external potential, where the  $\rho$ -dependence is not depicted. Two different equilibrium pairing densities are denoted by  $\kappa_{\text{ave}}^{(1,2)}$ . In (b),  $\delta$  is an infinitesimally small but non-zero number. Without the external potential,  $\kappa_{\text{ave}}$  is not determined uniquely in the variational way as  $I$  has the same value in the region shown in (a). With a small external field being applied, the equilibrium density [ $\kappa_{\text{ave}}^{(1)}$  in (b)] may be obtained variationally since the flat region is slightly tilted.

density  $\kappa^{(*)}(\bar{\xi}^{\kappa^{(*)}})$ , which will, however, be taken to be zero in the end of calculation. We shall consider a generic case where the chemical potential  $\mu_a$  may depend on the internal degree of freedom  $a$ ; however, notice that the possible spatial dependence of  $\mu_a$  can be neglected without loss of generality because it can be absorbed away into the redefinition of  $V_a(\mathbf{x})$ .

Now under the condition that the external potential  $\delta_{i\rho} \mathcal{V}(\bar{\xi}^\rho) - \mu^i(\bar{\xi}^i)$  is applied to the system, consider the variational problem of the following functional:

$$I[\vec{\rho}] = \Gamma[\vec{\rho}] - \sum_i \int_{\bar{\xi}^i} \mu^i(\bar{\xi}^i) \rho_i(\bar{\xi}^i), \tag{8}$$

where  $\vec{\mu} = (\mu^\rho(\bar{\xi}^\rho), \mu^\kappa(\bar{\xi}^\kappa), \mu^{\kappa^*}(\bar{\xi}^{\kappa^*})) = (\mu_a, \mu^\kappa(\bar{\xi}^\kappa), \mu^{\kappa^*}(\bar{\xi}^{\kappa^*}))$ .

The solution  $\vec{\rho}_{\text{ave}}$  of the variational equation  $\delta I[\vec{\rho}] / \delta \rho_i(\bar{\xi}^i) = 0$  satisfies  $J_{\text{sup}}^i[\vec{\rho}_{\text{ave}}](\bar{\xi}^i) = \mu^i(\bar{\xi}^i)$ , and thus one obtains

$$\rho_{\text{ave},i}(\bar{\xi}^i) = \frac{1}{Z[\vec{\mu}]} \int \mathcal{D}\psi \mathcal{D}\psi^* \hat{\rho}_i(\bar{\xi}^i) e^{-S[\psi, \psi^*] + \sum_{j=\rho, \kappa, \kappa^*} \int_{\bar{\xi}^j} \mu^j(\bar{\xi}^j) \hat{\rho}_j(\bar{\xi}^j)}, \tag{9}$$

by the use of Eqs. (2) and (7). Equation (9) shows that  $\vec{\rho}_{\text{ave}}$  is the average of the density in the equilibrium state in the presence of the external potential  $\delta_{i\rho} \mathcal{V}(\bar{\xi}^\rho) - \mu^i(\bar{\xi}^i)$ .

A remark is in order here: Although the vanishing limit is formally taken for  $\mu^{\kappa^{(*)}}(\bar{\xi}^{\kappa^{(*)}})$ , this limit should be taken with a care when SSB is concerned; it should be interpreted as  $0+$  in the mathematical notation, meaning an infinitesimally small but non-zero value to obtain  $\vec{\rho}_{\text{ave}}$  variationally. Figure 1 shows a schematic picture of  $I[\vec{\rho}]$  solely as a function of  $\kappa$ , say, with  $\rho$  fixed. If we have two solutions,  $\kappa_{\text{ave}}^{(1)}$  and  $\kappa_{\text{ave}}^{(2)}$ , as the pairing density in equilibrium,  $I[\vec{\rho}]$  with  $\mu^{\kappa^{(*)}} = 0$  is actually flat in the interpolated densities [ $\kappa = \alpha \kappa_{\text{ave}}^{(1)} + (1 - \alpha) \kappa_{\text{ave}}^{(2)}$ ,  $0 \leq \alpha \leq 1$ ] since  $\Gamma[\vec{\rho}]$  is a convex functional as a result of the Legendre transformation. This prevents one from determining the equilibrium density uniquely by a variational method. As long as  $\mu^{\kappa^{(*)}}$  is kept small but non-vanishing, however, the flat region of  $I[\vec{\rho}]$  is slightly tilted; then one can uniquely identify the equilibrium density in the variational method.

◦ **One-to-one map between the external fields and the densities.**

From Eq. (6), we obtain

$$\begin{aligned} \Gamma[\vec{\rho}] &= \sup_{\vec{J}} \left( \sum_i \int_{\bar{\xi}^i} J^i(\bar{\xi}^i) \rho_i(\bar{\xi}^i) - W|_{\mathcal{V}=0}[\vec{J} - (\mathcal{V}, 0, 0)] \right) \\ &= \int_{\xi} \mathcal{V}(\xi) \rho(\xi) + \sup_{\vec{J}} \left( \sum_i \int_{\bar{\xi}^i} J^i(\bar{\xi}^i) \rho_i(\bar{\xi}^i) - W|_{\mathcal{V}=0}[\vec{J}] \right) \\ &= \int_{\xi} \mathcal{V}(\xi) \rho(\xi) + \Gamma|_{\mathcal{V}=0}[\vec{\rho}], \end{aligned} \tag{10}$$

where  $W|_{\mathcal{V}=0}[\vec{J}]$  and  $\Gamma|_{\mathcal{V}=0}[\vec{\rho}]$  are defined by the action with vanishing external potential. From the first to second line of Eq. (10), we have shifted  $\vec{J}$  as  $\vec{J} \rightarrow \vec{J} + (\mathcal{V}, 0, 0)$ . This shows that  $\Gamma[\vec{\rho}]$  can be decomposed into the universal part  $\Gamma|_{\mathcal{V}=0}[\vec{\rho}]$  independent of  $\mathcal{V}(\xi)$  and the term depending on  $\mathcal{V}(\xi)$  linearly.

Through Eq. (10) and the variational equation of  $I[\vec{\rho}]$ , the existence of the one-to-one map from  $\vec{\rho}_{\text{ave}}$  to  $\delta_{i\rho} \mathcal{V}(\bar{\xi}^\rho) - \mu^i(\bar{\xi}^i)$  is established. To show this, let us assume that two sets of the external potential and the chemical potential denoted by  $(\mathcal{V}_1, \vec{\mu}_1)$  and  $(\mathcal{V}_2, \vec{\mu}_2)$ , respectively, give the same densities  $\vec{\rho}_{\text{ave}}$ . By use of the variational equation of  $I[\vec{\rho}]$  and Eq. (10), however, we obtain

$$\begin{aligned} \frac{\delta \Gamma|_{\mathcal{V}=0}[\vec{\rho}_{\text{ave}}]}{\delta \rho_i(\bar{\xi}^i)} + \delta_{i\rho} \mathcal{V}_1(\bar{\xi}^\rho) - \mu_1^i(\bar{\xi}^i) &= 0, \\ \frac{\delta \Gamma|_{\mathcal{V}=0}[\vec{\rho}_{\text{ave}}]}{\delta \rho_i(\bar{\xi}^i)} + \delta_{i\rho} \mathcal{V}_2(\bar{\xi}^\rho) - \mu_2^i(\bar{\xi}^i) &= 0. \end{aligned}$$

Subtracting these equations from each other, we have the equality

$$\delta_{i\rho} \mathcal{V}_1(\bar{\xi}^\rho) - \mu_1^i(\bar{\xi}^i) = \delta_{i\rho} \mathcal{V}_2(\bar{\xi}^\rho) - \mu_2^i(\bar{\xi}^i), \tag{11}$$

which proves that  $\delta_{i\rho} \mathcal{V}(\bar{\xi}^\rho) - \mu^i(\bar{\xi}^i)$  is uniquely determined by  $\vec{\rho}_{\text{ave}}$ .

Thus the Hohenberg–Kohn theorem for superfluid systems with non-zero temperature, which was first demonstrated in Ref. [11], is established in terms of the effective action. Furthermore, it is also evident that  $\beta^{-1} \Gamma[\vec{\rho}]$  can be identified with Helmholtz free energy  $F_{\text{H}}[\vec{\rho}]$  at  $\vec{\rho} = \vec{\rho}_{\text{ave}}$  as

$$F_{\text{H}}[\vec{\rho}] = \frac{\Gamma[\vec{\rho}]}{\beta}. \tag{12}$$

In fact, in the limit of  $\mu^{\kappa^{(*)}} \rightarrow 0$ , Eq. (12) at  $\vec{\rho} = \vec{\rho}_{\text{ave}}$  becomes

$$F_{\text{H}}[\vec{\rho}_{\text{ave}}] = \frac{1}{\beta} \int_{\xi} \mu_a \rho_{\text{ave}}(\xi) - \frac{1}{\beta} W[\vec{\mu} = (\mu_a, 0, 0)], \tag{13}$$

because of the relation  $\vec{J}_{\text{sup}}[\vec{\rho}_{\text{ave}}] = \vec{\mu}$  and Eq. (6). In terms of words, since  $Z[\vec{\mu}]$  is the grand partition function in the presence of the chemical potential  $\vec{\mu}$ ,  $-W[\vec{\mu}]/\beta = -\ln Z[\mu]/\beta$  is the grand potential, and hence  $F_{\text{H}}[\vec{\rho}_{\text{ave}}]$  in Eq. (13) is identified with the Helmholtz free energy.

Finally, let us consider the case of a zero-temperature limit. At the zero-temperature limit  $\beta \rightarrow \infty$ ,  $F_{\text{H}}[\vec{\rho}_{\text{ave}}]$  becomes the ground-state energy  $E_{\text{gs}}$  because  $F_{\text{H}}[\vec{\rho}_{\text{ave}}]$  can be written as  $F_{\text{H}}[\vec{\rho}_{\text{ave}}] =$

$-\beta^{-1} \ln \sum_n \exp(-\beta E_n)$ , where  $\{E_n\}$  is the energy eigenvalues of the system and satisfies  $E_{\text{gs}} = E_0 < E_1 < \dots$ . Therefore, we can identify the EDF with the effective action as

$$E[\vec{\rho}] = \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[\vec{\rho}]. \quad (14)$$

In particular, the universal part of the EDF is obtained by the substitution of  $\Gamma$  with  $\Gamma|_{\mathcal{V}=0}$ . This concludes the generalization of the correspondence between the EDF and the effective action to the superfluid systems [27,28,44].

### 2.3. Flow equation

The effective action  $\Gamma[\vec{\rho}]$  contains the whole contents of the physics of the quantum system in a compact form of the functional integral. Although the compact and exact form of the action allows us to define consistent approximations, the problem is developing a computational method to perform the functional integral in a systematic and hopefully exact way. In this subsection, we are going to develop a practical method to calculate the effective action in such a manner.

A wise way originally developed by Wegner [35] and Wilson [36] is to convert the functional integral to a differential equation, which is called a renormalization-group (RG) equation or flow equation, and solve the equation with some systematic approximation being adopted. In the case of the effective action solely for the particle-number density and accordingly without SSB, a calculational framework is developed based on an RG/flow equation in Refs. [39,40]; see also Refs. [44,45]. Here, we generalize this framework to the case with SSB for the calculation of  $\Gamma[\vec{\rho}]$  containing the pairing density fields.

Following Refs. [39,40,44,45], we introduce a regulated two-body interaction  $\mathcal{U}_\lambda(\xi, \xi')$  with a flow parameter  $\lambda$  and define the regulated action as

$$\begin{aligned} S_\lambda[\psi, \psi^*] &= \int_\xi \psi^*(\xi + \epsilon_\tau) \left( \partial_\tau - \frac{\Delta}{2} + \mathcal{V}(\xi) \right) \psi(\xi) \\ &+ \frac{1}{2} \int_{\xi, \xi'} \mathcal{U}_\lambda(\xi, \xi') \psi^*(\xi + \epsilon_\tau) \psi^*(\xi' + \epsilon_\tau) \psi(\xi) \psi(\xi'), \end{aligned} \quad (15)$$

where  $\mathcal{U}_\lambda(\xi, \xi')$  is defined by

$$\mathcal{U}_\lambda(\xi, \xi') = \delta(\tau - \tau') U_{\lambda, aa'}(\mathbf{x} - \mathbf{x}'), \quad (16)$$

with a constraint

$$\begin{aligned} U_{\lambda=0, aa'}(\mathbf{x} - \mathbf{x}') &= 0, \\ U_{\lambda=1, aa'}(\mathbf{x} - \mathbf{x}') &= U_{aa'}(\mathbf{x} - \mathbf{x}'), \end{aligned}$$

so that the action evolves from the free  $S_{\lambda=0}$  to the fully interacting one  $S_{\lambda=1}$  as  $\lambda$  runs from 0 to 1. With this action, the  $\lambda$ -dependent generating functionals and effective action are defined in the same manner as in Sect. 2.1:

$$W_\lambda[\vec{J}] = \ln Z_\lambda[\vec{J}] = \ln \int \mathcal{D}\psi \mathcal{D}\psi^* e^{-S_\lambda[\psi, \psi^*] + \sum_{i=\rho, \kappa, \kappa^*} \int_{\bar{\xi}^i} J^i(\bar{\xi}^i) \hat{\rho}_i(\bar{\xi}^i)}, \quad (17)$$

$$\Gamma_\lambda[\vec{\rho}] = \sup_{\vec{J}} \left( \sum_i \int_{\bar{\xi}^i} J^i(\bar{\xi}^i) \rho_i(\bar{\xi}^i) - W_\lambda[\vec{J}] \right) =: \sum_i \int_{\bar{\xi}^i} J_{\text{sup}, \lambda}^i[\vec{\rho}](\bar{\xi}^i) \rho_i(\bar{\xi}^i) - W_\lambda[\vec{J}_{\text{sup}, \lambda}[\vec{\rho}]], \quad (18)$$



where  $J_{\text{sup},\lambda}^i[\vec{\rho}](\vec{\xi}^i)$  satisfies

$$\left. \frac{\delta W_\lambda[\vec{J}]}{\delta J^i(\vec{\xi}^i)} \right|_{\vec{J}=\vec{J}_{\text{sup},\lambda}[\vec{\rho}](\vec{\xi})} = \rho_i(\vec{\xi}^i). \tag{19}$$

Now utilizing the  $\lambda$ -dependence of the action (18), the flow equation of  $\Gamma_\lambda[\vec{\rho}]$  can be obtained simply by differentiating it with respect to  $\lambda$  [39,40,43–45]. It turns out, however, that the most convenient way to obtain the flow equation for  $\Gamma_\lambda[\vec{\rho}]$  is first to derive that for  $W_\lambda[\vec{J}]$  instead of  $\Gamma_\lambda[\vec{\rho}]$ . The differentiation of  $W_\lambda[\vec{J}]$  with respect to  $\lambda$  reads

$$\partial_\lambda W_\lambda[\vec{J}] = -\frac{1}{2} \int_{\vec{\xi}_1^\rho := (\tau_1, \mathbf{x}_1, a_1), \vec{\xi}_2^\rho := (\tau_2, \mathbf{x}_2, a_2)} \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \langle \psi^*(\vec{\xi}_1^\rho + \epsilon_\tau) \psi^*(\vec{\xi}_2^\rho + \epsilon_\tau) \psi(\vec{\xi}_2^\rho) \psi(\vec{\xi}_1^\rho) \rangle_{\lambda, \vec{J}}, \tag{20}$$

where

$$\langle \mathcal{O}[\psi, \psi^*] \rangle_{\lambda, \vec{J}} := \frac{1}{Z_\lambda[\vec{J}]} \int \mathcal{D}\psi \mathcal{D}\psi^* \mathcal{O}[\psi, \psi^*] e^{-S_\lambda[\psi, \psi^*] + \sum_{i=\rho, \kappa} \int_{\vec{\xi}^i} \vec{J}(\vec{\xi}^i) \hat{\rho}_i(\vec{\xi}^i)}, \tag{21}$$

with  $\mathcal{O}[\psi, \psi^*]$  being some functional of  $\psi$  and  $\psi^*$ . Noting that  $\mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho)$  defined in Eq. (16) involves the delta function of times, the integrand in Eq. (20) can be cast into the form of the density correlation functions with the use of the commutation relation:

$$\begin{aligned} & \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \langle \psi^*(\vec{\xi}_1^\rho + \epsilon_\tau) \psi^*(\vec{\xi}_2^\rho + \epsilon_\tau) \psi(\vec{\xi}_2^\rho) \psi(\vec{\xi}_1^\rho) \rangle_{\lambda, \vec{J}} \\ &= \delta(\tau_1 - \tau_2) \partial_\lambda U_{\lambda, aa'}(\mathbf{x} - \mathbf{x}') \langle \psi^*(\vec{\xi}_1^\rho + \epsilon_\tau) \psi^*(\vec{\xi}_2^\rho + \epsilon_\tau) \psi(\vec{\xi}_2^\rho) \psi(\vec{\xi}_1^\rho) \rangle_{\lambda, \vec{J}} \\ &= \delta(\tau_1 - \tau_2) \partial_\lambda U_{\lambda, aa'}(\mathbf{x} - \mathbf{x}') \left[ \langle \psi^*(\vec{\xi}_1^\rho + \epsilon'_\tau + \epsilon_\tau) \psi(\vec{\xi}_1^\rho + \epsilon'_\tau) \psi^*(\vec{\xi}_2^\rho + \epsilon_\tau) \psi(\vec{\xi}_2^\rho) \rangle_{\lambda, \vec{J}} \right. \\ & \quad \left. - \delta_{a_1, a_2} \langle \psi^*(\vec{\xi}_1^\rho + \epsilon_\tau) \psi(\vec{\xi}_1^\rho) \rangle_{\lambda, \vec{J}} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right], \end{aligned} \tag{22}$$

where an infinitesimal number  $\epsilon'_\tau$  plays the same role as  $\epsilon_\tau$  but its zero limit should be taken after that of  $\epsilon_\tau$ ; see the appendix in Ref. [44]. From Eq. (17), one can immediately see

$$\langle \hat{\rho}_i(\vec{\xi}^i) \rangle_{\lambda, \vec{J}} = \frac{\delta W_\lambda[\vec{J}]}{\delta J_i(\vec{\xi}^i)}, \tag{23}$$

$$\langle \psi^*(\vec{\xi}_1^\rho + \epsilon'_\tau + \epsilon_\tau) \psi(\vec{\xi}_1^\rho + \epsilon'_\tau) \psi^*(\vec{\xi}_2^\rho + \epsilon_\tau) \psi(\vec{\xi}_2^\rho) \rangle_{\lambda, \vec{J}} = \frac{\delta W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_1^\rho)} \frac{\delta W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_2^\rho)} + \frac{\delta^2 W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_1^\rho + \epsilon'_\tau) \delta J_\rho(\vec{\xi}_2^\rho)}. \tag{24}$$

Using these relations, one finds that Eq. (20) takes the form of the flow equation for  $W_\lambda[\vec{J}]$  as follows:

$$\begin{aligned} \partial_\lambda W_\lambda[\vec{J}] &= -\frac{1}{2} \int_{\vec{\xi}_1^\rho, \vec{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \\ & \quad \times \left( \frac{\delta W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_1^\rho)} \frac{\delta W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_2^\rho)} + \frac{\delta^2 W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_1^\rho + \epsilon'_\tau) \delta J_\rho(\vec{\xi}_2^\rho)} - \frac{\delta W_\lambda[\vec{J}]}{\delta J_\rho(\vec{\xi}_1^\rho)} \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right). \end{aligned} \tag{25}$$



Next we shall show that this flow equation is in turn converted to that for  $\Gamma_\lambda[\vec{\rho}]$  on account of Eq. (18). By differentiating Eq. (19) with respect to  $\vec{J}_{\text{sup},\lambda}[\vec{\rho}]$ , we have

$$\frac{\delta^2 W_\lambda[\vec{J}_{\text{sup},\lambda}[\vec{\rho}]]}{\delta J_i(\vec{\xi}_1^i)\delta J_j(\vec{\xi}_2^j)} = \frac{\delta \rho_i(\vec{\xi}_1^i)}{\delta J_j(\vec{\xi}_2^j)} \Big|_{\vec{J}=\vec{J}_{\text{sup},\lambda}[\vec{\rho}]}. \tag{26}$$

By taking the second derivative of Eq. (6) with respect to  $\vec{\rho}$ , we have

$$\frac{\delta^2 \Gamma_\lambda[\vec{\rho}]}{\delta \rho_i(\vec{\xi}_1^i)\delta \rho_j(\vec{\xi}_2^j)} = \frac{\delta J_{\text{sup},\lambda}^j[\vec{\rho}](\vec{\xi}_2^j)}{\delta \rho_i(\vec{\xi}_1^i)}. \tag{27}$$

One finds that Eq. (26) is the inverse of Eq. (27):

$$\frac{\delta^2 W_\lambda[\vec{J}_{\text{sup},\lambda}[\vec{\rho}]]}{\delta J_i(\vec{\xi}_1^i)\delta J_j(\vec{\xi}_2^j)} = \left( \frac{\delta^2 \Gamma_\lambda}{\delta \vec{\rho} \delta \vec{\rho}} \right)^{-1}_{ij} [\vec{\rho}](\vec{\xi}_1^i, \vec{\xi}_2^j). \tag{28}$$

Here,  $(\delta^2 \Gamma_\lambda / \delta \vec{\rho} \delta \vec{\rho})^{-1}_{ij}[\vec{\rho}](\vec{\xi}^i, \vec{\xi}^j)$  is defined as follows:

$$\sum_{k=\rho, \kappa, \kappa^*} \int_{\vec{\xi}^k} \left( \frac{\delta^2 \Gamma_\lambda}{\delta \vec{\rho} \delta \vec{\rho}} \right)^{-1}_{ik} [\vec{\rho}](\vec{\xi}^i, \vec{\xi}^k) \frac{\delta^2 \Gamma_\lambda[\vec{\rho}]}{\delta \rho_k(\vec{\xi}^k) \delta \rho_j(\vec{\xi}^j)} = \delta(\vec{\xi}^i, \vec{\xi}^j), \tag{29}$$

and  $\delta(\vec{\xi}^i, \vec{\xi}^j)$  is defined by

$$\delta(\vec{\xi}^i, \vec{\xi}^j) = \begin{cases} \delta(\xi, \xi') & (i = j = \rho, \vec{\xi}^\rho = \xi, \vec{\xi}^\rho = \xi') \\ \delta(\xi_1, \xi'_1) \delta(\xi_2, \xi'_2) & (i = j = \kappa^*, \vec{\xi}^{\kappa^*} = (\xi_1, \xi_2), \vec{\xi}^{\kappa^*} = (\xi'_1, \xi'_2)), \\ 0 & (\text{otherwise}) \end{cases}$$

with  $\delta(\xi = (\tau, \mathbf{x}, a), \xi' = (\tau', \mathbf{x}', a')) = \delta_{a,a'} \delta(\tau - \tau') \delta(\mathbf{x} - \mathbf{x}')$ . By taking the derivative of Eq. (6) with respect to  $\lambda$ , we obtain

$$\partial_\lambda \Gamma_\lambda[\vec{\rho}] = -(\partial_\lambda W_\lambda)[\vec{J}_{\text{sup},\lambda}[\vec{\rho}]]. \tag{30}$$

Substituting Eqs. (19), (28), and (30) into Eq. (25), we eventually arrive at the formal flow equation for  $\Gamma_\lambda[\vec{\rho}]$ :

$$\begin{aligned} \partial_\lambda \Gamma_\lambda[\vec{\rho}] &= \frac{1}{2} \int_{\vec{\xi}_1^\rho=(\tau_1, \mathbf{x}_1, a_1), \vec{\xi}_2^\rho=(\tau_2, \mathbf{x}_2, a_2)} \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \\ &\times \left[ \rho(\vec{\xi}_1^\rho) \rho(\vec{\xi}_2^\rho) + \left( \frac{\delta^2 \Gamma_\lambda}{\delta \vec{\rho} \delta \vec{\rho}} \right)^{-1}_{\rho\rho} [\vec{\rho}](\vec{\xi}_1^\rho + \epsilon'_\tau, \vec{\xi}_2^\rho) - \rho(\vec{\xi}_1^\rho) \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right]. \end{aligned} \tag{31}$$

Now Eqs. (24) and (28) together with Eq. (19) tell us that  $[(\delta^2\Gamma_\lambda)/(\delta\bar{\rho}\delta\bar{\rho})]_{\rho\rho}^{-1}$  gives essentially the correlation functions of the densities  $\bar{\rho}$ , which collectively denote the particle-number and pairing densities. To see more explicitly the physical contents of the flow equation (31), in particular, the contributions of the pairing densities, we find it convenient to separate the  $\lambda = 0$  part of the correlation function where the particle operators are free ones:

$$\begin{aligned} & \left(\frac{\delta^2\Gamma_\lambda}{\delta\bar{\rho}\delta\bar{\rho}}\right)_{\rho\rho}^{-1} [\bar{\rho}](\bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) - \rho(\bar{\xi}_1^\rho)\delta_{a_1,a_2}\delta(\mathbf{x}_1 - \mathbf{x}_2) \\ &= \langle \psi^*(\bar{\xi}_1^\rho + \epsilon_\tau + \epsilon'_\tau)\psi(\bar{\xi}_1^\rho + \epsilon'_\tau)\psi^*(\bar{\xi}_2^\rho + \epsilon_\tau)\psi(\bar{\xi}_2^\rho) \rangle_{\lambda, \vec{j}_{\text{sup},\lambda}[\bar{\rho}]} - \rho(\bar{\xi}_1^\rho + \epsilon'_\tau)\rho(\bar{\xi}_2^\rho) \\ & \quad - \rho(\bar{\xi}_1^\rho)\delta_{a_1,a_2}\delta(\mathbf{x}_1 - \mathbf{x}_2) \\ &= \langle \psi^*(\bar{\xi}_1^\rho + \epsilon_\tau + \epsilon'_\tau)\psi(\bar{\xi}_1^\rho + \epsilon'_\tau)\psi^*(\bar{\xi}_2^\rho + \epsilon_\tau)\psi(\bar{\xi}_2^\rho) \rangle_{\lambda=0, \vec{j}_{\text{sup},\lambda=0}[\bar{\rho}]} - \rho(\bar{\xi}_1^\rho + \epsilon'_\tau)\rho(\bar{\xi}_2^\rho) \\ & \quad - \rho(\bar{\xi}_1^\rho)\delta_{a_1,a_2}\delta(\mathbf{x}_1 - \mathbf{x}_2) + \mathcal{O}(\lambda). \end{aligned}$$

By applying the Wick's theorem, we obtain

$$\begin{aligned} & \left(\frac{\delta^2\Gamma_\lambda}{\delta\bar{\rho}\delta\bar{\rho}}\right)_{\rho\rho}^{-1} [\bar{\rho}](\bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) - \rho(\bar{\xi}_1^\rho)\delta_{a_1,a_2}\delta(\mathbf{x}_1 - \mathbf{x}_2) \\ &= \kappa^*(\bar{\xi}_{12}^{\kappa*})\kappa(\bar{\xi}_{12}^\kappa)|_{\bar{\xi}_{12}^{\kappa(*)}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \\ & \quad - \langle \psi^*(\bar{\xi}_1^\rho + \epsilon_\tau + \epsilon'_\tau)\psi(\bar{\xi}_2^\rho) \rangle_{\lambda=0, \vec{j}_{\text{sup},\lambda=0}[\bar{\rho}]} \langle \psi^*(\bar{\xi}_2^\rho + \epsilon_\tau)\psi(\bar{\xi}_1^\rho + \epsilon'_\tau) \rangle_{\lambda=0, \vec{j}_{\text{sup},\lambda=0}[\bar{\rho}]} \\ & \quad - \rho(\bar{\xi}_1^\rho)\delta_{a_1,a_2}\delta(\mathbf{x}_1 - \mathbf{x}_2) + \mathcal{O}(\lambda), \end{aligned} \tag{32}$$

where we have used the equality  $\langle \hat{\rho}_i(\bar{\xi}^i) \rangle_{\lambda, \vec{j}_{\text{sup},\lambda}[\bar{\rho}]} = \rho_i(\bar{\xi}^i)$  which follows from Eqs. (23) and (19). One sees that the first term given by a product of the pairing condensates in Eq. (32) is the counterpart to that of the particle-number densities given in the first term of Eq. (31), while the terms in the second line and the remaining order- $\lambda$  terms are identified with the exchange and correlation terms, respectively. Thus one finds that it is natural to represent Eq. (31) in a form where the terms with different physical significance are written separately, as,

$$\begin{aligned} \partial_\lambda \Gamma_\lambda[\bar{\rho}] &= \frac{1}{2} \int_{\bar{\xi}_1^\rho=(\tau_1, \mathbf{x}_1, a_1), \bar{\xi}_2^\rho=(\tau_2, \mathbf{x}_2, a_2)} \partial_\lambda \mathcal{U}_\lambda(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\ & \quad \times \left[ \rho(\bar{\xi}_1^\rho)\rho(\bar{\xi}_2^\rho) + \kappa^*(\bar{\xi}_{12}^{\kappa*})\kappa(\bar{\xi}_{12}^\kappa)|_{\bar{\xi}_{12}^{\kappa(*)}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} + G_{\text{xc},\lambda}^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \right], \end{aligned} \tag{33}$$

where  $G_{\text{xc},\lambda}^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)$  denotes the exchange–correlation term given by

$$G_{\text{xc},\lambda}^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) = G_x^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) + G_{c,\lambda}^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho), \tag{34}$$

with

$$\begin{aligned} G_x^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) &= \left(\frac{\delta^2\Gamma_{\lambda=0}}{\delta\bar{\rho}\delta\bar{\rho}}\right)_{\rho\rho}^{-1} [\bar{\rho}](\bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) - \kappa^*(\bar{\xi}_{12}^{\kappa*})\kappa(\bar{\xi}_{12}^\kappa)|_{\bar{\xi}_{12}^{\kappa(*)}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \\ & \quad - \rho(\bar{\xi}_1^\rho)\delta_{a_1,a_2}\delta(\mathbf{x}_1 - \mathbf{x}_2), \end{aligned} \tag{35}$$

$$G_{c,\lambda}^{(2)}[\vec{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) = \left( \frac{\delta^2 \Gamma_\lambda}{\delta \vec{\rho} \delta \vec{\rho}} \right)_{\rho\rho}^{-1} [\vec{\rho}](\bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) - \left( \frac{\delta^2 \Gamma_{\lambda=0}}{\delta \vec{\rho} \delta \vec{\rho}} \right)_{\rho\rho}^{-1} [\vec{\rho}](\bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho). \quad (36)$$

We call  $G_x^{(2)}[\vec{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)$  and  $G_{c,\lambda}^{(2)}[\vec{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)$  the exchange and correlation terms, respectively.

We note that the flow equation gives the systematic way to calculate the higher-order contribution for  $\Gamma_\lambda[\vec{\rho}]$ , or  $G_{c,\lambda}^{(2)}[\vec{\rho}]$ , since it is not only an exact but also closed equation for  $\Gamma_\lambda[\vec{\rho}]$ . Moreover, it also provides us with the basis for defining consistent approximations, say, respecting symmetries, if necessary. In this respect, some approximation schemes developed for the study of the normal phase such as the vertex expansion [39,40] is expected to be utilized for the determination of  $\Gamma_\lambda[\vec{\rho}]$  also in the case of superfluid systems.

#### 2.4. Expressions of Helmholtz free energy and ground-state energy

Having derived the flow equation (33) for the effective action  $\Gamma_\lambda[\vec{\rho}]$ , we here give a reduced formula for the Helmholtz free energy which is given in terms of the effective action.

The Helmholtz free energy given in Eq. (12) now takes the form

$$F_H[\vec{\rho}_{\text{ave}}] = \frac{\Gamma_{\lambda=1}[\vec{\rho}_{\text{ave}}]}{\beta}, \quad (37)$$

where  $\vec{\rho}_{\text{ave}}$  is the equilibrium density of the fully-interacting ( $\lambda = 1$ ) system in the presence of a given chemical potential  $\vec{\mu}$ :

$$\rho_{\text{ave},i}(\bar{\xi}^i) = \frac{1}{Z_{\lambda=1}[\vec{\mu}]} \int \mathcal{D}\psi \mathcal{D}\psi^* \hat{\rho}_i(\bar{\xi}^i) e^{-S_{\lambda=1}[\psi, \psi^*] + \sum_{j=\rho, \kappa, \kappa^*} \int_{\bar{\xi}_1^j} \mu^j(\bar{\xi}_1^j) \hat{\rho}_j(\bar{\xi}_1^j)}, \quad (38)$$

which is nothing but Eq. (9) with a replacement of  $Z[\vec{\mu}] \rightarrow Z_{\lambda=1}[\vec{\mu}]$ . The expression for  $\Gamma_{\lambda=1}[\vec{\rho}_{\text{ave}}]$  is obtained by integrating Eq. (33) with respect to  $\lambda$ . Inserting the expression into Eq. (37) and using Eq. (10) for  $\Gamma_{\lambda=0}$ , we have

$$\begin{aligned} F_H[\vec{\rho}_{\text{ave}}] &= \frac{\Gamma_{\lambda=0}|_{\mathcal{V}=0}[\vec{\rho}_{\text{ave}}]}{\beta} + \frac{1}{\beta} \int_{\xi} \mathcal{V}(\xi) \rho_{\text{ave}}(\xi) \\ &+ \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \left[ \rho_{\text{ave}}(\bar{\xi}_1^\rho) \rho_{\text{ave}}(\bar{\xi}_2^\rho) + \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{\kappa^*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^{\kappa}) \Big|_{\bar{\xi}_{12}^{(\kappa^*)} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \right] \\ &+ \int_0^1 d\lambda \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) G_{xc,\lambda}^{(2)}[\vec{\rho}_{\text{ave}}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho). \end{aligned} \quad (39)$$

The ground-state energy is obtained by taking the zero-temperature limit in Eq. (39):

$$\begin{aligned} E_{\text{gs}} &= \lim_{\beta \rightarrow \infty} F_H[\vec{\rho}_{\text{ave}}] \\ &= T[\vec{\rho}_{\text{gs}}] + \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_{\xi} \mathcal{V}(\xi) \rho_{\text{ave}}(\xi) \\ &+ \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \left[ \rho_{\text{ave}}(\bar{\xi}_1^\rho) \rho_{\text{ave}}(\bar{\xi}_2^\rho) + \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{\kappa^*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^{\kappa}) \Big|_{\bar{\xi}_{12}^{(\kappa^*)} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \right] \\ &+ \lim_{\beta \rightarrow \infty} \int_0^1 d\lambda \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) G_{xc,\lambda}^{(2)}[\vec{\rho}_{\text{ave}}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho), \end{aligned} \quad (40)$$

where  $T[\vec{\rho}_{\text{gs}}] := \lim_{\beta \rightarrow \infty} \Gamma_{\lambda=0|_{\nu=0}}[\vec{\rho}_{\text{ave}}]/\beta$ , with  $\vec{\rho}_{\text{gs}} := \lim_{\beta \rightarrow \infty} \vec{\rho}_{\text{ave}}$  being the ground-state density, is interpreted as the kinetic energy. Notice that  $T[\vec{\rho}_{\text{gs}}]$  is neither the kinetic energy of a free gas nor that of the interacting system, but that of the non-interacting system with an appropriate potential, as may be utilized in KS formalism. Indeed, we shall show in the following subsection that the KS theory for superfluid systems at finite temperature emerges naturally in the present formalism.

### 2.5. The Kohn–Sham potential

In our formulation of the FRG-DFT theory for superfluid systems, the starting action with  $\lambda = 0$  is that for a non-interacting system with the external forces ensuring the densities. Thus it is natural that  $\vec{J}_{\text{sup},\lambda}[\vec{\rho}]$  is related to the KS potential  $\vec{V}_{\text{KS}}[\vec{\rho}]$  that is generalized so as to incorporate the anomalous or pair potentials besides the normal ones: The KS potential is defined by the derivative of the EDF subtracted by the non-interacting kinetic energy part at zero temperature. In terms of the effective action at finite temperature, the kinetic energy part  $T_{\text{KS}}[\vec{\rho}]$  may be identified with  $\Gamma_{\lambda=0|_{\nu=0}}$ , and then we naturally arrive at the definition of the KS potential as

$$\mathcal{V}_{\text{KS}}^i[\vec{\rho}](\vec{\xi}^i) = \frac{\delta}{\delta \rho_i(\vec{\xi}^i)} (\Gamma_{\lambda=1}[\vec{\rho}] - \Gamma_{\lambda=0|_{\nu=0}}[\vec{\rho}]). \quad (41)$$

By differentiating Eq. (18) with respect to the densities, we obtain

$$\frac{\delta \Gamma_{\lambda}[\vec{\rho}]}{\delta \rho_i(\vec{\xi}^i)} = J_{\text{sup},\lambda}^i[\vec{\rho}](\vec{\xi}^i). \quad (42)$$

Using this relation and Eq. (10) for  $\Gamma = \Gamma_{\lambda=0}$ , Eq. (41) is rewritten as follows:

$$\mathcal{V}_{\text{KS}}^i[\vec{\rho}](\vec{\xi}^i) = \delta_{i\rho} \mathcal{V}(\vec{\xi}^i) + J_{\text{sup},\lambda=1}^i[\vec{\rho}] - J_{\text{sup},\lambda=0}^i[\vec{\rho}]. \quad (43)$$

The KS potential determines  $\vec{\rho}_{\text{ave}}$  for given chemical potentials  $\vec{\mu}$ : Since  $J_{\text{sup},\lambda=1}^i[\vec{\rho}_{\text{ave}}](\vec{\xi}^i) = \mu^i(\vec{\xi}^i)$  is satisfied, Eq. (43) at  $\vec{\rho} = \vec{\rho}_{\text{ave}}$  reads

$$\frac{\delta \Gamma_{\lambda=0|_{\nu=0}}[\vec{\rho}_{\text{ave}}]}{\delta \rho_i(\vec{\xi}^i)} + \mathcal{V}_{\text{KS}}^i[\vec{\rho}_{\text{ave}}](\vec{\xi}^i) = \mu^i(\vec{\xi}^i), \quad (44)$$

which is equivalent to the variational equation in the KS DFT [49] and determines  $\vec{\rho}_{\text{ave}}$  from the KS potential (41). Although the variational equation (44) has been derived only in terms of the densities, the practical solution to the equation may utilize the notion of single-particle orbitals as is done in Ref. [8]. Note that Eq. (44) does possess the property of a self-consistency in terms of the densities. In fact, the equilibrium density of the fully interacting system with a given chemical potential  $\vec{\mu}$  is also the equilibrium density of the non-interacting system under the external potential  $\vec{\mu} - \vec{V}_{\text{KS}}[\vec{\rho}_{\text{ave}}]$ , as we will now show explicitly: First of all, we notice that Eq. (44) is also expressed as  $J_{\text{sup},\lambda=0}^i[\vec{\rho}_{\text{ave}}](\vec{\xi}^i) = \delta_{i\rho} \mathcal{V}(\vec{\xi}^i) + \mu^i(\vec{\xi}^i) - \mathcal{V}_{\text{KS}}^i[\vec{\rho}_{\text{ave}}](\vec{\xi}^i)$  on account of the relation  $J_{\text{sup},\lambda=1}^i[\vec{\rho}_{\text{ave}}](\vec{\xi}^i) = \mu^i(\vec{\xi}^i)$  and Eq. (43). Inserting this relation into Eqs. (17) and (19), one finds that Eq. (19) tells us that the equilibrium density  $\vec{\rho}_{\text{ave}}$  in Eq. (38) also has the following expression:

$$\rho_{\text{ave},i}(\vec{\xi}^i) = \frac{1}{Z_{\lambda=0|_{\nu=0}}[\vec{\mu} - \vec{V}_{\text{KS}}[\vec{\rho}_{\text{ave}}]]} \int \mathcal{D}\psi \mathcal{D}\psi^* \hat{\rho}_i(\vec{\xi}^i) \times e^{-S_{\lambda=0|_{\nu=0}}[\psi^*, \psi] + \sum_{j=\rho, \kappa, \kappa^*} \int_{\vec{\xi}_1^j} (\mu^j(\vec{\xi}_1^j) - \mathcal{V}_{\text{KS}}^j[\vec{\rho}_{\text{ave}}](\vec{\xi}_1^j)) \hat{\rho}_j(\vec{\xi}_1^j)}, \quad (45)$$

where  $Z_\lambda|_{\mathcal{V}=0}[\vec{J}]$  is defined by the action  $S_\lambda|_{\mathcal{V}=0}[\psi^*, \psi]$  with no external potential in Eq. (17). Note that Eq. (45) is a self-consistent equation for  $\vec{\rho}_{\text{ave}}$  since  $\vec{\mathcal{V}}_{\text{KS}}[\vec{\rho}_{\text{ave}}]$  in the right-hand side depends on  $\vec{\rho}_{\text{ave}}$  in the left-hand side, as noted before.

Next, let us reduce the exact expression of the central quantity  $\vec{\mathcal{V}}_{\text{KS}}[\vec{\rho}]$  in our formalism in a more calculable form from the flow equation (33). After differentiating Eq. (33) with respect to  $\vec{\rho}$  and then integrating it with respect to  $\lambda$ , we have

$$\begin{aligned} J_{\text{sup},\lambda=1}^i[\vec{\rho}](\vec{\xi}^i) &= J_{\text{sup},\lambda=0}^i[\vec{\rho}](\vec{\xi}^i) + \delta_{i,\rho} \int_{\vec{\xi}_1^\rho} \mathcal{U}_{\lambda=1}(\vec{\xi}^\rho, \vec{\xi}_1^\rho) \rho(\vec{\xi}_1^\rho) + \frac{\delta_{i,\kappa}}{2} \bar{\mathcal{U}}_{\lambda=1}(\vec{\xi}^{\kappa*}) \kappa^*(\vec{\xi}^{\kappa*}) \\ &+ \frac{\delta_{i,\kappa*}}{2} \bar{\mathcal{U}}_{\lambda=1}(\vec{\xi}^\kappa) \kappa(\vec{\xi}^\kappa) + \frac{1}{2} \int_0^1 d\lambda \int_{\vec{\xi}_1^\rho, \vec{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \frac{\delta G_{\text{xc},\lambda}^{(2)}[\vec{\rho}](\vec{\xi}_1^\rho, \vec{\xi}_2^\rho)}{\delta \rho_i(\vec{\xi}^i)}, \end{aligned} \quad (46)$$

where  $\bar{\mathcal{U}}_\lambda(\vec{\xi}^{\kappa*}) := (\xi, \xi') = \mathcal{U}_\lambda(\xi, \xi')$  and Eq. (42) has been used. With use of Eq. (43), we finally arrive at the following expression for  $\vec{\mathcal{V}}_{\text{KS}}[\vec{\rho}]$ :

$$\begin{aligned} \mathcal{V}_{\text{KS}}^i[\vec{\rho}](\vec{\xi}^i) &= \delta_{i,\rho} \mathcal{V}(\vec{\xi}^\rho) + \delta_{i,\rho} \int_{\vec{\xi}_1^\rho} \mathcal{U}_{\lambda=1}(\vec{\xi}^\rho, \vec{\xi}_1^\rho) \rho(\vec{\xi}_1^\rho) \\ &+ \left( \frac{\delta_{i,\kappa}}{2} \bar{\mathcal{U}}_{\lambda=1}(\vec{\xi}^{\kappa*}) \kappa^*(\vec{\xi}^{\kappa*}) + \frac{\delta_{i,\kappa*}}{2} \bar{\mathcal{U}}_{\lambda=1}(\vec{\xi}^\kappa) \kappa(\vec{\xi}^\kappa) \right) \\ &+ \frac{1}{2} \int_0^1 d\lambda \int_{\vec{\xi}_1^\rho, \vec{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \frac{\delta G_{\text{xc},\lambda}^{(2)}[\vec{\rho}](\vec{\xi}_1^\rho, \vec{\xi}_2^\rho)}{\delta \rho_i(\vec{\xi}^i)}. \end{aligned} \quad (47)$$

It is noteworthy that  $\mathcal{V}_{\text{KS}}^i[\vec{\rho}]$  is now naturally decomposed into four terms, which denote the external, Hartree, pairing, and exchange–correlation terms, respectively. In particular, a microscopic expression of the exchange–correlation term  $\mathcal{V}_{\text{KS,xc}}^i[\vec{\rho}]$  is explicitly given in terms of  $G_{\text{xc},\lambda}^{(2)}[\vec{\rho}]$ :

$$\mathcal{V}_{\text{KS,xc}}^i[\vec{\rho}](\vec{\xi}^i) = \frac{1}{2} \int_0^1 d\lambda \int_{\vec{\xi}_1^\rho, \vec{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\vec{\xi}_1^\rho, \vec{\xi}_2^\rho) \frac{\delta G_{\text{xc},\lambda}^{(2)}[\vec{\rho}](\vec{\xi}_1^\rho, \vec{\xi}_2^\rho)}{\delta \rho_i(\vec{\xi}^i)}. \quad (48)$$

We emphasize that our FRG-DFT formalism applied to superfluid systems has naturally led to the self-consistent equation for the densities that are kept the same between the non-interacting and interacting systems together with the microscopic expressions of the KS potential and the kinetic energy without recourse to notions of single-particle orbitals. It is also noted here that the effective action formalism with the inversion method was applied to a microscopic construction of the KS potential for a normal system [50] and a superfluid system of the local singlet pairs [33]. However, the exact expression of the KS potential is not derived in the inversion method. Furthermore, the single-particle basis are introduced in developing the KS DFT.<sup>1</sup>

In the next section, we are going to show that Eq. (39) together with Eqs. (44) and (47) leads to the ground-state energy in the Hartree–Fock–Bogoliubov approximation, which is furthermore reduced to the well-known gap equations of BCS theory in the case of short-range interaction.

<sup>1</sup> In Ref. [34], it was anticipated that the KS DFT may be constructed without single-particle orbitals in the FRG-DFT.

### 3. Analysis in the lowest order approximation: neglect of correlations

We demonstrate that our formalism actually reproduces the results of the mean field theory at the lowest-order truncation, implying that  $G_{xc,\lambda}^{(2)}$  does not have  $\lambda$  dependence:  $G_{xc,\lambda}^{(2)} \approx G_x^{(2)}$ .

#### 3.1. The case of a generic interaction

Applying the lowest-order truncation to Eq. (47), we have

$$\begin{aligned} \mathcal{V}_{\text{KS}}^i[\bar{\rho}](\bar{\xi}^i) &= \delta_{i,\rho} \left( \mathcal{V}(\bar{\xi}^\rho) + \int_{\bar{\xi}_1^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}^\rho, \bar{\xi}_1^\rho) \rho(\bar{\xi}_1^\rho) \right) + \frac{\delta_{i,\kappa}}{2} \bar{\mathcal{U}}_{\lambda=1}(\bar{\xi}^\kappa) \kappa^*(\bar{\xi}^\kappa) \\ &+ \frac{\delta_{i,\kappa^*}}{2} \bar{\mathcal{U}}_{\lambda=1}(\bar{\xi}^{\kappa^*}) \kappa(\bar{\xi}^{\kappa^*}) + \frac{1}{2} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \partial_\lambda \mathcal{U}_\lambda(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \frac{\delta G_x^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)}{\delta \rho_i(\bar{\xi}^i)}, \end{aligned} \quad (49)$$

for the KS potential. On account of Eq. (35),  $\delta G_x^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)/\delta \rho_i(\bar{\xi}^i)$  is represented as follows:

$$\begin{aligned} &\frac{\delta G_x^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)}{\delta \rho_i(\bar{\xi}^i)} \\ &= - \sum_{i_1', i_2'} \int_{\bar{\xi}_2^{i_1'}, \bar{\xi}_2^{i_2'}} \Gamma_{\lambda=0, \rho i_1'}^{(2)-1}[\bar{\rho}](\bar{\xi}_1^\rho + \epsilon'_t, \bar{\xi}_1^{i_1'}) \Gamma_{\lambda=0, \rho i_2'}^{(2)-1}[\bar{\rho}](\bar{\xi}_2^\rho, \bar{\xi}_2^{i_2'}) \Gamma_{\lambda=0, i_1' i_2'}^{(3)}[\bar{\rho}](\bar{\xi}^i, \bar{\xi}_1^{i_1'}, \bar{\xi}_2^{i_2'}) \\ &- \delta(\bar{\xi}^i, \bar{\xi}_{12}^\kappa) \kappa^*(\bar{\xi}_{12}^{\kappa^*}) \Big|_{\bar{\xi}_{12}^{(\kappa^*)} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} - \delta(\bar{\xi}^i, \bar{\xi}_{12}^{\kappa^*}) \kappa(\bar{\xi}_{12}^\kappa) \Big|_{\bar{\xi}_{12}^{(\kappa)} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} - \delta(\bar{\xi}^i, \bar{\xi}_1^\rho) \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2). \end{aligned} \quad (50)$$

Here, the following notation has been introduced:

$$\Gamma_{\lambda, i_1 \dots i_n}^{(n)}[\bar{\rho}](\bar{\xi}_1^{i_1}, \dots, \bar{\xi}_n^{i_n}) := \frac{\delta^n \Gamma_\lambda[\bar{\rho}]}{\delta \rho_{i_1}(\bar{\xi}_1^{i_1}) \dots \delta \rho_{i_n}(\bar{\xi}_n^{i_n})},$$

and  $\Gamma_{\lambda, ij}^{(2)-1}[\bar{\rho}](\bar{\xi}^i, \bar{\xi}^j)$  is equivalent to  $(\delta^2 \Gamma_\lambda / \delta \bar{\rho} \delta \bar{\rho})_{ij}^{-1}[\bar{\rho}](\bar{\xi}^i, \bar{\xi}^j)$  defined in Eq. (29).  $\Gamma_{\lambda=0}^{(n \geq 2)}$  are expressed in terms of the density correlation functions of the non-interacting system, which can be further reduced to simpler forms using the Wick's theorem. When the superfluidity is not considered [43,44],  $\Gamma_\lambda^{(n \geq 2)}$  are also written in terms of the connected density correlation functions. We are going to extend them so as to incorporate the anomalous density correlation functions as

$$\Gamma_{\lambda, i_1 i_2}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1}, \bar{\xi}_2^{i_2}) = G_{\lambda, i_1 i_2}^{(2)-1}[\bar{\rho}](\bar{\xi}_1^{i_1}, \bar{\xi}_2^{i_2}), \quad (51)$$

$$\begin{aligned} \Gamma_{\lambda, i_1 i_2 i_3}^{(3)}[\bar{\rho}](\bar{\xi}_1^{i_1}, \bar{\xi}_2^{i_2}, \bar{\xi}_3^{i_3}) &= - \sum_{i_4, i_5, i_6} \int_{\bar{\xi}_4^{i_4}, \bar{\xi}_5^{i_5}, \bar{\xi}_6^{i_6}} G_{\lambda, i_1 i_4}^{(2)-1}[\bar{\rho}](\bar{\xi}_1^{i_1}, \bar{\xi}_4^{i_4}) G_{\lambda, i_2 i_5}^{(2)-1}[\bar{\rho}](\bar{\xi}_2^{i_2}, \bar{\xi}_5^{i_5}) \\ &\times G_{\lambda, i_3 i_6}^{(2)-1}[\bar{\rho}](\bar{\xi}_3^{i_3}, \bar{\xi}_6^{i_6}) G_{\lambda, i_4 i_5 i_6}^{(3)}[\bar{\rho}](\bar{\xi}_4^{i_4}, \bar{\xi}_5^{i_5}, \bar{\xi}_6^{i_6}), \end{aligned} \quad (52)$$

where  $G_{\lambda, i_1 \dots i_n}^{(n)}$  ( $\bar{\xi}_1^{i_1}, \dots, \bar{\xi}_n^{i_n}$ ) is the connected correlation function given by

$$G_{\lambda, i_1 \dots i_n}^{(n)}[\bar{\rho}](\bar{\xi}_1^{i_1}, \dots, \bar{\xi}_n^{i_n}) = \frac{\delta^n W_\lambda[\vec{J}_{\text{sup}, \lambda}[\bar{\rho}]]}{\delta J_{i_1}(\bar{\xi}_1^{i_1}) \dots \delta J_{i_n}(\bar{\xi}_n^{i_n})},$$

and  $G_{\lambda=0, i_1 i_2}^{(2)-1}(\bar{\xi}_1^{i_1}, \bar{\xi}_2^{i_2})$  satisfies

$$\sum_{i_3} \int_{\bar{\xi}_3^{i_3}} G_{\lambda, i_1 i_3}^{(2)-1}[\bar{\rho}](\bar{\xi}_1^{i_1}, \bar{\xi}_3^{i_3}) G_{\lambda, i_3 i_2}^{(2)}[\bar{\rho}](\bar{\xi}_3^{i_3}, \bar{\xi}_2^{i_2}) = \delta(\bar{\xi}_1^{i_1}, \bar{\xi}_2^{i_2}).$$

Using these relations, the last term in the right-hand side of Eq. (49) is rewritten as follows:

$$\begin{aligned}
 & \frac{1}{2} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \frac{\delta G_x^{(2)}[\bar{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)}{\delta \rho_i(\bar{\xi}^i)} \\
 &= \frac{1}{2} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \left[ \sum_{i_1'} \int_{\bar{\xi}_1^{i_1'}} G_{\lambda=0, i_1'}^{(2)-1}[\bar{\rho}](\bar{\xi}^i, \bar{\xi}^{i_1'}) G_{\lambda=0, i_1', \rho\rho}^{(3)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) \right. \\
 & \quad \left. - \delta(\bar{\xi}_1^i, \bar{\xi}_{12}^k) \kappa^*(\bar{\xi}_{12}^{k*}) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} - \delta(\bar{\xi}^i, \bar{\xi}_{12}^{k*}) \kappa(\bar{\xi}_{12}^k) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} - \delta(\bar{\xi}^i, \bar{\xi}_1^\rho) \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right] \\
 &= \frac{1}{2} \sum_{i_1'} \int_{\bar{\xi}_1^{i_1'}} G_{\lambda=0, i_1'}^{(2)-1}[\bar{\rho}](\bar{\xi}^i, \bar{\xi}^{i_1'}) \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\
 & \quad \times \left[ G_{\lambda=0, i_1', \rho\rho}^{(3)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) - G_{\lambda=0, i_1', \kappa}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_{12}^k) \kappa^*(\bar{\xi}_{12}^{k*}) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \right. \\
 & \quad \left. - G_{\lambda=0, i_1', \kappa^*}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_{12}^{k*}) \kappa(\bar{\xi}_{12}^k) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} - G_{\lambda=0, i_1', \rho}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_2^\rho) \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right]. \tag{53}
 \end{aligned}$$

By use of the Wick's theorem,  $G_{\lambda=0, i_1', \rho\rho}^{(3)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho)$  is evaluated as follows:

$$\begin{aligned}
 & G_{\lambda=0, i_1', \rho\rho}^{(3)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) \\
 &= \langle \psi^*(\xi_1) \psi^*(\xi_2 + \epsilon'_\tau) \rangle_{\bar{\rho}} \left( \langle \psi(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\
 & \quad + \langle \psi(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \left( \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi^*(\xi_2) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi^*(\xi_2) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\
 & \quad - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \left( \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\
 & \quad - \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \left( \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\
 &= \kappa^*(\bar{\xi}_{12}^{k*}) G_{\lambda=0, i_1', \kappa}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_{12}^k) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} + \kappa(\bar{\xi}_{12}^k) G_{\lambda=0, i_1', \kappa^*}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_{12}^{k*}) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\
 & \quad - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \left( \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\
 & \quad - \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \left( \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right).
 \end{aligned}$$

Here, we have introduced

$$\langle \mathcal{O}[\psi, \psi^*] \rangle_{\bar{\rho}} := \langle \mathcal{O}[\psi, \psi^*] \rangle_{\lambda=0, \vec{j}_{\text{sup}}, \lambda=0[\bar{\rho}]}, \tag{54}$$

the right-hand side of which is defined by Eq. (21) for a functional  $\mathcal{O}[\psi, \psi^*]$ . The integral with respect to  $\bar{\xi}_1^\rho$  and  $\bar{\xi}_2^\rho$  in Eq. (53) is then evaluated as follows:

$$\begin{aligned}
 & \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \left[ G_{\lambda=0, i_1', \rho\rho}^{(3)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_1^\rho + \epsilon'_\tau, \bar{\xi}_2^\rho) \right. \\
 & \quad - G_{\lambda=0, i_1', \kappa}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_{12}^k) \kappa^*(\bar{\xi}_{12}^{k*}) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} - G_{\lambda=0, i_1', \kappa^*}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_{12}^{k*}) \kappa(\bar{\xi}_{12}^k) \Big|_{\bar{\xi}_{12}^{k*}=(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\
 & \quad \left. - G_{\lambda=0, i_1', \rho}^{(2)}[\bar{\rho}](\bar{\xi}_1^{i_1'}, \bar{\xi}_1^\rho) \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right]
 \end{aligned}$$



$$\begin{aligned}
 &= -2 \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \\
 &\quad \times \left( \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right), \tag{55}
 \end{aligned}$$

where we have used the equal-time commutation relation:

$$\begin{aligned}
 \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} &= \delta(\tau_1 - \tau_2) U_{\lambda, a_1 a_2}(\mathbf{x}_1 - \mathbf{x}_2) \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \\
 &= \delta(\tau_1 - \tau_2) U_{\lambda, a_1 a_2}(\mathbf{x}_1 - \mathbf{x}_2) \left( \langle \psi^*(\xi_1) \psi(\xi_2 + \epsilon'_\tau) \rangle_{\bar{\rho}} \right. \\
 &\quad \left. - \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right).
 \end{aligned}$$

Substituting Eq. (55) into Eq. (53), we have

$$\begin{aligned}
 \mathcal{V}_{\text{KS}}^i[\vec{\rho}](\bar{\xi}^i) &= \delta_{i, \rho} \left( \mathcal{V}(\bar{\xi}^\rho) + \int_{\bar{\xi}_1^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}^\rho, \bar{\xi}_1^\rho) \rho(\bar{\xi}_1^\rho) \right) \\
 &\quad + \frac{\delta_{i, \kappa}}{2} \bar{\mathcal{U}}_{\lambda=1}(\bar{\xi}^\kappa) \kappa^*(\bar{\xi}^\kappa) + \frac{\delta_{i, \kappa^*}}{2} \bar{\mathcal{U}}_{\lambda=1}(\bar{\xi}^{\kappa^*}) \kappa(\bar{\xi}^{\kappa^*}) \\
 &\quad - \sum_{i_1'} \int_{\bar{\xi}_1^{i_1'}} G_{\lambda=0, ii_1'}^{(2)-1}[\vec{\rho}](\bar{\xi}^i, \bar{\xi}_1^{i_1'}) \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \\
 &\quad \times \left( \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right). \tag{56}
 \end{aligned}$$

Although it is difficult to obtain an explicit representation of the last term in the right-hand side in terms of the density correlation functions in general, it can be further simplified for an arbitrary  $\mathcal{U}_\lambda$ . In the next subsection, we shall discuss the case with short-range interactions and then show that the last term of Eq. (56) is approximately represented in terms of the density correlation functions.

Finally, let us discuss the Helmholtz free energy. Applying the approximation  $G_{\text{xc}, \lambda}^{(2)} \approx G_{\text{x}}^{(2)}$  to Eq. (39), we have

$$\begin{aligned}
 F_{\text{H}}[\vec{\rho}_{\text{ave}}] &= \frac{\Gamma_{\lambda=0} |_{\nu=0} [\vec{\rho}_{\text{ave}}]}{\beta} + \frac{1}{\beta} \int_{\xi} \mathcal{V}(\xi) \rho_{\text{ave}}(\xi) \\
 &\quad + \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \left[ \rho_{\text{ave}}(\bar{\xi}_1^\rho) \rho_{\text{ave}}(\bar{\xi}_2^\rho) + \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{\kappa^*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^{\kappa}) \Big|_{\bar{\xi}_{12}^{\kappa^*} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \right] \\
 &\quad + \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) G_{\text{x}}^{(2)}[\vec{\rho}_{\text{ave}}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho). \tag{57}
 \end{aligned}$$

From Eqs. (32) and (35),  $G_{\text{x}}^{(2)}[\vec{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)$  is rewritten as

$$G_{\text{x}}^{(2)}[\vec{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) = -\langle \psi^*(\xi_1 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \langle \psi^*(\xi_2 + \epsilon_\tau) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} - \rho(\bar{\xi}_1^\rho) \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2).$$

Then the integral with respect to  $\bar{\xi}_1^\rho$  and  $\bar{\xi}_2^\rho$  in the third line of Eq. (57) is evaluated as follows:

$$\begin{aligned}
 &\int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) G_{\text{x}}^{(2)}[\vec{\rho}_{\text{ave}}](\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\
 &= - \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_1 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}_{\text{ave}}} \langle \psi^*(\xi_2 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_1) \rangle_{\bar{\rho}_{\text{ave}}}, \tag{58}
 \end{aligned}$$

where we have used the equal-time commutation relation:

$$\begin{aligned} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_2 + \epsilon_\tau) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \\ = \delta(\tau_1 - \tau_2) U_{\lambda, a_1 a_2}(\mathbf{x}_1 - \mathbf{x}_2) \langle \psi^*(\xi_2 + \epsilon_\tau) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \\ = \delta(\tau_1 - \tau_2) U_{\lambda, a_1 a_2}(\mathbf{x}_1 - \mathbf{x}_2) \left( \langle \psi^*(\xi_2 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_1) \rangle_{\bar{\rho}} - \delta_{a_1, a_2} \delta(\mathbf{x}_1 - \mathbf{x}_2) \right). \end{aligned}$$

Substituting Eq. (58) into Eq. (57), we have

$$\begin{aligned} F_H[\bar{\rho}_{\text{ave}}] &= \frac{\Gamma_{\lambda=0} |v=0| [\bar{\rho}_{\text{ave}}]}{\beta} + \frac{1}{\beta} \int_{\xi} \mathcal{V}(\xi) \rho_{\text{ave}}(\xi) \\ &+ \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\ &\times \left[ \rho_{\text{ave}}(\bar{\xi}_1^\rho) \rho_{\text{ave}}(\bar{\xi}_2^\rho) - \langle \psi^*(\xi_1 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}_{\text{ave}}} \langle \psi^*(\xi_2 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_1) \rangle_{\bar{\rho}_{\text{ave}}} \right] \\ &+ \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{\kappa^*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^{\kappa}) \Big|_{\bar{\xi}_{12}^{\kappa^*} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)}. \end{aligned} \quad (59)$$

At the zero-temperature limit  $\beta \rightarrow \infty$ , it gives the ground-state energy:

$$\begin{aligned} E_{\text{gs}} &= T[\bar{\rho}_{\text{gs}}] + \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int_{\xi} \mathcal{V}(\xi) \rho_{\text{ave}}(\xi) \\ &+ \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \\ &\times \left[ \rho_{\text{ave}}(\bar{\xi}_1^\rho) \rho_{\text{ave}}(\bar{\xi}_2^\rho) - \langle \psi^*(\xi_1 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}_{\text{ave}}} \langle \psi^*(\xi_2 + \epsilon_\tau + \epsilon'_\tau) \psi(\xi_1) \rangle_{\bar{\rho}_{\text{ave}}} \right] \\ &+ \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{\kappa^*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^{\kappa}) \Big|_{\bar{\xi}_{12}^{\kappa^*} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)}. \end{aligned}$$

The third term in the right-hand side is interpreted as the Hartree–Fock energy; the fourth term is the contribution from the pairing condensate. This formula of the ground-state energy is identical to that given in the Hartree–Fock–Bogoliubov approximation [51–53].

### 3.2. The case of short-range interactions in the weak coupling

Let us take the case where the inter-particle interaction is short-range in the weak coupling limit of the pairing force as in the BCS theory [54]. Then it will be found that Eq. (56) is reduced to a simple and familiar form.

In the case of short-range interactions, the integral in the last term of Eq. (56) is dominated by the contribution from the region where  $\mathbf{x}_2$  is close to  $\mathbf{x}_1$ . Therefore, we can make the following approximation for short-range interactions that holds exactly for the zero-range interaction:

$$\begin{aligned} &\int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \\ &\times \left( \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_{1'}^{i_1'}) \rangle_{\bar{\rho}} - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_{1'}^{i_1'}) \rangle_{\bar{\rho}} \right) \\ &\approx \int_{\bar{\xi}_1^\rho = (\tau_1, \mathbf{x}_1, a_1), \bar{\xi}_2^\rho = (\tau_2, \mathbf{x}_2, a_2)} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \rho_{a_1 a_2}(\tau_2, \mathbf{x}_2) \end{aligned}$$

$$\begin{aligned} & \times \left( \langle \psi^*(\tau_1, \mathbf{x}_1, a_2) \psi(\tau_1 + \epsilon'_\tau, \mathbf{x}_1, a_1) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right. \\ & \left. - \langle \psi^*(\tau_1, \mathbf{x}_1, a_2) \psi(\tau_1 + \epsilon'_\tau, \mathbf{x}_1, a_1) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right), \end{aligned} \tag{60}$$

where we have used

$$\mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho := (\tau_1, \mathbf{x}_1, a_1), \bar{\xi}_2^\rho := (\tau_2, \mathbf{x}_2, a_2)) = \delta(\tau_1 - \tau_2) \mathcal{U}_{\lambda=1}(\tau_1, \mathbf{x}_1, a_1; \tau_1, \mathbf{x}_2, a_2),$$

and introduced  $\rho_{a_1 a_2}(\tau, \mathbf{x}) = \langle \psi^*(\tau + \epsilon'_\tau, \mathbf{x}, a_1) \psi(\tau, \mathbf{x}, a_2) \rangle_{\bar{\rho}}$ .

We evaluate  $\rho_{a_1 a_2}(\tau, \mathbf{x})$  in the weak coupling limit leading to small  $\kappa$  in comparison with the particle density  $\rho$ . In the non-interacting case  $\lambda = 0$ , the vanishing external field  $J_{\text{sup}, \lambda=0}^{\kappa^{(*)}}[\vec{\rho}] = 0$  gives  $\kappa^{(*)} = 0$ . Conversely, we have  $\lim_{\kappa, \kappa^* \rightarrow 0} J_{\text{sup}, \lambda=0}^{\kappa^{(*)}}[\vec{\rho}] = 0$  since  $\kappa^{(*)}$  uniquely determines the external field. Therefore, by use of Eqs. (54) and (21),  $\rho_{a_1 a_2}(\tau, \mathbf{x})$  is approximated in the weak coupling as

$$\begin{aligned} \rho_{a_1 a_2}(\tau, \mathbf{x}) & \approx \frac{1}{Z_{\lambda=0}[J_{\text{sup}, \lambda=0}^\rho[\vec{\rho}], 0, 0]} \int \mathcal{D}\psi \mathcal{D}\psi^* \psi^*(\tau + \epsilon'_\tau, \mathbf{x}, a_1) \psi(\tau, \mathbf{x}, a_2) \\ & \times e^{-S_{\lambda=0}[\psi, \psi^*] + \int_{\xi} J_{\text{sup}, \lambda=0}^\rho[\vec{\rho}](\xi) \hat{\rho}(\xi)}. \end{aligned} \tag{61}$$

Notice that there is no term causing a mixing between different components of  $\psi^{(*)}(\tau, \mathbf{x}, a)$  with different  $a$  in the exponent  $S_{\lambda=0}[\psi, \psi^*] - \int_{\xi} J_{\text{sup}, \lambda=0}^\rho[\vec{\rho}](\xi) \hat{\rho}(\xi)$  any more. Thus we have  $\rho_{a_1 a_2}(\tau, \mathbf{x}) \simeq 0$  for  $a_1 \neq a_2$  in the weak coupling limit. In other words,  $\rho_{a_1 a_2}(\tau, \mathbf{x})$  with  $a_1 \neq a_2$  is negligible in comparison with the diagonal component  $\rho_{a_1 a_1}(\tau, \mathbf{x}) = \rho(\tau, \mathbf{x}, a_1)$  in the weak coupling limit or small  $\kappa^{(*)}$ . Thus, we can make the approximation for  $\rho_{a_1 a_2}(\tau, \mathbf{x})$  as follows:

$$\rho_{a_1 a_2}(\tau, \mathbf{x}) \approx \delta_{a_1, a_2} \rho(\tau, \mathbf{x}, a_1). \tag{62}$$

Then, Eq. (60) is reduced as follows,

$$\begin{aligned} & \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \langle \psi^*(\xi_1 + \epsilon'_\tau) \psi(\xi_2) \rangle_{\bar{\rho}} \left( \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right. \\ & \left. - \langle \psi^*(\xi_2) \psi(\xi_1 + \epsilon'_\tau) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\ & \approx \int_{\bar{\xi}_1^\rho = (\tau_1, \mathbf{x}_1, a_1), \bar{\xi}_2^\rho = (\tau_2, \mathbf{x}_2, a_2)} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \delta_{a_1 a_2} \rho(\tau_2, \mathbf{x}_2, a_2) \\ & \times \left( \langle \psi^*(\tau_1, \mathbf{x}_1, a_1) \psi(\tau_1 + \epsilon'_\tau, \mathbf{x}_1, a_1) \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right. \\ & \left. - \langle \psi^*(\tau_1, \mathbf{x}_1, a_1) \psi(\tau_1 + \epsilon'_\tau, \mathbf{x}_1, a_1) \rangle_{\bar{\rho}} \langle \hat{\rho}_{i_1'}(\bar{\xi}_1^{i_1'}) \rangle_{\bar{\rho}} \right) \\ & = \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \delta_{a_1, a_2} \rho(\bar{\xi}_2^\rho) G_{\lambda=0, \rho i_1'}^{(2)}[\vec{\rho}](\bar{\xi}_1^\rho, \bar{\xi}_1^{i_1'}). \end{aligned} \tag{63}$$

Applying this approximation to Eq. (56), we arrive at the following expression of the basic equation for the KS theory for the case of short-range interactions in the weak coupling:

$$\begin{aligned} \mathcal{V}_{\text{KS}}^i[\vec{\rho}](\bar{\xi}^i) & = \delta_{i, \rho} \left( \mathcal{V}(\bar{\xi}^\rho) + \int_{\bar{\xi}_1^\rho} (1 - \delta_{a, a_1}) \mathcal{U}_{\lambda=1}(\bar{\xi}^\rho, \bar{\xi}_1^\rho) \rho(\bar{\xi}_1^\rho) \right) \\ & + \frac{\delta_{i, \kappa}}{2} \overline{\mathcal{U}}_{\lambda=1}(\bar{\xi}^\kappa) \kappa^*(\bar{\xi}^\kappa) + \frac{\delta_{i, \kappa^*}}{2} \overline{\mathcal{U}}_{\lambda=1}(\bar{\xi}^{\kappa^*}) \kappa(\bar{\xi}^{\kappa^*}). \end{aligned} \tag{64}$$

### 3.3. Homogeneous systems

In this subsection, we are going to discuss a homogeneous system with  $\mathcal{V}(\xi) = 0$  in Eq. (1), and show that Eq. (64) together with Eq. (44) is reduced to the well-known gap equation in the BCS theory [55]. For simplicity, we consider fermions with spin but not any other internal degrees of freedom: we assume that the spin is saturated in the system, and accordingly the chemical potential  $\mu$  has no spin dependence. We also assume that the two-body interaction is a spin-independent short-range one,  $U_{ab}(\mathbf{x}) = U(\mathbf{x})$ , and consider the weak-coupling limit so that the approximated equation Eq. (63) is applicable. Although we treat the spin-singlet condensate in the present investigation exclusively in the present article, the extension to the spin-triplet case is straightforward by considering the vector pairing densities.

Here, we introduce the following notation:  $\mathcal{V}_{\text{KS}}^i(\bar{\xi}^i) := \mathcal{V}_{\text{KS}}^i[\bar{\rho}_{\text{ave}}](\bar{\xi}^i)$ . Owing to the translational symmetry, the coordinate dependence of  $\mathcal{V}_{\text{KS}}^\rho(\bar{\xi}^\rho)$  is simplified as follows:

$$\mathcal{V}_{\text{KS}}^\rho(\bar{\xi}^\rho := (\tau, \mathbf{x}, a)) = \mathcal{V}_{\text{KS}}^\rho(0, \mathbf{0}, a) =: \mathcal{V}_{\text{KS},a}^\rho,$$

$$\mathcal{V}_{\text{KS}}^{\kappa^{(*)}}(\xi := (\tau, \mathbf{x}, a), \xi' := (\tau', \mathbf{x}', a')) = \mathcal{V}_{\text{KS}}^{\kappa^{(*)}}(\tau - \tau', \mathbf{x} - \mathbf{x}', a, 0, \mathbf{0}, a') =: \mathcal{V}_{\text{KS},aa'}^{\kappa^{(*)}}(\tau - \tau', \mathbf{x} - \mathbf{x}').$$

Similarly, we have

$$\rho_{\text{ave}}(\xi := (\tau, \mathbf{x}, a)) = \rho_{\text{ave}}(\tau = 0, \mathbf{x} = \mathbf{0}, a) =: \rho_{\text{ave}}^a,$$

$$\kappa_{\text{ave}}^{(*)}(\xi := (\tau, \mathbf{x}, a), \xi' := (\tau', \mathbf{x}', a')) = \kappa_{\text{ave}}^{(*)}(\tau - \tau', \mathbf{x} - \mathbf{x}', a, 0, \mathbf{0}, a') =: \kappa_{\text{ave}}^{aa'(*)}(\tau - \tau', \mathbf{x} - \mathbf{x}').$$

Since the spin-saturated system under consideration has the time-reversal symmetry, we have

$$\mathcal{V}_{\text{KS},aa'}^{\kappa^{*}}(\tau, \mathbf{x}) = \mathcal{V}_{\text{KS},a'a}^{\kappa}(\tau, \mathbf{x})^*.$$

Furthermore, the following relation should be satisfied because of the spin symmetry:

$$\begin{aligned} \rho_{\text{ave}}^\uparrow &= \rho_{\text{ave}}^\downarrow =: \rho_{\text{ave}}/2, \\ \mathcal{V}_{\text{KS},\uparrow}^\rho &= \mathcal{V}_{\text{KS},\downarrow}^\rho =: \mathcal{V}_{\text{KS}}^\rho, \\ \kappa_{\text{ave}}^{\uparrow\downarrow}(\tau, \mathbf{x}) &= -\kappa_{\text{ave}}^{\downarrow\uparrow}(\tau, \mathbf{x}) =: \kappa_{\text{ave}}^{\text{S}}(\tau, \mathbf{x}), \\ \mathcal{V}_{\text{KS},\uparrow\downarrow}^\kappa(\tau, \mathbf{x}) &= -\mathcal{V}_{\text{KS},\downarrow\uparrow}^\kappa(\tau, \mathbf{x}) =: \mathcal{V}_{\text{KS}}^{\kappa,\text{S}}(\tau, \mathbf{x}). \end{aligned}$$

Here,  $\rho_{\text{ave}} = \rho_{\text{ave}}^\uparrow + \rho_{\text{ave}}^\downarrow$  is the total particle-number density. Other components for  $\kappa_{\text{ave}}^{ab}(\tau, \mathbf{x})$  and  $\mathcal{V}_{\text{KS},ab}^\kappa(\tau, \mathbf{x})$  are assumed to be zero since we focus on the systems with the spin-singlet condensate.

For convenience for the description of the homogeneous system, let us move to the momentum representation. Then Eq. (64) is reduced to the following two equations for the particle and pairing densities, respectively,

$$\begin{cases} \mathcal{V}_{\text{KS}}^\rho = \frac{1}{2} \tilde{U}(\mathbf{0}) \rho_{\text{ave}} \\ \tilde{\mathcal{V}}_{\text{KS}}^{\kappa,\text{S}}(P) = \frac{1}{2} \int_Q \tilde{U}(\mathbf{q} - \mathbf{p}) \tilde{\kappa}_{\text{ave}}^{\text{S}}(Q)^* \end{cases} \quad (65)$$

Here, we have introduced the notations as  $P = (p_0, \mathbf{p})$  and  $Q = (q_0, \mathbf{q})$  with the Matsubara frequencies  $p_0$  and  $q_0$  and the spacial momenta  $\mathbf{p}$  and  $\mathbf{q}$ , and  $\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,\text{S}}(P)$ ,  $\tilde{U}(\mathbf{p})$  and  $\tilde{\kappa}_{\text{ave}}^{\text{S}}(P)$  are the Fourier

transforms of  $\mathcal{V}_{\text{KS}}^{\kappa,S}(\tau, \mathbf{x})$ ,  $U(\mathbf{x})$ , and  $\kappa_{\text{ave}}^s(\tau, \mathbf{x})$ , respectively. The following abbreviation is also used for the  $Q$ -“integrations”:

$$\int_Q = \beta^{-1} \sum_{q_0} \int d\mathbf{q}/(2\pi)^3.$$

Notice that the right-hand side of Eq. (65) and hence  $\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(P)$  in the left-hand side are independent of  $p_0$ . Thus we write as  $\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(P) = \tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p})$  from now on.

Now we calculate the equilibrium densities in the KS system via the variational equation (44) with the obtained KS potential Eq. (65). However, we have already seen that the solution  $\vec{\rho}_{\text{ave}}$  of Eq. (44) satisfies the self-consistent equation Eq. (45), which is now simplified to

$$\rho_{\text{ave},i}(\bar{\xi}^i) = \frac{1}{Z_{\lambda=0}[\vec{\mu} - \tilde{\mathcal{V}}_{\text{KS}}]} \int \mathcal{D}\psi \mathcal{D}\psi^* \hat{\rho}_i(\bar{\xi}^i) e^{-S_{\lambda=0}[\psi^*, \psi] + \sum_{j=\rho, \kappa, \kappa^*} \int_{\bar{\xi}_1^j} (\mu^j - \mathcal{V}_{\text{KS}}^j(\bar{\xi}_1^j)) \hat{\rho}_j(\bar{\xi}_1^j)}.$$

Furthermore, since the exponent in the integral becomes a bilinear form when Eq. (65) is inserted, we can perform the path integral analytically to give

$$\rho_{\text{ave}} = \int_{\mathbf{p}} \left( 1 - \frac{\varepsilon(\mathbf{p})}{E(\mathbf{p})} \tanh \frac{\beta E(\mathbf{p})}{2} \right), \tag{66}$$

$$\tilde{\kappa}_{\text{ave}}^s(P) = - \frac{2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p})^*}{p_0^2 + E(\mathbf{p})^2}, \tag{67}$$

where  $\int_{\mathbf{p}} = \int d\mathbf{p}/(2\pi)^3$ ,  $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2 + \mathcal{V}_{\text{KS}}^\rho - \mu$ , and  $E(\mathbf{p}) = \sqrt{\varepsilon(\mathbf{p})^2 + |2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p})|^2}$ , as is detailed in Appendix. Substitution of Eq. (67) into the second equation of Eq. (65) in turn leads to

$$\begin{cases} \tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p}) = - \int_{\mathbf{q}} \tilde{U}(\mathbf{q} - \mathbf{p}) \frac{\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{q})}{2\sqrt{\varepsilon(\mathbf{q})^2 + |2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{q})|^2}} \tanh \frac{\beta\sqrt{\varepsilon(\mathbf{q})^2 + |2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{q})|^2}}{2} \\ \varepsilon(\mathbf{p}) = \frac{\mathbf{p}^2}{2} + \frac{1}{2} \tilde{U}(\mathbf{0}) \rho_{\text{ave}} - \mu \end{cases} \tag{68}$$

Equation (67) implies that  $\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p})$  is identified with the energy gap  $\Delta^s(\mathbf{p})$  in the BCS theory as  $\Delta^s(\mathbf{p}) = -2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p})^*$ . With this identification, we find that Eq. (68) is nothing else than the celebrated gap equation in the BCS theory [54].

As is also shown in the Appendix, the Helmholtz free energy is calculated from Eq. (59) to yield

$$\begin{aligned} \frac{F_{\text{H}}[\vec{\rho}_{\text{ave}}]}{V} &= \frac{\Gamma_{\lambda=0}[\gamma=0][\vec{\rho}_{\text{ave}}]}{\beta V} + \frac{1}{2} \tilde{U}(\mathbf{0}) \rho_{\text{ave}}^2 \\ &\quad - \frac{1}{4} \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \left( 1 - \frac{\varepsilon(\mathbf{p})}{E(\mathbf{p})} \tanh \frac{\beta E(\mathbf{p})}{2} \right) \left( 1 - \frac{\varepsilon(\mathbf{q})}{E(\mathbf{q})} \tanh \frac{\beta E(\mathbf{q})}{2} \right) \\ &\quad + \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \frac{\tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{p}) \tilde{\mathcal{V}}_{\text{KS}}^{\kappa,S}(\mathbf{q})^*}{E(\mathbf{p})E(\mathbf{q})} \tanh \frac{\beta E(\mathbf{p})}{2} \tanh \frac{\beta E(\mathbf{q})}{2}. \end{aligned} \tag{69}$$

where  $V = \int d\mathbf{x}$  is the volume of the system.

Taking the zero-temperature limit  $\beta \rightarrow \infty$  in Eq. (69), the ground-state energy is obtained as

$$\frac{E_{\text{gs}}}{V} = \frac{T[\vec{\rho}_{\text{gs}}]}{V} + \frac{1}{2} \rho_{\text{gs}}^2 \tilde{U}(\mathbf{0}) - \frac{1}{4} \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \left( 1 - \frac{\varepsilon(\mathbf{p})}{E(\mathbf{p})} \right) \left( 1 - \frac{\varepsilon(\mathbf{q})}{E(\mathbf{q})} \right)$$

$$+ \frac{1}{4} \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \frac{\Delta^s(\mathbf{p}) \Delta^s(\mathbf{q})^*}{E(\mathbf{p})E(\mathbf{q})}, \quad (70)$$

Our ground-state energy is identical to that obtained in the BCS theory with the identification  $\Delta^s(\mathbf{p}) = -2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa, s}(\mathbf{p})^*$  [51,53,54,56].

#### 4. Conclusion

On the basis of the effective action formalism, we have developed a generalized DFT for superfluid systems at finite temperature in a rigorous way. The rigorous formulation is combined with the renormalization group method by introducing a scale parameter that is multiplied to the inter-particle potential, which is reminiscent of the adiabatic connection method. A possible difficulty that the SSB is not described when the symmetry-breaking term is absent is nicely circumvented by a suitable choice of the external fields by making use of the FRG.

We have then established the Hohenberg–Kohn theorem with the SSB being taken into account. By introducing flow-parameter-dependent source terms appropriately fixing the ground-state densities during the flow, we have derived the flow equation for the effective action for the particle-number and non-local pairing densities where the flow parameter  $\lambda$  runs from 0 to 1, corresponding to the non-interacting and interacting systems, respectively.

Integrating this flow equation and using the variational equation for the thermal equilibrium densities, we have arrived at the exact self-consistent equation to determine the Kohn–Sham potential  $\mathcal{V}_{\text{KS}}^i[\vec{\rho}]$  generalized to include the pairing potentials at finite temperature without the introduction of single-particle orbitals. The resultant Kohn–Sham potential has a nice feature in that it expresses the microscopic formulae of the external, Hartree, pairing and exchange–correlation terms separately. In particular, the exchange–correlation term  $\mathcal{V}_{\text{KS}, \text{xc}}^i[\vec{\rho}]$  is given explicitly in terms of the corresponding density–density correlation functions  $G_{\text{xc}, \lambda}^{(2)}[\vec{\rho}]$ .

As a demonstration of the validity of our formulation as a microscopic theory of DFT for superfluidity, we have shown that our self-consistent equation with Kohn–Sham potential leads to the ground-state energy of the Hartree–Fock–Bogoliubov theory when the correlations are neglected. In addition, the self-consistent equation is further reduced for short-range interaction and in the weak-coupling limit to reproduce the gap equation of the BCS theory for the spin-singlet pairing.

Although we have shown the validity of our microscopic formulation of DFT based on FRG by applying it to simple cases, an advantage of our exact FRG-DFT formalism lies in the fact that it contains the equation (36), with which the correlation part can be improved systematically. One of the most effective systematic schemes used in the FRG-DFT is the vertex expansion, where the Taylor expansion around the equilibrium densities are applied to the flow equation for the effective action. In fact, it is shown [45] for the system without superfluidity that the vertex expansion only up to the second order gives an approximate scheme superior to the random phase approximation (RPA). Therefore it is naturally expected that a simple vertex expansion applied to the basic equation in the present work would lead to an approximation scheme that incorporates correlations beyond those given by the quasi-particle RPA. We hope to report on such an attempt in the near future.

Our formulation was given to general cases, i.e. any spatial profiles, and the dependence of the interaction on the internal degrees of freedom are not imposed. Such a general formulation may be helpful in the application to the superfluidity in various systems. Introduction of the non-local particle density is an interesting extension of the present formalism, with which we can describe the particle–hole and particle–particle correlations on the same footing. Furthermore, our general formulation for

non-local pairing should provide us with a sound basis for describing pairing phenomena with any symmetry such as spin-triplet superfluidity and/or the pairing with spin-orbit coupling incorporated. We hope that there will be a chance to report on such investigations.

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**Appendix A. Equilibrium densities and Helmholtz energy of homogeneous systems**

In this appendix we shall derive the equilibrium densities and Helmholtz free energy of homogeneous systems.

*Appendix A.1. Free propagators*

As was done in Sect. 3.3, we consider a system with the translational, time-reversal and spin symmetries. The generating functional for non-interacting fermions in the presence of  $\tau$ -independent external sources coupled to the total particle-number density and spin-singlet pairing density reads:

$$Z_0[\vec{J}] = \int \mathcal{D}\psi \mathcal{D}\psi^* e^{-S_0[\psi, \psi^*] + J_\rho \int_X \hat{\rho}(X) + \int_{X, X'} 2J_{\kappa^s}(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \hat{\kappa}^s(X, X') + \int_{X, X'} 2J_{\kappa^s}(\mathbf{x} - \mathbf{x}')^* \delta(\tau - \tau') \hat{\kappa}^{s*}(X, X')}, \tag{A.1}$$

where  $X = (\tau, \mathbf{x})$ ,  $\int_X := \int_0^\beta d\tau \int d\mathbf{x}$ ,  $\vec{J} = (J_\rho, J_{\kappa^s}(\mathbf{x}), J_{\kappa^s}(\mathbf{x})^*)$ , and

$$S_0[\psi, \psi^*] = \sum_{s=\uparrow\downarrow} \int_X \psi_s^*(X + \epsilon_\tau) \left( \partial_\tau - \frac{\Delta}{2} \right) \psi_s(X), \tag{A.2}$$

$$\hat{\rho}(X) = \sum_{s=\uparrow\downarrow} \psi_s^*(X + \epsilon_\tau) \psi_s(X), \tag{A.3}$$

$$\hat{\kappa}^s(X, X') = \frac{1}{2} (\psi_\uparrow(X) \psi_\downarrow(X') - \psi_\downarrow(X) \psi_\uparrow(X')), \tag{A.4}$$

$$\hat{\kappa}^{s*}(X, X') = \frac{1}{2} (\psi_\downarrow^*(X') \psi_\uparrow^*(X) - \psi_\uparrow^*(X') \psi_\downarrow^*(X)). \tag{A.5}$$

Here,  $X + \epsilon_\tau = (\tau + \epsilon, \mathbf{x})$ , and  $\epsilon (> 0)$  is the time step size of the path integral, which will be taken to be zero in the end of the calculation. We first note that the time derivative of the Grassmann field  $\partial_\tau \psi_s(X)$  in Eq. (A.2) is defined as

$$\partial_\tau \psi_s(X) := \frac{\psi_s(X + \epsilon_\tau) - \psi_s(X)}{\epsilon}. \tag{A.6}$$

By the Fourier transformation

$$\begin{aligned} \psi_s(X) &= \int_P e^{iP \cdot X} \tilde{\psi}_s(P) = \int_P e^{-i\omega_n \tau + i\mathbf{p} \cdot \mathbf{x}} \tilde{\psi}_s(P), \\ \psi_s^*(X) &= \int_P e^{-iP \cdot X} \tilde{\psi}_s^*(P), \end{aligned}$$



$$J_{\kappa^s}(\mathbf{x}) = \int_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}} \tilde{J}_{\kappa^s}(\mathbf{p}),$$

where  $P = (\omega_n, \mathbf{p})$  with the Matsubara frequency  $\omega_n = (2n + 1)/\beta$ ,  $\int_P := \beta^{-1} \sum_{\omega_n} \int d\mathbf{p}/(2\pi)^3$ , and  $\int_{\mathbf{p}} := \int d\mathbf{p}/(2\pi)^3$ , the generating functional is rewritten in the momentum representation as:

$$\begin{aligned} Z_0[\vec{J}] = & \int \mathcal{D}\tilde{\psi} \mathcal{D}\tilde{\psi}^* \exp \left\{ \sum_s \int_P \tilde{\psi}_s^*(P) \left[ \frac{e^{i\omega_n\epsilon} - 1}{\epsilon} - e^{i\omega_n\epsilon} \left( \frac{\mathbf{p}^2}{2} - J_\rho \right) \right] \tilde{\psi}_s(P) \right. \\ & + \int_P \tilde{J}_{\kappa^s}(\mathbf{p}) \left[ \tilde{\psi}_\uparrow(-P)\tilde{\psi}_\downarrow(P) - \tilde{\psi}_\downarrow(-P)\tilde{\psi}_\uparrow(P) \right] \\ & \left. + \int_P \tilde{J}_{\kappa^s}(\mathbf{p})^* \left[ \tilde{\psi}_\downarrow^*(P)\tilde{\psi}_\uparrow^*(-P) - \tilde{\psi}_\uparrow^*(P)\tilde{\psi}_\downarrow^*(-P) \right] \right\}. \end{aligned} \tag{A.7}$$

The usual treatment of the exponent in the first term may be to make a replacement  $(e^{i\omega_n\epsilon} - 1)/\epsilon \rightarrow i\omega_n$  while leaving  $e^{i\omega_n\epsilon}(\mathbf{p}^2/2 - J_\rho)$ . Indeed, nothing is wrong with this practical treatment and it will give the correct result. Instead, however, here we leave all  $\epsilon$ s until just before the end of the calculation for an instructive purpose.

Introducing  $\tilde{\Psi}(P) := \begin{bmatrix} \tilde{\psi}_\uparrow(P) & \tilde{\psi}_\downarrow^*(-P) \end{bmatrix}^\top$ , the exponent of the right-hand side of Eq. (A.7) is organized in a matrix form as in the Nambu–Gor’kov formalism:

$$Z_0[\vec{J}] = \int \mathcal{D}\tilde{\psi} \mathcal{D}\tilde{\psi}^* \exp \left\{ - \int_P \tilde{\Psi}^\dagger(P) \begin{bmatrix} \frac{1-e^{i\omega_n\epsilon}}{\epsilon} + \varepsilon(\mathbf{p}; J_\rho)e^{i\omega_n\epsilon} & 2\tilde{J}_{\kappa^s}(\mathbf{p})^* \\ 2\tilde{J}_{\kappa^s}(\mathbf{p}) & -\frac{1-e^{-i\omega_n\epsilon}}{\epsilon} - \varepsilon(\mathbf{p}; J_\rho)e^{-i\omega_n\epsilon} \end{bmatrix} \tilde{\Psi}(P) \right\}, \tag{A.8}$$

where  $\varepsilon(\mathbf{p}; J_\rho) := \mathbf{p}^2/2 - J_\rho$ . By adding external source terms  $\sum_{a=1,2} \left[ \int_P \tilde{\eta}_a^*(P)\tilde{\Psi}_a(P) + \int_P \tilde{\Psi}_a^*(P)\tilde{\eta}_a(P) \right]$  to the exponent of the right-hand side of Eq. (A.8) with  $\tilde{\eta}$  and  $\tilde{\eta}^*$  being Grassmann variables, and differentiating the generating functional with respect to  $\tilde{\eta}$  and  $\tilde{\eta}^*$ , the propagators are obtained in a matrix form:

$$\begin{aligned} & \left\langle \begin{bmatrix} \tilde{\psi}_\uparrow(P)\tilde{\psi}_\uparrow^*(P) & \tilde{\psi}_\uparrow(P)\tilde{\psi}_\downarrow(-P) \\ \tilde{\psi}_\downarrow^*(-P)\tilde{\psi}_\uparrow^*(P) & \tilde{\psi}_\downarrow^*(-P)\tilde{\psi}_\downarrow(-P) \end{bmatrix} \right\rangle_{\vec{J}} \\ &= \begin{bmatrix} \frac{1-e^{i\omega_n\epsilon}}{\epsilon} + \varepsilon(\mathbf{p}; J_\rho)e^{i\omega_n\epsilon} & 2\tilde{J}_{\kappa^s}(\mathbf{p})^* \\ 2\tilde{J}_{\kappa^s}(\mathbf{p}) & -\frac{1-e^{-i\omega_n\epsilon}}{\epsilon} - \varepsilon(\mathbf{p}; J_\rho)e^{-i\omega_n\epsilon} \end{bmatrix}^{-1} \\ &= \frac{1}{\left( \frac{2\sqrt{1-\varepsilon\varepsilon(\mathbf{p}; J_\rho)}}{\epsilon} \sin \frac{\omega_n\epsilon}{2} \right)^2 + E(\mathbf{p}; \vec{J})^2} \\ & \quad \times \begin{bmatrix} \frac{2ie^{-i\frac{\omega_n\epsilon}{2}}}{\epsilon} \sin \frac{\omega_n\epsilon}{2} + \varepsilon(\mathbf{p}; J_\rho)e^{-i\omega_n\epsilon} & 2\tilde{J}_{\kappa^s}(\mathbf{p})^* \\ 2\tilde{J}_{\kappa^s}(\mathbf{p}) & \frac{2ie^{i\frac{\omega_n\epsilon}{2}}}{\epsilon} \sin \frac{\omega_n\epsilon}{2} - \varepsilon(\mathbf{p}; J_\rho)e^{i\omega_n\epsilon} \end{bmatrix}, \end{aligned} \tag{A.9}$$

where  $E(\mathbf{p}; \vec{J}) := \sqrt{\varepsilon(\mathbf{p}; J_\rho)^2 + |2\tilde{J}_{\kappa^s}(\mathbf{p})|^2}$ , and  $\langle \mathcal{O}[\psi, \psi^*] \rangle_{\vec{J}}$  is defined as

$$\langle \mathcal{O}[\psi, \psi^*] \rangle_{\vec{J}} := \frac{1}{Z_0[\vec{J}]} \int \mathcal{D}\psi \mathcal{D}\psi^* \mathcal{O}[\psi, \psi^*]$$

$$\times e^{-S_0[\psi, \psi^*] + J_\rho \int_X \hat{\rho}(X) + \int_{X, X'} 2J_{\kappa^s}(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \hat{\kappa}^s(X, X') + \int_{X, X'} 2J_{\kappa^*}(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \hat{\kappa}^{s^*}(X, X')} \tag{A.10}$$

with an arbitrary functional  $\mathcal{O}[\psi, \psi^*]$  of  $\psi$  and  $\psi^*$  including the Fourier transforms of them.

*Appendix A.2. Equilibrium densities*

From Eq. (45) the equilibrium densities satisfy

$$\rho_{\text{ave}} = \langle \hat{\rho}(X) \rangle_{\vec{\mu} - \vec{\mathcal{V}}_{\text{KS}}}, \tag{A.11}$$

$$\kappa_{\text{ave}}^{s(*)}(X - X') = \langle \hat{\kappa}^{s(*)}(X, X') \rangle_{\vec{\mu} - \vec{\mathcal{V}}_{\text{KS}}}. \tag{A.12}$$

The equilibrium total particle-number density is calculated as follows:

$$\begin{aligned} \rho_{\text{ave}} &= \sum_s \langle \psi_s^*(X + \epsilon_\tau) \psi_s(X) \rangle_{\vec{\mu} - \vec{\mathcal{V}}_{\text{KS}}} \\ &= \int_P e^{i\omega_n \epsilon} \sum_s \langle \tilde{\psi}_s^*(P) \tilde{\psi}_s(P) \rangle_{\vec{\mu} - \vec{\mathcal{V}}_{\text{KS}}} \\ &= 2 \int_P \frac{-\frac{2ie^{i\frac{\omega_n \epsilon}{2}}}{\epsilon} \sin \frac{\omega_n \epsilon}{2} - \epsilon(\mathbf{p})}{\left(\frac{2\sqrt{1 - \epsilon \epsilon}(\mathbf{p})}{\epsilon} \sin \frac{\omega_n \epsilon}{2}\right)^2 + E(\mathbf{p})^2}, \end{aligned} \tag{A.13}$$

where  $\epsilon(\mathbf{p}) := \epsilon(\mathbf{p}; \mu - \mathcal{V}_{\text{KS}}^\rho) = \mathbf{p}^2/2 + \mathcal{V}_{\text{KS}}^\rho - \mu$ , and  $E(\mathbf{p}) := E(\mathbf{p}; \vec{\mu} - \vec{\mathcal{V}}_{\text{KS}}) = \sqrt{\epsilon(\mathbf{p})^2 + |2\tilde{\mathcal{V}}_{\text{KS}}^{\kappa, s}(\mathbf{p})|^2}$ . To calculate the Matsubara frequency summation in Eq. (A.13), let us introduce a complex function

$$h(z) = \frac{-\frac{2ie^{i\frac{z\epsilon}{2}}}{\epsilon} \sin \frac{z\epsilon}{2} - \epsilon}{\left(\frac{2\sqrt{1 - \epsilon \epsilon}}{\epsilon} \sin \frac{z\epsilon}{2}\right)^2 + E^2}$$

and a weighting function

$$g(z) = -\beta n_F(z) = \frac{-\beta}{1 + e^{\beta z}}.$$

It is observed that the product  $h(-iz)g(z)$  decays sufficiently fast as  $|z| \rightarrow \infty$ , and  $h(-iz)$  has simple poles at  $z = \pm(2/\epsilon) \sinh^{-1}[\epsilon E/(2\sqrt{1 - \epsilon \epsilon})]$ . Therefore,

$$\begin{aligned} \frac{1}{\beta} \sum_{\omega_n} h(\omega_n) &= -\frac{1}{\beta} \text{Res} \left( h(-iz)g(z), z = \frac{2}{\epsilon} \sinh^{-1} \frac{\epsilon E}{2\sqrt{1 - \epsilon \epsilon}} \right) \\ &\quad - \frac{1}{\beta} \text{Res} \left( h(-iz)g(z), z = -\frac{2}{\epsilon} \sinh^{-1} \frac{\epsilon E}{2\sqrt{1 - \epsilon \epsilon}} \right) \\ &= \frac{E + \epsilon}{2E} n_F(E) + \frac{E - \epsilon}{2E} n_F(-E) \\ &= \frac{1}{2} \left( 1 - \frac{\epsilon}{E} \tanh \frac{\beta E}{2} \right). \end{aligned} \tag{A.14}$$

In the second-to-last line, we have taken the limit  $\epsilon \rightarrow 0$  implicitly. Consequently, we arrive at

$$\rho_{\text{ave}} = \int_P \left( 1 - \frac{\epsilon(\mathbf{p})}{E(\mathbf{p})} \tanh \frac{\beta E(\mathbf{p})}{2} \right). \tag{A.15}$$

In the same way, the equilibrium spin-singlet pairing density is calculated as follows:

$$\begin{aligned}
\kappa_{\text{ave}}^s(X - X') &= \frac{1}{2} \langle \psi_{\uparrow}(X) \psi_{\downarrow}(X') - \psi_{\downarrow}(X) \psi_{\uparrow}(X') \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \\
&= \frac{1}{2} \int_P e^{iP \cdot (X - X')} \left[ \langle \tilde{\psi}_{\uparrow}(P) \tilde{\psi}_{\downarrow}(-P) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} - \langle \tilde{\psi}_{\downarrow}(P) \tilde{\psi}_{\uparrow}(-P) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \right] \\
&= \int_P e^{iP \cdot (X - X')} \frac{-2\tilde{\mathcal{V}}_{\text{KS}}^{k,s}(\mathbf{p})^*}{\left( \frac{2\sqrt{1-\epsilon\epsilon(\mathbf{p})}}{\epsilon} \sin \frac{\omega_n \epsilon}{2} \right)^2 + E(\mathbf{p})^2} \\
&= \int_{\mathbf{p}} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')} \frac{-\tilde{\mathcal{V}}_{\text{KS}}^{k,s}(\mathbf{p})^*}{E(\mathbf{p})} \left( \frac{e^{-E(\mathbf{p})|\tau - \tau'|}}{1 + e^{-\beta E(\mathbf{p})}} - \frac{e^{E(\mathbf{p})|\tau - \tau'|}}{1 + e^{\beta E(\mathbf{p})}} \right). \tag{A.16}
\end{aligned}$$

In particular, the local spin-singlet pairing density in equilibrium is given by

$$\kappa_{\text{ave}}^s(0) = \int_{\mathbf{p}} \frac{-\tilde{\mathcal{V}}_{\text{KS}}^{k,s}(\mathbf{p})^*}{E(\mathbf{p})} \tanh \frac{\beta E(\mathbf{p})}{2}. \tag{A.17}$$

### Appendix A.3. Helmholtz free energy

From Eq. (59) the Helmholtz energy in the lowest-order approximation is given by

$$\begin{aligned}
F_{\text{H}}[\bar{\rho}_{\text{ave}}] &= \frac{\Gamma_{\lambda=0}[\bar{\rho}_{\text{ave}}]}{\beta} + \frac{1}{2\beta} \int_{\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}) \rho_{\text{ave}}(\bar{\xi}_1^{\rho}) \rho_{\text{ave}}(\bar{\xi}_2^{\rho}) \\
&\quad - \frac{1}{2\beta} \int_{\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}) \langle \psi^*(\xi_1 + \epsilon_{\tau} + \epsilon'_{\tau}) \psi(\xi_2) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \langle \psi^*(\xi_2 + \epsilon_{\tau} + \epsilon'_{\tau}) \psi(\xi_1) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \\
&\quad + \frac{1}{2\beta} \int_{\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}) \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{k*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^k) \Big|_{\bar{\xi}_{12}^{k*} = (\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho})}. \tag{A.18}
\end{aligned}$$

The second term of the right-hand side of Eq. (A.18) is evaluated as follows:

$$\frac{1}{2\beta} \int_{\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}) \rho_{\text{ave}}(\bar{\xi}_1^{\rho}) \rho_{\text{ave}}(\bar{\xi}_2^{\rho}) = \frac{1}{2} \int_{\mathbf{x}_1, \mathbf{x}_2} U(\mathbf{x}_1 - \mathbf{x}_2) \sum_{s_1=\uparrow\downarrow} \rho_{\text{ave}}^{s_1} \sum_{s_2=\uparrow\downarrow} \rho_{\text{ave}}^{s_2} = \frac{V}{2} \tilde{U}(\mathbf{0}) \rho_{\text{ave}}^2, \tag{A.19}$$

where  $V = \int d\mathbf{x}$  is the volume and  $\tilde{U}(\mathbf{p}) = \int d\mathbf{x} e^{-i\mathbf{p} \cdot \mathbf{x}} U(\mathbf{x})$ . The third term is evaluated as follows:

$$\begin{aligned}
& - \frac{1}{2\beta} \int_{\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^{\rho}, \bar{\xi}_2^{\rho}) \langle \psi^*(\xi_1 + \epsilon_{\tau} + \epsilon'_{\tau}) \psi(\xi_2) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \langle \psi^*(\xi_2 + \epsilon_{\tau} + \epsilon'_{\tau}) \psi(\xi_1) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \\
&= - \frac{1}{2} \int_{\mathbf{x}_1, \mathbf{x}_2} U(\mathbf{x}_1 - \mathbf{x}_2) \sum_{s_1, s_2=\uparrow\downarrow} \left[ \langle \psi_{s_1}^*(X_1 + \epsilon_{\tau} + \epsilon'_{\tau}) \psi_{s_2}(X_2) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \right. \\
&\quad \left. \times \langle \psi_{s_2}^*(\xi_2 + \epsilon_{\tau} + \epsilon'_{\tau}) \psi_{s_1}(\xi_1) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \right]_{\tau_1 = \tau_2} \\
&= - \frac{V}{2} \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \sum_{s=\uparrow\downarrow} \frac{1}{\beta} \sum_m e^{i\omega_n(\epsilon + \epsilon')} \langle \tilde{\psi}_s^*(\omega_m, \mathbf{p}) \tilde{\psi}_s(\omega_m, \mathbf{p}) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}} \\
&\quad \times \frac{1}{\beta} \sum_n e^{i\omega_n(\epsilon + \epsilon')} \langle \tilde{\psi}_s^*(\omega_n, \mathbf{q}) \tilde{\psi}_s(\omega_n, \mathbf{q}) \rangle_{\bar{\mu} - \bar{\nu}_{\text{KS}}}
\end{aligned}$$

$$= -\frac{V}{4} \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \left(1 - \frac{\varepsilon(\mathbf{p})}{E(\mathbf{p})} \tanh \frac{\beta E(\mathbf{p})}{2}\right) \left(1 - \frac{\varepsilon(\mathbf{q})}{E(\mathbf{q})} \tanh \frac{\beta E(\mathbf{q})}{2}\right). \quad (\text{A.20})$$

The fourth term is evaluated as follows:

$$\begin{aligned} & \frac{1}{2\beta} \int_{\bar{\xi}_1^\rho, \bar{\xi}_2^\rho} \mathcal{U}_{\lambda=1}(\bar{\xi}_1^\rho, \bar{\xi}_2^\rho) \kappa_{\text{ave}}^*(\bar{\xi}_{12}^{\kappa^*}) \kappa_{\text{ave}}(\bar{\xi}_{12}^\kappa) \Big|_{\bar{\xi}_{12}^{\kappa^*} = (\bar{\xi}_1^\rho, \bar{\xi}_2^\rho)} \\ &= \frac{1}{2} \int_{\mathbf{x}_1, \mathbf{x}_2} U(\mathbf{x}_1 - \mathbf{x}_2) \left[ \kappa_{\text{ave}}^{\uparrow\downarrow*}(X_1, X_2) \kappa_{\text{ave}}^{\uparrow\downarrow}(X_1, X_2) + \kappa_{\text{ave}}^{\downarrow\uparrow*}(X_1, X_2) \kappa_{\text{ave}}^{\downarrow\uparrow}(X_1, X_2) \right]_{\tau_1 = \tau_2} \\ &= \int_{\mathbf{x}_1, \mathbf{x}_2} U(\mathbf{x}_1 - \mathbf{x}_2) \kappa_{\text{ave}}^{s*}(X_1, X_2) \Big|_{\tau_1 = \tau_2} \kappa_{\text{ave}}^s(X_1, X_2) \Big|_{\tau_1 = \tau_2} \\ &= V \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \frac{\tilde{\mathcal{V}}_{\text{KS}}^{\kappa, s}(\mathbf{p}) \tilde{\mathcal{V}}_{\text{KS}}^{\kappa, s}(\mathbf{q})^*}{E(\mathbf{p})E(\mathbf{q})} \tanh \frac{\beta E(\mathbf{p})}{2} \tanh \frac{\beta E(\mathbf{q})}{2}. \end{aligned} \quad (\text{A.21})$$

Consequently, we have

$$\begin{aligned} \frac{F_{\text{H}}[\bar{\rho}_{\text{ave}}]}{V} &= \frac{\Gamma_{\lambda=0} |_{\nu=0} [\bar{\rho}_{\text{ave}}]}{\beta V} + \frac{1}{2} \tilde{U}(\mathbf{0}) \rho_{\text{ave}}^2 \\ &\quad - \frac{1}{4} \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \left(1 - \frac{\varepsilon(\mathbf{p})}{E(\mathbf{p})} \tanh \frac{\beta E(\mathbf{p})}{2}\right) \left(1 - \frac{\varepsilon(\mathbf{q})}{E(\mathbf{q})} \tanh \frac{\beta E(\mathbf{q})}{2}\right) \\ &\quad + \int_{\mathbf{p}, \mathbf{q}} \tilde{U}(\mathbf{p} - \mathbf{q}) \frac{\tilde{\mathcal{V}}_{\text{KS}}^{\kappa, s}(\mathbf{p}) \tilde{\mathcal{V}}_{\text{KS}}^{\kappa, s}(\mathbf{q})^*}{E(\mathbf{p})E(\mathbf{q})} \tanh \frac{\beta E(\mathbf{p})}{2} \tanh \frac{\beta E(\mathbf{q})}{2}. \end{aligned} \quad (\text{A.22})$$

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