Extension of time-dependent Hartree-Fock-Bogoliubov equations

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An extension of the time-dependent Hartree-Fock-Bogoliubov theory (ETDHFB) which includes higher-order effects such as screening of the pairing correlation is proposed. ETDHFB is applied to a pairing model and a fermion system trapped in a harmonic potential to test its feasibility by comparison with exact solutions. With the use of perturbative expressions for the pairing tensor and the two-body density matrix derived from ETDHFB, the screening effect is investigated for atomic fermion systems and isotopes of tin nuclei. It is found that the screening effect on the pairing correlation is not significant.

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I. INTRODUCTION

The study of higher-order effects on superfluidity has been attracting strong theoretical interests in many fields of physics including nuclear physics. Many-body effects that go beyond the Bardeen-Cooper-Schrieffer theory (BCS) may include the medium polarization known as Gorkov and Melik-Barkhudarov (GMB) correction [1], the self-energy correction, the vertex correction, and so on. Most calculations for neutron matter [2–5] and dilute Fermi gases [1,5–7] show suppression of the pairing correlation due to the medium polarization, whereas studies of finite nuclei treating the medium polarization as low-lying vibrations give opposite results [8]. Theoretical studies on the higher-order effects usually start from the generalized gap equation [9] which consists of the particle-particle irreducible kernel and the anomalous propagator, and higher-order corrections are made for these quantities. The fact that various approaches give contradictory results suggests the necessity of a consistent microscopic treatment of various higher-order effects on the same footing. Monte Carlo calculations [5,10–12] and, eventually, exact diagonalization are certainly consistent approaches but are restricted to rather small systems (and configuration spaces for the latter) and, thus, have also their limitations. It is, therefore, desirable to develop many body techniques which go beyond the standard BCS theory in a systematic way as has been done in Refs. [13–15] and check their validity for cases where exact solutions can be obtained [16].

In the present paper we propose an extension of the time-dependent Hartree-Bogoliubov theory (TDHFB) to include higher-order effects. We formulate the extended TDHFB (ETDHFB) using a truncation scheme similar to that used in the time-dependent density-matrix theory (TDDM) in the normal-fluid regime [17,18], where higher-order reduced density matrices are approximated by lower-order density matrices to truncate the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy for reduced density matrices. TDDM has in the past demonstrated its effectiveness in various applications [18–20] and it can reasonably be assumed that its extension to the superfluid case will show equally good performance. The advantages of ETDHFB are that it has a direct connection to TDHFB and that various correction terms are expressed explicitly, contrary to Monte Carlo approaches. To show the feasibility of ETDHFB, we apply it to a pairing model and a fermion system trapped in a harmonic potential where comparison with the exact solution can be made. Using perturbative expressions for the pairing tensor and two-body density matrix derived from ETDHFB, we study the screening effect on the pairing correlation for trapped fermion systems and nuclei of tin isotopes and make contact with earlier work.

The paper is organized as follows. The ETDHFB equations and the perturbative expressions for the pairing tensor and the two-body correlation matrix are given in Sec. II. The obtained results for the pairing model, trapped fermions, and tin isotopes are presented in Sec. III, and Sec. IV is devoted to the summary.

II. FORMULATION

A. ETDHFB equations

We consider a Hamiltonian consisting of a one-body part and a two-body interaction:

$$H = \sum_{\alpha\alpha'} \langle \alpha | t | \alpha' \rangle a^\dagger_\alpha a_{\alpha'} + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} \langle \alpha\beta | v | \alpha'\beta' \rangle a^\dagger_\alpha a^\dagger_\beta a_{\beta'} a_{\alpha'}, \tag{1}$$

where $a^\dagger_\alpha$ and a_α are the creation and annihilation operators of a fermion in a time-independent single-particle state α.

We first consider the equation of motion for the density matrix $n_{\alpha\alpha'}$ which is defined as $n_{\alpha\alpha'} = \langle \Phi(t) | a^\dagger_{\alpha'} a_\alpha | \Phi(t) \rangle$. Here, $|\Phi(t)\rangle$ is the time-dependent total wave function $|\Phi(t)\rangle = \exp(-i(H - \mu\hat{N})/\hbar)|\Phi(0)\rangle$, where $\hat{N}$ is the number operator and μ is the chemical potential. In the equation of motion for the density matrix $i\hbar\dot{n}_{\alpha\alpha'} = \langle \Phi(t) | [a^\dagger_{\alpha'} a_\alpha, H - \mu\hat{N}] | \Phi(t) \rangle$, there appears a two-body density matrix

$\rho_{\alpha\beta\alpha'\beta'} = \langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\beta a_\alpha|\Phi(t)\rangle$. We decompose it as

$$\rho_{\alpha\beta\alpha'\beta'} = n_{\alpha\alpha'}n_{\beta\beta'} - n_{\alpha\beta'}n_{\beta\alpha'} + \kappa_{\alpha\beta}\kappa^*_{\alpha'\beta'} + \mathcal{C}_{\alpha\beta\alpha'\beta'}. \quad (2)$$

Here, $\kappa_{\alpha\beta}$ is the pairing tensor given by $\kappa_{\alpha\beta} = \langle\Phi(t)|a_\beta a_\alpha|\Phi(t)\rangle$. The matrix $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ describes two-body correlations which are not included through the pairing tensor. In TDHFB the last term in Eq. (2), that is $\mathcal{C}_{\alpha\beta\alpha'\beta'}$, is neglected. Similarly, in the equation of motion for the pairing tensor $i\hbar\dot{\kappa}_{\alpha\beta} = \langle\Phi(t)|[a_\beta a_\alpha, H - \mu\hat{N}]|\Phi(t)\rangle$, there appears a matrix given by $\langle\Phi(t)|a^\dagger_{\alpha'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle$. We decompose it as

$$\langle\Phi(t)|a^\dagger_{\alpha'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = n_{\gamma\alpha'}\kappa_{\alpha\beta} - n_{\beta\alpha'}\kappa_{\alpha\gamma} + n_{\alpha\alpha'}\kappa_{\beta\gamma} + K_{\alpha\beta\gamma:\alpha'}. \quad (3)$$

The last term in the above equation is omitted in TDHFB. The matrices $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ and $K_{\alpha\beta\gamma:\alpha'}$ describe higher-order effects. The equation for the density matrix is now extended as

$$\begin{aligned} i\hbar\dot{n}_{\alpha\alpha'} = &\sum_\lambda(\epsilon_{\alpha\lambda}n_{\lambda\alpha'} - n_{\alpha\lambda}\epsilon_{\lambda\alpha'}) + \sum_\lambda(\Delta_{\alpha\lambda}\kappa^*_{\alpha'\lambda} - \Delta^*_{\alpha'\lambda}\kappa_{\alpha\lambda}), \\ &+ \sum_{\lambda_1\lambda_2\lambda_3}[\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle\mathcal{C}_{\lambda_2\lambda_3\alpha'\lambda_1} \\ &- \mathcal{C}_{\alpha\lambda_1\lambda_2\lambda_3}\langle\lambda_2\lambda_3|v|\alpha'\lambda_1\rangle], \end{aligned} \quad (4)$$

where $\epsilon_{\alpha\alpha'}$ is given by

$$\epsilon_{\alpha\alpha'} = \langle\alpha|t|\alpha'\rangle + \sum_{\lambda_1\lambda_2}\langle\alpha\lambda_1|v|\alpha'\lambda_2\rangle_A n_{\lambda_2\lambda_1}, \quad (5)$$

and the pairing potential $\Delta_{\alpha\beta}$ by

$$\Delta_{\alpha\beta} = \frac{1}{2}\sum_{\lambda_1\lambda_2}\langle\alpha\beta|v|\lambda_1\lambda_2\rangle_A\kappa_{\lambda_1\lambda_2}. \quad (6)$$

Here, the subscript A means that the corresponding matrix is antisymmetrized. Equations (5) and (6) denote the energy-independent (static) part of the single-particle normal and anomalous self energies in Gorkov Green's function theory, respectively [13,21]. The equation of motion for $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ is given by

$$\begin{aligned} i\hbar\dot{\mathcal{C}}_{\alpha\beta\alpha'\beta'} = &\sum_\lambda(\epsilon_{\alpha\lambda}\mathcal{C}_{\lambda\beta\alpha'\beta'} + \epsilon_{\beta\lambda}\mathcal{C}_{\alpha\lambda\alpha'\beta'} - \epsilon_{\lambda\alpha'}\mathcal{C}_{\alpha\beta\lambda\beta'} \\ &- \epsilon_{\lambda\beta'}\mathcal{C}_{\alpha\beta\alpha'\lambda}) + B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'} \\ &+ S_{\alpha\beta\alpha'\beta'} + T_{\alpha\beta\alpha'\beta'}. \end{aligned} \quad (7)$$

In order to close the coupled chain of equations of motion, we approximated the matrix $\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a^\dagger_{\gamma'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle$ by antisymmetrized product combinations of $n_{\alpha\alpha'}$, $\kappa_{\alpha\beta}$, $\mathcal{C}_{\alpha\beta\alpha'\beta'}$, and $K_{\alpha\beta\gamma:\alpha'}$ such as $n_{\alpha\alpha'}n_{\beta\beta'}n_{\gamma\gamma'}$, $n_{\alpha\alpha'}\mathcal{C}_{\beta\gamma\beta'\gamma'}$, $n_{\alpha\alpha'}\kappa_{\beta\gamma}\kappa^*_{\beta'\gamma'}$, $\kappa_{\alpha\beta}K^*_{\alpha'\beta'\gamma':\gamma}$, and $\kappa^*_{\alpha'\beta'}K_{\alpha\beta\gamma:\gamma'}$. In Eq. (7) $B_{\alpha\beta\alpha'\beta'}$ describes the two-particle (2p)–two-hole (2h) and 2h-2p excitations, $P_{\alpha\beta\alpha'\beta'}$ p-p (and h-h) correlations which are not included in the pairing tensor, and $H_{\alpha\beta\alpha'\beta'}$ p-h correlations. The terms in $S_{\alpha\beta\alpha'\beta'}$ and $T_{\alpha\beta\alpha'\beta'}$ express the coupling to $\kappa_{\alpha\beta}$ and $K_{\alpha\beta\gamma:\alpha'}$, respectively. The expressions for the matrices in Eq. (7) are given in Appendix A. The equation for $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ without $S_{\alpha\beta\alpha'\beta'}$ and $T_{\alpha\beta\alpha'\beta'}$ are the same as that in TDDM [18]. Since the total wave function $|\Phi(t)\rangle$ is not an eigenstate of the number operator, the couplings to $\kappa_{\alpha\beta}$ and $K_{\alpha\beta\gamma:\alpha'}$ appear in Eq. (7).

The equation for the pairing tensor is also extended so that

$$\begin{aligned} i\hbar\dot{\kappa}_{\alpha\beta} = &\sum_\lambda(\tilde{\epsilon}_{\alpha\lambda}\kappa_{\lambda\beta} + \tilde{\epsilon}_{\beta\lambda}\kappa_{\alpha\lambda}) + \Delta_{\alpha\beta} \\ &+ \sum_\lambda(\Delta_{\beta\lambda}n_{\alpha\lambda} - \Delta_{\alpha\lambda}n_{\beta\lambda}) \\ &- \sum_{\lambda_1\lambda_2\lambda_3}(\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle K_{\beta\lambda_2\lambda_3:\lambda_1} \\ &+ \langle\lambda_1\beta|v|\lambda_2\lambda_3\rangle K_{\alpha\lambda_2\lambda_3:\lambda_1}), \end{aligned} \quad (8)$$

where $\tilde{\epsilon}_{\alpha\alpha'} = \epsilon_{\alpha\alpha'} - \mu\delta_{\alpha\alpha'}$. The equation for $K_{\alpha\beta\gamma:\alpha'}$ is written as

$$\begin{aligned} i\hbar\dot{K}_{\alpha\beta\gamma:\alpha'} = &\sum_\lambda(\tilde{\epsilon}_{\alpha\lambda}K_{\lambda\beta\gamma:\alpha'} + \tilde{\epsilon}_{\beta\lambda}K_{\alpha\lambda\gamma:\alpha'} + \tilde{\epsilon}_{\gamma\lambda}K_{\alpha\beta\lambda:\alpha'} \\ &- \tilde{\epsilon}_{\lambda\alpha'}K_{\alpha\beta\gamma:\lambda}) + D_{\alpha\beta\gamma:\alpha'} + E_{\alpha\beta\gamma:\alpha'}, \\ &+ F_{\alpha\beta\gamma:\alpha'} + G_{\alpha\beta\gamma:\alpha'}. \end{aligned} \quad (9)$$

We approximated the matrix $\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle$ by antisymmetrized product combinations of $n_{\alpha\alpha'}$, $\kappa_{\alpha\beta}$, $\mathcal{C}_{\alpha\beta\alpha'\beta'}$, and $K_{\alpha\beta\gamma:\alpha'}$. The terms in $D_{\alpha\beta\gamma:\alpha'}$ and $E_{\alpha\beta\gamma:\alpha'}$ describe the coupling to the pairing tensor and to the product of three pairing tensors, respectively. The terms in $F_{\alpha\beta\gamma:\alpha'}$ describe correlations involving $K_{\alpha\beta\gamma:\alpha'}$. The coupling to $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ is contained in $G_{\alpha\beta\gamma:\alpha'}$. The matrices in Eq. (9) are given in Appendix A. Equations (4) and (8) may be written in matrix form as in TDHFB:

$$i\hbar\dot{\mathcal{R}} - [\mathcal{H},\mathcal{R}] = [\mathcal{V},\mathcal{K}], \quad (10)$$

where in obvious notation

$$\mathcal{R} = \begin{pmatrix} n & \kappa \\ -\kappa^* & 1-n^* \end{pmatrix}, \quad (11)$$

$$\mathcal{H} = \begin{pmatrix} \epsilon & \Delta \\ -\Delta^* & -\epsilon^* \end{pmatrix}, \quad (12)$$

$$\mathcal{K} = \begin{pmatrix} \mathcal{C} & K \\ -K^* & -\mathcal{C}^* \end{pmatrix}, \quad (13)$$

$$\mathcal{V} = \begin{pmatrix} v & 0 \\ 0 & -v^* \end{pmatrix}. \quad (14)$$

The ETDHFB equation (4) conserves on average the total number of particles $N = \sum_\alpha n_{\alpha\alpha}$ as is easily shown by taking the trace of Eq. (4). Since our formalism is designed to deal with small fluctuations around the HFB ground state, ETDHFB cannot recover number symmetry broken by HFB, though higher-order effects are included, as will be shown below. The total energy $E_{\rm tot}$,

$$E_{\rm tot} = \sum_\alpha\epsilon_\alpha n_{\alpha\alpha} + \frac{1}{2}\sum_{\alpha\beta\alpha'\beta'}\langle\alpha\beta|v|\alpha'\beta'\rangle\rho_{\alpha'\beta'\alpha\beta}, \quad (15)$$

may be divided into the mean-field energy $E_{\rm MF}$, the pairing energy $E_{\rm pair}$ and the correlation energy $E_{\rm corr}$ given by

$$E_{\rm MF} = \sum_{\alpha} \epsilon_{\alpha} n_{\alpha\alpha} + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} \langle \alpha\beta | v | \alpha'\beta' \rangle_A n_{\alpha'\alpha} n_{\beta'\beta}, \quad (16)$$

$$E_{\rm pair} = \frac{1}{2} \sum_{\alpha\beta} \Delta_{\alpha\beta} \kappa^*_{\alpha\beta}, \quad (17)$$

$$E_{\rm corr} = \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} \langle \alpha\beta | v | \alpha'\beta' \rangle \mathcal{C}_{\alpha'\beta'\alpha\beta}. \quad (18)$$

To conserve $E_{\rm tot}$, we need all ETDHFB equations (4) and (7)–(9).

B. Perturbative expression

To understand various higher-order effects included in ETDHFB, we derive perturbative expressions for the pairing tensor and the two-body correlation matrix and show how the screening effect is treated in ETDHFB.

1. Pairing tensor

First we derive a perturbative expression for the pairing tensor using the equations of motion of ETDHFB. Since the F and G terms in Eq. (9) which include $K_{\alpha\beta\gamma:\alpha'}$ and $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ are of higher order, we consider only the D term and assume that the single-particle energy $\tilde{\epsilon}_{\alpha\alpha'}$, the density matrix $n_{\alpha\alpha'}$ and the pairing tensor $\kappa_{\alpha\beta}$ are diagonal: $\tilde{\epsilon}_{\alpha\alpha'} = \tilde{\epsilon}_{\alpha}\delta_{\alpha\alpha'}$, $n_{\alpha\alpha'} = n_{\alpha}\delta_{\alpha\alpha'}$, and $\kappa_{\alpha\beta} = \kappa_{\alpha}\delta_{\beta\bar{\alpha}}$ where $\bar{\alpha}$ stands for the time-reversal state of α. The E term is also neglected because $\kappa_{\alpha}\kappa_{\beta}$ is small for the p-h transition where $\bar{n}_{\alpha}n_{\beta} \approx 1$. Then Eq. (9) is written as

$$\begin{aligned} i\hbar\dot{K}_{\alpha\beta\gamma:\alpha'} \approx\ & (\tilde{\epsilon}_{\alpha} + \tilde{\epsilon}_{\beta} + \tilde{\epsilon}_{\gamma} - \tilde{\epsilon}_{\alpha'}) K_{\alpha\beta\gamma:\alpha'} \\ & - \langle \alpha\beta | v | \alpha'\bar{\gamma} \rangle_A (\bar{n}_{\alpha}\bar{n}_{\beta}n_{\alpha'} + n_{\alpha}n_{\beta}\bar{n}_{\alpha'})\kappa_{\gamma} \\ & - \langle \beta\gamma | v | \alpha'\bar{\alpha} \rangle_A (\bar{n}_{\beta}\bar{n}_{\gamma}n_{\alpha'} + n_{\beta}n_{\gamma}\bar{n}_{\alpha'})\kappa_{\alpha} \\ & + \langle \alpha\gamma | v | \alpha'\bar{\beta} \rangle_A (\bar{n}_{\alpha}\bar{n}_{\gamma}n_{\alpha'} + n_{\alpha}n_{\gamma}\bar{n}_{\alpha'})\kappa_{\beta}, \end{aligned} \quad (19)$$

where $\bar{n}_{\alpha} = 1 - n_{\alpha}$. The stationary condition $\dot{K}_{\alpha\beta\gamma:\alpha'} = 0$ gives a perturbative expression for $K_{\alpha\beta\gamma:\alpha'}$. Inserting it into Eq. (8) and using the stationary condition $\dot{\kappa}_{\alpha\beta} = 0$, we can write the equation for the pairing tensor as

$$\begin{aligned} 2\tilde{\epsilon}_{\alpha}\kappa_{\alpha} \approx\ & -(1 - 2n_{\alpha})\Delta_{\alpha} + 2 \sum_{\lambda_1\lambda_2\lambda_3} \langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle_A \\ & \times \frac{\bar{n}_{\alpha}\bar{n}_{\lambda_3}n_{\lambda_1} + n_{\alpha}n_{\lambda_3}\bar{n}_{\lambda_1}}{\tilde{\epsilon}_{\alpha} + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \langle \bar{\alpha}\lambda_3 | v | \bar{\lambda}_2\lambda_1 \rangle_A \kappa_{\lambda_2} \\ & + \sum_{\lambda_1\lambda_2\lambda_3} \langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle_A \frac{\bar{n}_{\lambda_2}\bar{n}_{\lambda_3}n_{\lambda_1} + n_{\lambda_2}n_{\lambda_3}\bar{n}_{\lambda_1}}{\tilde{\epsilon}_{\alpha} + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \\ & \times \langle \lambda_2\lambda_3 | v | \alpha\lambda_1 \rangle_A \kappa_{\alpha}. \end{aligned} \quad (20)$$

The second term on the right-hand side can be interpreted as a correction to Δ_{α} because it contains the sum over the pairing tensor as the pair potential does. The corresponding diagram is shown in Fig. 1(a). We call it the screening term because a similar process has been shown responsible for the screening of the pairing correlation [1–3,6]. The last term on

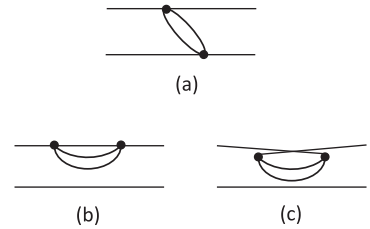

FIG. 1. Schematic presentation of higher-order effects: (a) Screening effect, and (b) and (c) self-energy correction. Lines depict single-particle states and dots the residual interaction.

the right-hand side of Eq. (20) can be interpreted as the self-energy correction to the single-particle energies $2\tilde{\epsilon}_{\alpha}$ because it is proportional to κ_{α} as the term on the left-hand side of Eq. (20). The corresponding diagrams are schematically shown in Figs. 1(b) and 1(c). Using the BCS relations

$$n^0_{\alpha} = v^2_{\alpha} = \frac{1}{2}\left(1 - \frac{\tilde{\epsilon}_{\alpha}}{E_{\alpha}}\right), \quad (21)$$

$$\kappa^0_{\alpha} = v_{\alpha}u_{\alpha} = -\frac{1}{2\tilde{\epsilon}_{\alpha}}(1 - 2n^0_{\alpha})\Delta_{\alpha} = -\frac{1}{2E_{\alpha}}\Delta_{\alpha}, \quad (22)$$

where κ^0_{α} is the pairing tensor in BCS and E_{α} is the quasiparticle energy $E_{\alpha} = \sqrt{\tilde{\epsilon}^2_{\alpha} + \Delta^2_{\alpha}}$, and expressing $2\tilde{\epsilon}_{\alpha}\kappa_{\alpha} - 2n_{\alpha}\Delta_{\alpha}$ as $2E_{\alpha}\kappa_{\alpha}$, we solve Eq. (20) for the pairing tensor:

$$\begin{aligned} \kappa_{\alpha} \approx\ & \kappa^0_{\alpha} + \frac{1}{E_{\alpha}} \sum_{\lambda_1\lambda_2\lambda_3} \langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle_A \frac{\bar{n}^0_{\alpha}\bar{n}^0_{\lambda_3}n^0_{\lambda_1} + n^0_{\alpha}n^0_{\lambda_3}\bar{n}^0_{\lambda_1}}{\tilde{\epsilon}_{\alpha} + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \\ & \times \langle \bar{\alpha}\lambda_3 | v | \bar{\lambda}_2\lambda_1 \rangle_A \kappa^0_{\lambda_2} + \frac{\kappa^0_{\alpha}}{2E_{\alpha}} \sum_{\lambda_1\lambda_2\lambda_3} \langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle_A \\ & \times \frac{\bar{n}^0_{\lambda_2}\bar{n}^0_{\lambda_3}n^0_{\lambda_1} + n^0_{\lambda_2}n^0_{\lambda_3}\bar{n}^0_{\lambda_1}}{\tilde{\epsilon}_{\alpha} + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \langle \lambda_2\lambda_3 | v | \alpha\lambda_1 \rangle_A. \end{aligned} \quad (23)$$

Inserting the above expression for κ_{α} into Eq. (6), we obtain the pair potential and also the correction to the pairing energy Eq. (17). In the case of the simple contact interaction $v(\boldsymbol{r} - \boldsymbol{r}') = g\delta^3(\boldsymbol{r} - \boldsymbol{r}')$ which is often used in the study of pairing correlations the spin state of the single-particle state λ_2 in the screening term of Eq. (23) must be the same as $\bar{\alpha}$. This means that $\kappa^0_{\lambda_2}$ has a sign opposite to κ^0_{α}. Therefore, the screening effect is compensated by the self-energy correction. The effects of the mean-field contribution and the partial occupation of the single-particle states are also included through $\tilde{\epsilon}_{\alpha}$ and the Pauli blocking factor, respectively.

2. Relation to other perturbative approaches

Next we discuss the relation of our perturbative formulation and the expression used in Refs. [2,3,6] to study the screening effect. The latter is related to the self-energy $\Sigma_{1\alpha}$ of the Gorkov Green's function (see Appendix B), where

$$\begin{aligned} \Sigma_{1\alpha} =\ & \sum_{\lambda_1\lambda_2\lambda_3} \langle \alpha\lambda_1 | v | \lambda_2\lambda_3 \rangle_A \\ & \times \frac{n_{\lambda_3} - n_{\lambda_1}}{\omega_{\mu} + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \langle \bar{\alpha}\lambda_3 | v | \bar{\lambda}_2\lambda_1 \rangle_A \kappa_{\lambda_2}. \end{aligned} \quad (24)$$

We focus on the second term on the right-hand side of Eq. (20) and neglect for the purpose of discussion for the moment the last term (the self-energy correction). Rewriting the numerator of the second term as

$$\bar{n}_\alpha \bar{n}_{\lambda_3} n_{\lambda_1} + n_\alpha n_{\lambda_3} \bar{n}_{\lambda_1} = \bar{n}_{\lambda_3} n_{\lambda_1} + n_\alpha \left(n_{\lambda_3} \bar{n}_{\lambda_1} - \bar{n}_{\lambda_3} n_{\lambda_1} \right) = \bar{n}_{\lambda_3} n_{\lambda_1} + n_\alpha \left(n_{\lambda_3} - n_{\lambda_1} \right), \quad (25)$$

we can express Eq. (20) without the self-energy contribution such that

$$2\tilde{\epsilon}_\alpha \kappa_\alpha = -(\Delta_\alpha + \Sigma_\alpha) + 2n_\alpha \Delta'_\alpha, \quad (26)$$

where

$$\Sigma_\alpha = -2 \sum_{\lambda_1 \lambda_2 \lambda_3} \langle \alpha \lambda_1 | v | \lambda_2 \lambda_3 \rangle_A \frac{\bar{n}_{\lambda_3} n_{\lambda_1}}{\tilde{\epsilon}_\alpha + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \times \langle \bar{\alpha} \lambda_3 | v | \bar{\lambda}_2 \lambda_1 \rangle_A \kappa_{\lambda_2} \quad (27)$$

and $\Delta'_\alpha = \Delta_\alpha + \Sigma_{1\alpha}(\omega_\mu = \tilde{\epsilon}_\alpha)$. If we consider the single-particle state near μ ($\tilde{\epsilon}_\alpha \approx 0$) and assume that the pairing tensor for the single-particle state around μ dominates (this means also $\tilde{\epsilon}_{\lambda_2} \approx 0$), $\Sigma_{1\alpha}$ is simplified to

$$\Sigma_{1\alpha}(\omega_\mu \approx 0) \approx \sum_{\lambda_1 \lambda_2 \lambda_3} \langle \alpha \lambda_1 | v | \lambda_2 \lambda_3 \rangle_A \frac{n_{\lambda_3} - n_{\lambda_1}}{\tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \langle \bar{\alpha} \lambda_3 | v | \bar{\lambda_2} \lambda_1 \rangle_A \kappa_{\lambda_2} \quad (28)$$

and Σ_α is also given by

$$\Sigma_\alpha \approx -2 \sum_{\lambda_1 \lambda_2 \lambda_3} \langle \alpha \lambda_1 | v | \lambda_2 \lambda_3 \rangle_A \frac{\bar{n}_{\lambda_3} n_{\lambda_1}}{\tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \langle \bar{\alpha} \lambda_3 | v | \bar{\lambda}_2 \lambda_1 \rangle_A \kappa_{\lambda_2} = \sum_{\lambda_1 \lambda_2 \lambda_3} \langle \alpha \lambda_1 | v | \lambda_2 \lambda_3 \rangle_A \frac{n_{\lambda_3} - n_{\lambda_1}}{\tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \langle \bar{\alpha} \lambda_3 | v | \bar{\lambda}_2 \lambda_1 \rangle_A \kappa_{\lambda_2}. \quad (29)$$

In this limit the relation $\Sigma_\alpha \approx \Sigma_{1\alpha}$ holds and Eq. (26) is written as

$$2\tilde{\epsilon}_\alpha \kappa_\alpha = -(1 - 2n_\alpha)\Delta'_\alpha. \quad (30)$$

If Eq. (30) is treated as the BCS equation for κ_α, we obtain the modified quasiparticle energy $E'_\alpha = \sqrt{\tilde{\epsilon}_\alpha^2 + \Delta_\alpha'^2}$ and pairing tensor $\kappa'_\alpha = -\Delta'_\alpha / 2E'_\alpha$. The modified gap equation is written as

$$\Delta'_\alpha = -\sum_\lambda F_{\alpha:\lambda} \frac{\Delta'_\lambda}{2E'_\lambda}, \quad (31)$$

where $F_{\alpha:\lambda}$ is given by

$$F_{\alpha:\lambda} = \frac{1}{2} \langle \alpha \bar{\alpha} | v | \lambda \bar{\lambda} \rangle_A + \sum_{\lambda_1 \lambda_2} \langle \alpha \lambda_1 | v | \lambda \lambda_2 \rangle_A \frac{n_{\lambda_2} - n_{\lambda_1}}{\tilde{\epsilon}_{\lambda_2} - \tilde{\epsilon}_{\lambda_1}} \times \langle \bar{\alpha} \lambda_2 | v | \bar{\lambda} \lambda_1 \rangle_A. \quad (32)$$

When we further assume that $n_\alpha = 0$ or 1, we arrive at the perturbative expression of Refs. [2,3,6]. For a simple contact interaction $g\delta^3(\boldsymbol{r} - \boldsymbol{r}')$ Eq. (28) always gives a positive value (screening). The difference between Eqs. (26) and (30) stems from the difference in the occupation factors in the numerator between Eqs. (20) and (24). The occupation factor in Eq. (20) describes a blocking effect of the p-h excitation caused by the existence of another particle. As discussed, this difference may be small if pairing is concentrated to states close to the Fermi level (weak coupling).

3. *Two-body correlation matrix*

Now we consider the corrections to the correlation energy Eq. (18) which are given by the pertubative expression for the two-body correlation matrix. In Eq. (7) the terms in $P_{\alpha\beta\alpha'\beta'}$ and $H_{\alpha\beta\alpha'\beta'}$ contain $\mathcal{C}_{\alpha\beta\alpha'\beta'}$, and $T_{\alpha\beta\alpha'\beta'}$ includes $K_{\alpha\beta\gamma:\alpha'}$. Therefore, the lowest-order corrections are from $B_{\alpha\beta\alpha'\beta'}$ and $S_{\alpha\beta\alpha'\beta'}$. The pertubative expression for $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ obtained using only the terms in $S_{\alpha\beta\alpha'\beta'}$ in Eq. (7) is given by

$$\mathcal{C}_{1\alpha\beta\alpha'\beta'} = \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_{\alpha'} - \epsilon_{\beta'}} \left[\langle \alpha \bar{\beta}' | v | \alpha' \bar{\beta} \rangle_A \kappa^0_\beta \kappa^{0*}_{\beta'} \left(n^0_\alpha - n^0_{\alpha'} \right) + \langle \beta \bar{\alpha}' | v | \beta' \bar{\alpha} \rangle_A \kappa^0_\alpha \kappa^{0*}_{\alpha'} \left(n^0_\beta - n^0_{\beta'} \right) - \langle \alpha \bar{\alpha}' | v | \beta' \bar{\beta} \rangle_A \kappa^0_\beta \kappa^{0*}_{\alpha'} \left(n^0_\alpha - n^0_{\beta'} \right) - \langle \beta \bar{\beta}' | v | \alpha' \bar{\alpha} \rangle_A \kappa^0_\alpha \kappa^{0*}_{\beta'} \left(n^0_\beta - n^0_{\alpha'} \right) \right]. \quad (33)$$

The perturbative expression for $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ obtained from Eq. (7) with only the $B_{\alpha\beta\alpha'\beta'}$ is written as

$$\mathcal{C}_{2\alpha\beta\alpha'\beta'} = -\frac{\langle \alpha\beta | v | \alpha'\beta' \rangle_A}{\epsilon_\alpha + \epsilon_\beta - \epsilon_{\alpha'} - \epsilon_{\beta'}} \times \left(\bar{n}^0_\alpha \bar{n}^0_\beta n^0_{\alpha'} n^0_{\beta'} - n^0_\alpha n^0_\beta \bar{n}^0_{\alpha'} \bar{n}^0_{\beta'} \right), \quad (34)$$

which describes the 2p-2h and 2h-2p excitations. The corrections to the correlation energy obtained from $\mathcal{C}_{1\alpha\beta\alpha'\beta'}$ and $\mathcal{C}_{2\alpha\beta\alpha'\beta'}$ are related to the self-energies $\Sigma_{1\alpha}$ (Eq. (24)) and $\Sigma_{2\alpha}$ of the Gorkov Green's function (see Appendix B), where

$$\Sigma_{2\alpha} = -\frac{1}{2} \sum_{\lambda_1 \lambda_2 \lambda_3} \langle \alpha \lambda_1 | v | \lambda_2 \lambda_3 \rangle_A \frac{\bar{n}_{\lambda_2} \bar{n}_{\lambda_3} n_{\lambda_1} + n_{\lambda_2} n_{\lambda_3} \bar{n}_{\lambda_1}}{\omega_\mu + \tilde{\epsilon}_{\lambda_2} + \tilde{\epsilon}_{\lambda_3} - \tilde{\epsilon}_{\lambda_1}} \times \langle \lambda_2 \lambda_3 | v | \alpha \lambda_1 \rangle_A. \quad (35)$$

The self-energy $\Sigma_{1\alpha}$ describes a correction to the pair potential Δ_α, similarly to the screening term in Eq. (23), whereas $\Sigma_{2\alpha}$ is a correction to the mean-field potential as is the case of the normal single-particle Green's function. The correlation energy obtained from $\mathcal{C}_{1\alpha\beta\alpha'\beta'}$ corresponds to the contribution of $\Sigma_{1\alpha}$ to the total energy because it is written as $\sum_\alpha \Sigma_{1\alpha} \kappa^*_\alpha$, whereas the correlation energy obtained from $\mathcal{C}_{2\alpha\beta\alpha'\beta'}$ corresponds to the contribution of $\Sigma_{2\alpha}$. The correlation energy obtained from $\mathcal{C}_{2\alpha\beta\alpha'\beta'}$ gives a significant correction to the BCS total energy in the case of the pairing Hamiltonian [22–24].

III. NUMERICAL RESULTS

A. Pairing Hamiltonian

To check the validity of ETDHFB, we first apply it to the well-known pairing Hamiltonian [22]

$$H = \sum_{i=1}^{\Omega} \epsilon_\alpha (a^\dagger_i a_i + a^\dagger_{\bar{i}} a_{\bar{i}}) - g \sum_{i \neq j}^{\Omega} a^\dagger_i a^\dagger_{\bar{i}} a_{\bar{j}} a_j. \quad (36)$$

Here g is the strength of the pairing force acting in a space of Ω twofold degenerate equidistant orbitals with the single-particle energies $\epsilon_i = (i - 1)\Delta\epsilon$. This Hamiltonian has extensively

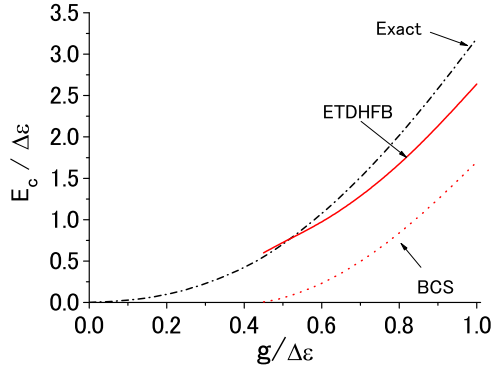

FIG. 2. (Color online) Interaction energy E_c as a function of g calculated in ETDHFB (solid line) for $N = \Omega = 6$. The dotted line depict the results in BCS. The dot-dashed line shows the exact solutions.

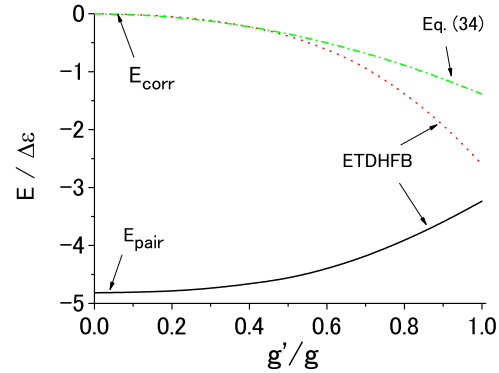

FIG. 3. (Color online) Pairing energy $E_{\rm pair}$ (solid line) and correlation energy $E_{\rm corr}$ (dotted line) as a function of g'/g calculated in ETDHFB for $N = \Omega = 6$ and $g/\Delta\epsilon = 1$. The correlation energy calculated using the perturbative expression for the two-body correlation matrix Eq. (34) is shown with the dot-dashed line. The values at $g'/g = 0$ correspond to the results in BCS.

been used to investigate the validity of theoretical models; see, e.g., [22–24]. The ground state in ETDHFB is obtained using an adiabatic method [25]: Starting from the BCS ground state, we solve the ETDHFB equations [Eqs. (4) and (7)–(9) together with the expressions given in Appendix A] by gradually increasing the residual interaction such that $g' = g \times t/T$. This method is motivated by the Gell-Mann–Low theorem [26] and has often been used to obtain approximate ground states [19]. To suppress oscillating components which come from the mixing of excited states, we must take large T: We use $T = 2400$ fm/c for $\Delta\epsilon = 1$ MeV.

The interaction energy E_c, which is defined by the difference between the energy of the HF configuration $E_{\rm HF}$ and the total energy $E(g)$ at g as $E_c = E_{\rm HF} - E(g)$, is shown in Fig. 2 as a function of g for $N = \Omega = 6$. It is well known [22–24] that BCS underestimates the interaction energy for the pairing Hamiltonian. ETDHFB significantly improves BCS because additional two-body correlations such as 2p-2h excitations are included through the two-body correlation matrix $\mathcal{C}_{\alpha\beta\alpha'\beta'}$. However, ETDHFB still slightly underestimates the correlation energy as shown in Fig. 2. This indicates that three-body correlations or higher play a role in the case of the pairing Hamiltonian [23].

The pairing energy $E_{\rm pair}$ (solid line) and the correlation energy $E_{\rm corr}$ (dotted line) calculated in ETDHFB are shown in Fig. 3 as a function of g'/g for $N = \Omega = 6$ and $g/\Delta\epsilon = 1$. Note that $E_{\rm pair}$ and $E_{\rm corr}$ in ETDHFB are defined by Eqs. (17) and (18). The values at $g'/g = 0$ correspond to the BCS results. The correlation energy calculated using the perturbative expression for the two-body correlation matrix Eq. (34) is also shown by the dot-dashed line. The pairing Hamiltonian Eq. (36) has no matrix elements for 1p-1h excitations and, therefore, cannot induce the screening effect: The screening term in Eq. (23) and the correlation energy from Eq. (33) vanish. The self-energy correction in Eq. (23) is also canceled out in the case of the half-filling $N = \Omega$. Therefore, the increase in the pairing energy calculated in ETDHFB is caused by higher-order correlations in Eq. (9). The difference between the dashed and dot-dahsed lines in Fig. 3 also indicates the importance of higher-order effects. The increase in the pairing energy is overcompensated by the decrease in the correlation energy, and the correlation energy gives a significant correction to the results in BCS as has been pointed out in Refs. [23,24].

The ratio E_c(ETDHFB)/E_c(exact) is 0.83 at $N = \Omega = 6$ and $g/\Delta\epsilon = 1$. Since BCS becomes better approximation with increasing N, the ratio increases with N: We found that the ratio in ETDHFB for $N = \Omega = 12$ and $g/\Delta\epsilon = 1$ is 0.88. This is of the same order as the result from the quasiparticle coupled-cluster approach for the same number of particles [16]. On the other hand, the higher-order effects included in ETDHFB also play a role in reducing the number fluctuation measured by $\sigma_N = \sqrt{\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2}$: σ_N in BCS for $N = \Omega = 6$ and $g/\Delta\epsilon = 1$ is 2.00 whereas the corresponding value in ETDHFB is 1.65. The reduction of σ_N may be associated with the increase in $E_{\rm pair}$ shown in Fig. 3. The reduction of σ_N in ETDHFB is not so drastic as in the quasiparticle coupled-cluster approach [16].

In this subsection we found that ETDHFB yields substantial improvement over BCS for the pairing Hamiltonian. It should be pointed out, however, that important aspects such as screening due to particle-hole correlations are absent in the pairing Hamiltonian and, therefore, important terms in ETDHFB are not activated and, thus, not tested. In the following model cases this aspect will be addressed.

B. Trapped fermions

We consider a system of fermions with spin one half, which is trapped in a spherically symmetric harmonic potential with frequency ω. The system is described by the Hamiltonian

$$H = \sum_{\alpha} \epsilon_\alpha a^\dagger_\alpha a_\alpha + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} \langle\alpha\beta|v|\alpha'\beta'\rangle a^\dagger_\alpha a^\dagger_\beta a_{\beta'} a_{\alpha'}, \qquad (37)$$

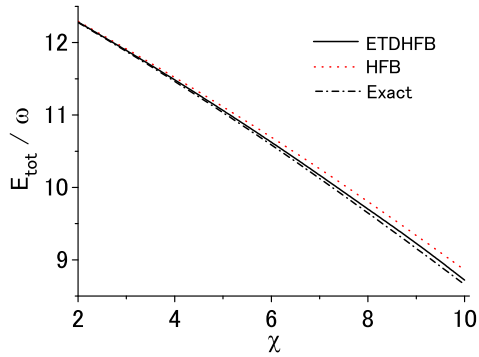

FIG. 4. (Color online) Total energy as a function of χ calculated in ETDHFB (solid line). The dotted line depicts the results in HFB. The exact solutions are given by the dot-dashed line.

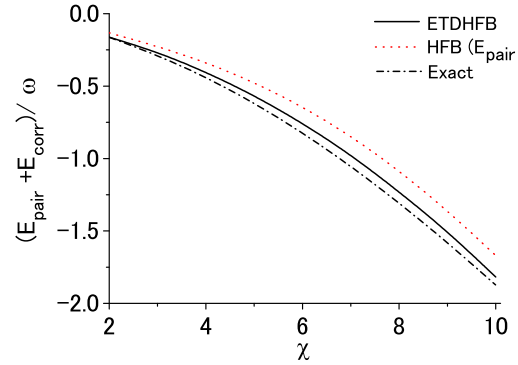

FIG. 5. (Color online) Sum $E_{\rm pair} + E_{\rm corr}$ as as a function of χ calculated in ETDHFB (solid line). The dot-dashed line depicts the exact solutions. $E_{\rm pair}$ in HFB is shown with the dotted line.

where $a^\dagger_\alpha$ and a_α are the creation and annihilation operators of an atom at a harmonic oscillator state α corresponding to the trapping potential $V(r) = m\omega^2 r^2/2$ and $\epsilon_\alpha = \hbar\omega(n + 3/2)$ with $n = 0,1,2,\ldots$. We assume that α contains the spin quantum number σ. In Eq. (37) $\langle\alpha\beta|v|\alpha'\beta'\rangle$ is the matrix element of an attractive contact interaction $v(\boldsymbol{r} - \boldsymbol{r}') = g\delta^3(\boldsymbol{r} - \boldsymbol{r}')$.

We consider a system consisting of six fermions whose noninteracting configuration consists of the partially filled $1p$ state. Besides a trap with a small number of cold atoms, our system may correspond to neutrons in carbon isotopes. For numerical reasons we only can handle a very restricted space and small number of particles, since we want to compare with exact solutions. Using a limited number of the single-particle states, the $1s$, $1p$, $1d$, and $2s$ states, we obtain the ground states in the Hartree-Fock-Bogoliubov (HFB) theory and the ETDHFB theory, and compare with the exact solution obtained from the diagonalization of the Hamiltonian using the same single-particle space. The ground state in ETDHFB is obtained using the adiabatic method [25]: Starting from the HFB ground state, we solve the coupled set of the ETDHFB equations by gradually increasing the residual interaction $g' = g \times t/T$. We use $T = 4 \times 2\pi/\omega$.

The total energy calculated in ETDHFB (solid line) is shown in Fig. 4 as a function of χ, where χ is given by $\chi = |g|/\hbar\omega\xi^3$ with ξ being the oscillator length ($\xi = \sqrt{\hbar/m\omega}$). In the case of nuclei for which $\hbar\omega \approx 10$ MeV is applied, $\chi = 5$ corresponds to $|g| \approx 400$ MeV fm^3, which is similar to the strength of nuclear pairing interactions commonly used for a small single-particle space [23]. Both the ETDHFB and HFB results (dotted line) agree well with the exact solutions (dot-dashed line). The better agreement of the ETDHFB results is due to the contribution of the correlation energy as shown in Fig. 5, where the sum $E_{\rm pair} + E_{\rm corr}(= E_{\rm tot} - E_{\rm MF})$ calculated in ETDHFB (solid line) is given as a function of χ. In HFB the pairing energy $E_{\rm pair}(= E_{\rm tot} - E_{\rm MF})$ is shown. In the exact case the difference $\Delta E = E_{\rm tot} - E_{\rm MF}$ is shown (dot-dashed line). HFB underestimates the correlation energy, which agrees with the results of the pairing model [22–24] and finite nuclei [23]. The small deviation of the ETDHFB results from the exact values in Fig. 5 means that $n_{\alpha\alpha'}$ and $\rho_{\alpha\beta\alpha'\beta'}$ in ETDHFB also agree with the exact solutions. The difference in the total energy is smaller than that in the correlation energy. This is due to a cancellation of errors between the mean-field energy and the correlation energy [23].

The pairing energy $E_{\rm pair}$ (solid line) and $E_{\rm corr}$ (dot-dashed line) calculated with ETDHFB are shown in Fig. 6 as a function of g'/g for $\chi = 5$. The perturbatively calculated correlation energies using Eq. (33) [the green (gray) dashed line] and Eq. (34) [green (gray) double-dot–dashed line] are also shown. The latter has a significant contribution, which is in agreement with the results for the pairing Hamiltonian [23,24]. As mentioned above, the former describes a correction to the total energy due to the screening effect. In the case of the trapped fermions it is quite small and plays a role opposite to screening. The sum $\Delta_\alpha + \Sigma_{1\alpha}$ is shown in Fig. 7 for each single-particle state. The self-energy is calculated

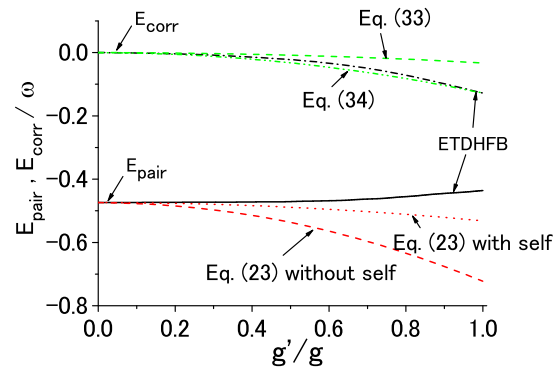

FIG. 6. (Color online) Pairing energy $E_{\rm pair}$ (solid line) and $E_{\rm corr}$ (dot-dashed line) calculated in ETDHFB for $\chi = 5$ as a function of g'/g. The correlation energy calculated using the perturbative expression for the two-body correlation matrix Eq. (34) is shown with the green (gray) double-dot–dashed line. The correlation energy obtained from the two-body correlation matrix Eq. (33) is also shown with the green (gray) dashed line. The dotted and dashed lines depict the results of the perturbative approach Eq. (23) with and without the self-energy correction, respectively. $E_{\rm pair}$ and $E_{\rm corr}$ at $g'/g = 0$ correspond to the values in HFB.

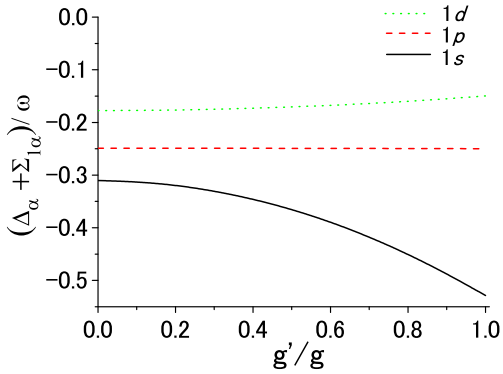

FIG. 7. (Color online) Pair potential plus the screening term $\Delta_\alpha + \Sigma_{1\alpha}$ as a function of g'/g for $\chi = 5$. The solid, dashed, and dotted lines depict the results for the $1s$, $1p$, and $1d$ states, respectively. The self-energy is calculated at $\omega_\mu = -\tilde{\epsilon}_\alpha$. The values at $g'/g = 0$ correspond to the results in HFB.

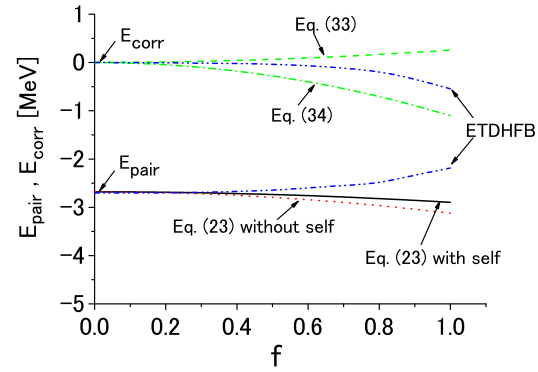

FIG. 8. (Color online) Pairing energy as a function of f calculated in the perturbative approaches for ^{106}Sn. The solid and dotted lines depict the results with and without the self-energy correction, respectively. The correlation energy calculated using the perturbative expressions for the two-body correlation matrix, Eqs. (33) and (34), are shown with the green (gray) dashed and dot-dashed lines, respectively. The pairing energy and correlation energy in ETDHFB are shown with the upper and lower double-dot–dashed lines, respectively. The values at $g'/g = 0$ correspond to the results in BCS.

at $\omega_\mu = -\tilde{\epsilon}_\alpha$. The anti-screening behavior of the correlation energy calculated with $\mathcal{C}_{1\alpha\beta\alpha'\beta'}$ is determined by the self-energy $\Sigma_{1\alpha}$ of the $1s$ state. This indicates that the conditions used to derive Eq. (28) are not fulfilled for the $1s$ state.

We also test the perturbative approximations for the pairing tensor. The dotted and dashed lines in Fig. 6 show the results obtained using Eq. (23) with and without the self-energy correction, respectively. In these calculations the pairing tensor given by Eq. (23) where g' is used for the higher-order terms (the v^2 terms) and the pairing potentials in HFB are used in Eq. (17). Comparison of the results shown by the dotted and dashed lines indicates that the self-energy correction is significant and almost cancels the screening effect for the pairing tensor. This strong cancellation is explained by the facts that the dominant contributions to the sums in Eq. (23) come from the $1p$ states because the pairing tensor is the largest for these states, and that only the doubly exchanged matrices in the screening term contribute because of their spin characters of the matrix elements. As shown in Fig. 6, the pairing energy in ETDHFB is slightly increased from the HFB value while the perturbative approach (dotted line) gives a slight decrease of the pairing energy. We found that the coupling to $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ in $G_{\alpha\beta\gamma:\alpha'}$ is responsible for the slight reduction of the pairing correlation in ETDHFB.

C. Tin isotopes

In the case of tin isotopes we first perform the BCS+HF calculations following the numerical procedure used in Ref. [27]. The Skyrme III interaction is used to calculate the single-particle states. For the BCS calculations of n_α and κ_α we take the neutron single-particle states, the $1g_{7/2}$, $2d_{5/2}$, $1h_{11/2}$, $3s_{1/2}$, and $2d_{3/2}$ states. As the pairing interaction we use $v = f_0(t_0 + t_3\rho_p)\delta^3(\boldsymbol{r} - \boldsymbol{r}')$ derived from the Skyrme III force with $x_0 = 0$, where ρ_p is the proton density. A reduction factor $f_0 = 0.55$ is used to approximately reproduce the excitation energy of the first 2^+ state in ^{108}Sn in an extended version of the random-phase approximation (RPA) [27]. This interaction is similar to a density-dependent pairing interaction $v_0(1 - \rho/\rho_0)\delta^3(\boldsymbol{r} - \boldsymbol{r}')$, which has often been used in the HFB and quasiparticle RPA calculations. To simulate the p-h excitations of the core in the pertubative calculations of the higher-order effects, we add several neutron states in the range $-20 \leqslant \epsilon_\alpha \leqslant 1$ MeV: The continuum states are discretized by confining the wave functions in a sphere with radius 15 fm [27]. There are two occupied states, ($2p_{1/2}$ and $1g_{9/2}$) and 1 to 4 unoccupied states ($2f_{7/2}$, $3p_{1/2}$, $3p_{3/2}$, and $1h_{9/2}$), depending on the isotope. We use the same pairing interaction in the perturbative calculations.

The pairing energies calculated in HF+BCS are -2.68, -4.65, and -4.27 MeV for ^{106}Sn, ^{116}Sn, and ^{126}Sn, respectively. These isotopes correspond to the beginning, middle, and end of the subshell. The pairing energies calculated using the perturbative expression for the pairing tensor Eq. (23) are shown in Figs. 8–10 as a function of the strength f of the residual interaction: The pairing interaction v used in the

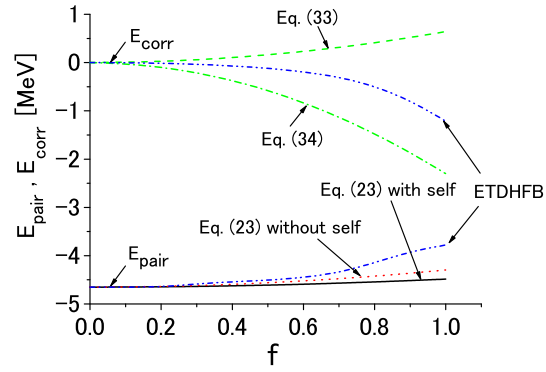

FIG. 9. (Color online) Same as Fig. 8 but for ^{116}Sn.

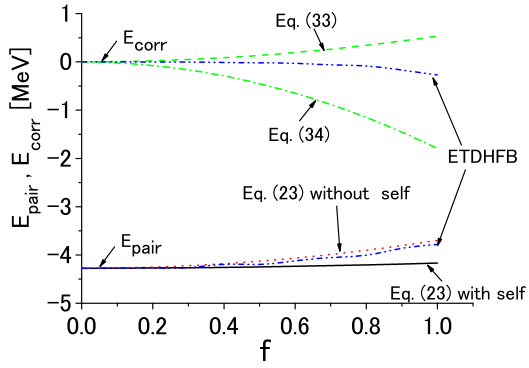

FIG. 10. (Color online) Same as Fig. 8 but for ^{126}Sn.

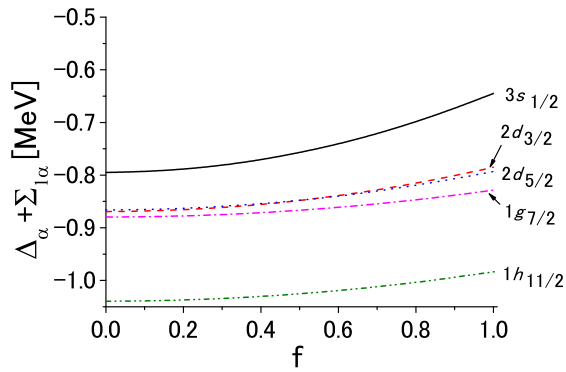

FIG. 11. (Color online) Sum $\Delta_\alpha + \Sigma_{1\alpha}$ as a function of f for ^{116}Sn. The solid, dashed, dotted, dot-dashed and double-dot–dashed lines depict the results for the $3s_{1/2}$, $2d_{3/2}$, $2d_{5/2}$, $1g_{7/2}$, and $1h_{11/2}$ states, respectively. The self-energy is calculated at $\omega_\mu = -\tilde{\epsilon}_\alpha$. The values at $g'/g = 0$ correspond to the results in BCS.

second-order terms in Eq. (23) is multiplied with an artificial factor f ($f = 1$ corresponds to the full strength). As is the case of the trapped fermion system, there is a cancellation between the screening term and the self-energy term. However, the perturbative correction to the pairing tensor is quite small in the case of the tin isotopes. This may be explained by the fact that the p-h excitation energies in the tin isotopes normalized by the averaged pairing potential are a few times larger than those in the trapped fermion systems. We also performed perturbative calculations for the pairing energy including the proton single-particle states in the energy range from -20 to 1 MeV to see the effects of proton p-h excitations on the screening. The results depend on isotope. We found a small antiscreening in ^{106}Sn and ^{116}Sn and an increase in screening in ^{126}Sn: The change in the pairing energy due to the proton p-h excitations is less than 2.5%.

The correlation energies calculated using Eq. (33) [green (gray) dashed line] and Eq. (34) [green (gray) dot-dashed line] are also shown in Figs. 8–10. The corrections to the total energy from the two-body correlation matrix are much larger than those from the pairing tensor. The correlation energies calculated using Eq. (33) are positive, which means that the pairing correlation is screened by the process given by the self-energy $\Sigma_{1\alpha}$ as is shown in Fig. 11, where the sum $\Delta_\alpha + \Sigma_{1\alpha}$ is given for each single-particle state of ^{116}Sn. The self-energy is calculated at $\omega_\mu = -\tilde{\epsilon}_\alpha$. The results shown in Fig 11 indicate that the conditions used in the derivation of Eq. (28) are approximately fulfilled.

In the ETDHFB calculations we use a small single-particle space consisting of the neutron $1g_{7/2}$, $2d_{5/2}$, $1h_{11/2}$, $3s_{1/2}$, and $2d_{3/2}$ states because it is hard to calculate the two-body matrices using the same single-particle space as used in the perturbative calculations. The ETDHFB results for the pairing energy (lower double dot-dashed line) and the correlation energy (upper double-dot–dashed line) are shown in Figs. 8–10 as a function of $f = t/T$, where $T = 1200$ fm/c is used. The pairing energies in ETDHFB are slightly increased from the perturbative results, indicating the contribution of nonperturbative effects as is the case of the trapped fermion system. The correlation energies in ETDHF are similar to the sum of the perturbative results from Eqs. (33) and (34) except for ^{126}Sn. In the case of ^{126}Sn the subshell is almost filled and the p-h excitations are limited within the small single-particle space used.

IV. SUMMARY

In order to study higher-order effects on the pairing correlation, we formulated an extended time-dependent Hartree-Fock-Bogoliubov theory (ETDHFB) using a truncation scheme of the time-dependent density matrix theory. This approach allows us to calculate the pairing tensor and the two-body correlation matrix in a nonperturbative way and it also is used to derive their perturbative expressions. We showed that the perturbative expression for the two-body correlation matrix which contains the pairing tensor has a direct connection to other approaches used in the study of the screening effect of the pairing correlation. We tested ETDHFB for a pairing model and fermions trapped in a harmonic potential where comparison with the exact solution could be made and obtained reasonable agreement with the exact solutions. We applied the perturbative expressions to the trapped fermion system and the tin isotopes, and compared with the results in ETDHFB. It was found thatm for the systems considered, the perturbative correction to the pairing energy is small both in the trapped fermion system and tin isotopes, whereas ETDHFB always gives a slight increase of the pairing energy, indicating the importance of nonperturbative effects. It was found that the perturbative correction to the correlation energy expressed by the pairing tensor shows a screening effect in the case of the tin isotopes. It was also found that the perturbative corrections to the correlation energy supplemented by the contribution of two-particle–two-hole excitations are similar to the results from full ETDHFB. The results of our calculations indicate that the screening correction to the results in HFB or BCS+HF is at most a few tens percent in the case of small finite systems considered here, although more quantitative analysis using larger single-particle space is required.

APPENDIX A

We present the terms in the equations of motion for $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ and $K_{\alpha\beta\gamma:\alpha'}$. Since decomposition of higher-order density matrices to lower-order ones involves various combinations due to the fact that the total wave function is not an eigenstate of the number operator, these equations contain many terms. We try to explain the meanings of each term as clearly as possible.

1. Terms in Eq. (7)

The terms in Eq. (7) are given below. $B_{\alpha\beta\alpha'\beta'}$ describes the 2p-2h and 2h-2p excitations as in TDDM [18].

$$B_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \big[\big(\delta_{\alpha\lambda_1} - n_{\alpha\lambda_1}\big)\big(\delta_{\beta\lambda_2} - n_{\beta\lambda_2}\big)n_{\lambda_3\alpha'}n_{\lambda_4\beta'} - n_{\alpha\lambda_1}n_{\beta\lambda_2}\big(\delta_{\lambda_3\alpha'} - n_{\lambda_3\alpha'}\big)\big(\delta_{\lambda_4\beta'} - n_{\lambda_4\beta'}\big)\big]. \tag{A1}$$

Particle-particle and h-h correlations which are not included in the pairing tensor are described by $P_{\alpha\beta\alpha'\beta'}$:

$$P_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle \big[\big(\delta_{\alpha\lambda_1}\delta_{\beta\lambda_2} - \delta_{\alpha\lambda_1}n_{\beta\lambda_2} - n_{\alpha\lambda_1}\delta_{\beta\lambda_2}\big)\mathcal{C}_{\lambda_3\lambda_4\alpha'\beta'} - \big(\delta_{\lambda_3\alpha'}\delta_{\lambda_4\beta'} - \delta_{\lambda_3\alpha'}n_{\lambda_4\beta'} - n_{\lambda_3\alpha'}\delta_{\lambda_4\beta'}\big)\mathcal{C}_{\alpha\beta\lambda_1\lambda_2}\big]. \tag{A2}$$

$H_{\alpha\beta\alpha'\beta'}$ describes p-h correlations:

$$\begin{aligned} H_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \big[&\delta_{\alpha\lambda_1}\big(n_{\lambda_3\alpha'}\mathcal{C}_{\lambda_4\beta\lambda_2\beta'} - n_{\lambda_3\beta'}\mathcal{C}_{\lambda_4\beta\lambda_2\alpha'}\big) + \delta_{\beta\lambda_2}\big(n_{\lambda_4\beta'}\mathcal{C}_{\lambda_3\alpha\lambda_1\alpha'} - n_{\lambda_4\alpha'}\mathcal{C}_{\lambda_3\alpha\lambda_1\beta'}\big) \\ &- \delta_{\alpha'\lambda_3}\big(n_{\alpha\lambda_1}\mathcal{C}_{\lambda_4\beta\lambda_2\beta'} - n_{\beta\lambda_1}\mathcal{C}_{\lambda_4\alpha\lambda_2\beta'}\big) - \delta_{\beta'\lambda_4}\big(n_{\beta\lambda_2}\mathcal{C}_{\lambda_3\alpha\lambda_1\alpha'} - n_{\alpha\lambda_2}\mathcal{C}_{\lambda_3\beta\lambda_1\alpha'}\big)\big]. \end{aligned} \tag{A3}$$

The coupling to the pairing tensor is given by $S_{\alpha\beta\alpha'\beta'}$:

$$\begin{aligned} S_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \big[&\delta_{\alpha\lambda_1}\big(n_{\lambda_3\alpha'}\kappa_{\lambda_4\beta}\kappa^*_{\lambda_2\beta'} - n_{\lambda_3\beta'}\kappa_{\lambda_4\beta}\kappa^*_{\lambda_2\alpha'}\big) + \delta_{\beta\lambda_2}\big(n_{\lambda_4\beta'}\kappa_{\lambda_3\alpha}\kappa^*_{\lambda_1\alpha'} - n_{\lambda_4\alpha'}\kappa_{\lambda_3\alpha}\kappa^*_{\lambda_1\beta'}\big) \\ &- \delta_{\alpha'\lambda_3}\big(n_{\alpha\lambda_1}\kappa_{\lambda_4\beta}\kappa^*_{\lambda_2\beta'} - n_{\beta\lambda_1}\kappa_{\lambda_4\alpha}\kappa^*_{\lambda_2\beta'}\big) - \delta_{\beta'\lambda_4}\big(n_{\beta\lambda_2}\kappa_{\lambda_3\alpha}\kappa^*_{\lambda_1\alpha'} - n_{\alpha\lambda_2}\kappa_{\lambda_3\beta}\kappa^*_{\lambda_1\alpha'}\big)\big]. \end{aligned} \tag{A4}$$

From the decomposition

$$\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a^\dagger_{\gamma'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = \langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}|\Phi(t)\rangle\langle\Phi(t)|a^\dagger_{\gamma'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle + \cdots \tag{A5}$$

we obtain $T_{\alpha\beta\alpha'\beta'}$ which expresses the coupling to $K_{\alpha\beta\gamma:\alpha'}$:

$$\begin{aligned} T_{\alpha\beta\alpha'\beta'} = &\sum_\lambda (\Delta_{\alpha\lambda}K^*_{\lambda\beta'\alpha':\beta} - \Delta_{\beta\lambda}K^*_{\lambda\beta'\alpha':\alpha} - \Delta^*_{\alpha'\lambda}K_{\alpha\beta\lambda:\beta'} + \Delta^*_{\beta'\lambda}K_{\alpha\beta\lambda:\alpha'}) + \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \\ &\times \big[\delta_{\alpha\lambda_1}\big(2\kappa_{\beta\lambda_4}K^*_{\beta'\lambda_2\alpha':\lambda_3} + \kappa^*_{\beta'\lambda_2}K_{\beta\lambda_4\lambda_3:\alpha'} - \kappa^*_{\alpha'\lambda_2}K_{\beta\lambda_4\lambda_3:\beta'}\big) - \delta_{\beta\lambda_1}\big(2\kappa_{\alpha\lambda_4}K^*_{\beta'\lambda_2\alpha':\lambda_3} + \kappa^*_{\beta'\lambda_2}K_{\alpha\lambda_4\lambda_3:\alpha'} - \kappa^*_{\alpha'\lambda_2}K_{\alpha\lambda_4\lambda_3:\beta'}\big) \\ &- \delta_{\alpha'\lambda_3}\big(2\kappa^*_{\lambda_2\beta'}K_{\alpha\lambda_4\beta:\lambda_1} + \kappa_{\alpha\lambda_4}K^*_{\lambda_1\lambda_2\beta':\beta} - \kappa_{\beta\lambda_4}K^*_{\lambda_1\lambda_2\beta':\alpha}\big) + \delta_{\beta'\lambda_3}\big(2\kappa^*_{\lambda_2\alpha'}K_{\alpha\lambda_4\beta:\lambda_1} + \kappa_{\alpha\lambda_4}K^*_{\lambda_1\lambda_2\alpha':\beta} - \kappa_{\beta\lambda_4}K^*_{\lambda_1\lambda_2\alpha':\alpha}\big)\big]. \end{aligned} \tag{A6}$$

The terms in the first sum describe the coupling to the pairing potential. Since the terms in the second sum contain both p-p (and h-h) and p-h correlations, they may describe corrections to $P_{\alpha\beta\alpha'\beta'}$ and $H_{\alpha\beta\alpha'\beta'}$. In the derivation of Eq. (7) we neglected the genuine three-body density matrix $\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a^\dagger_{\gamma'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle$ as in TDDM.

2. Terms in Eq. (9)

The terms in Eq. (9) are given below. $D_{\alpha\beta\gamma:\alpha'}$ describes the coupling to one pairing tensor:

$$\begin{aligned} D_{\alpha\beta\gamma:\alpha'} = &-\sum_{\lambda_1\lambda_2}(\langle\alpha\beta|v|\lambda_1\lambda_2\rangle_A\kappa_{\gamma\lambda_2} + \langle\beta\gamma|v|\lambda_1\lambda_2\rangle_A\kappa_{\alpha\lambda_2} - \langle\alpha\gamma|v|\lambda_1\lambda_2\rangle_A\kappa_{\beta\lambda_2})n_{\lambda_1\alpha'} \\ &+ \sum_{\lambda_1\lambda_2\lambda_3}\big[\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\big(n_{\beta\lambda_1}\kappa_{\gamma\lambda_3} - n_{\gamma\lambda_1}\kappa_{\beta\lambda_3}\big) + \langle\beta\lambda_1|v|\lambda_2\lambda_3\rangle_A\big(n_{\gamma\lambda_1}\kappa_{\alpha\lambda_3} - n_{\alpha\lambda_1}\kappa_{\gamma\lambda_3}\big) \\ &+ \langle\gamma\lambda_1|v|\lambda_2\lambda_3\rangle_A\big(n_{\alpha\lambda_1}\kappa_{\beta\lambda_3} - n_{\beta\lambda_1}\kappa_{\alpha\lambda_3}\big)\big]n_{\lambda_2\alpha'} + \sum_{\lambda_1\lambda_2\lambda_3}\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle_A\big(n_{\alpha\lambda_1}n_{\gamma\lambda_2}\kappa_{\beta\lambda_3} - n_{\beta\lambda_1}n_{\gamma\lambda_2}\kappa_{\alpha\lambda_3} - n_{\alpha\lambda_1}n_{\beta\lambda_2}\kappa_{\gamma\lambda_3}\big). \end{aligned} \tag{A7}$$

The terms in the first sum originate from the decomposition

$$\langle\Phi(t)|a^\dagger_{\alpha'}a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = \langle\Phi(t)|a^\dagger_{\alpha'}a_\gamma|\Phi(t)\rangle\langle\Phi(t)|a_\beta a_\alpha|\Phi(t)\rangle + \cdots, \tag{A8}$$

whereas those in the second and third sums from

$$\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = \langle\Phi(t)|a^\dagger_{\alpha'}a_\alpha|\Phi(t)\rangle\langle\Phi(t)|a^\dagger_{\beta'}a_\delta|\Phi(t)\rangle\langle\Phi(t)|a_\gamma a_\beta|\Phi(t)\rangle + \cdots. \tag{A9}$$

The perturbative expression for the pairing tensor Eq. (23) is obtained from the first term and $D_{\alpha\beta\gamma:\alpha'}$ in Eq. (9). From the decomposition of the matrix

$$\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = \langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}|\Phi(t)\rangle\langle\Phi(t)|a_\delta a_\gamma|\Phi(t)\rangle\langle\Phi(t)|a_\beta a_\alpha|\Phi(t)\rangle + \cdots, \tag{A10}$$

we also obtain the coupling to three paring tensors given by $E_{\alpha\beta\gamma:\alpha'}$,

$$E_{\alpha\beta\gamma:\alpha'} = -\sum_{\lambda_1\lambda_2\lambda_3}(\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\kappa_{\beta\lambda_2}\kappa_{\gamma\lambda_3} - \langle\beta\lambda_1|v|\lambda_2\lambda_3\rangle_A\kappa_{\alpha\lambda_2}\kappa_{\gamma\lambda_3} + \langle\gamma\lambda_1|v|\lambda_2\lambda_3\rangle_A\kappa_{\alpha\lambda_2}\kappa_{\beta\lambda_3})\kappa^*_{\alpha'\lambda_1}. \tag{A11}$$

These terms express the modification of the two-particle propagator due to the pairing correlations with other particles. The terms in $F_{\alpha\beta\gamma:\alpha'}$ are from

$$\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = \langle\Phi(t)|a^\dagger_{\alpha'}a_\alpha|\Phi(t)\rangle\langle\Phi(t)|a^\dagger_{\beta'}a_\delta a_\gamma a_\beta|\Phi(t)\rangle + \cdots \tag{A12}$$

and describe correlations among $K_{\alpha\beta\gamma:\alpha'}$:

$$\begin{aligned}F_{\alpha\beta\gamma:\alpha'} = \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A\big[&\big(\delta_{\alpha\lambda_1}\delta_{\beta\lambda_2} - \delta_{\alpha\lambda_1}n_{\beta\lambda_2} - \delta_{\beta\lambda_2}n_{\alpha\lambda_1}\big)K_{\gamma\lambda_3\lambda_4:\alpha'} + \big(\delta_{\beta\lambda_1}\delta_{\gamma\lambda_2} - \delta_{\beta\lambda_1}n_{\gamma\lambda_2} - \delta_{\gamma\lambda_2}n_{\beta\lambda_1}\big)K_{\alpha\lambda_3\lambda_4:\alpha'}\\ &- \big(\delta_{\alpha\lambda_1}\delta_{\gamma\lambda_2} - \delta_{\alpha\lambda_1}n_{\gamma\lambda_2} - \delta_{\gamma\lambda_2}n_{\alpha\lambda_1}\big)K_{\beta\lambda_3\lambda_4:\alpha'}\big] + \sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A\bigg[\frac{1}{2}\big(\delta_{\alpha\lambda_1}K_{\beta\gamma\lambda_3:\lambda_2} - \delta_{\beta\lambda_1}K_{\alpha\gamma\lambda_3:\lambda_2}\\ &+ \delta_{\gamma\lambda_1}K_{\alpha\beta\lambda_3:\lambda_2}\big)n_{\lambda_4\alpha'} + \delta_{\lambda_3\alpha'}\big(n_{\gamma\lambda_2}K_{\alpha\beta\lambda_4:\lambda_1} - n_{\beta\lambda_2}K_{\alpha\gamma\lambda_4:\lambda_1} - n_{\alpha\lambda_2}K_{\gamma\beta\lambda_4:\lambda_1}\big)\bigg].\end{aligned} \tag{A13}$$

The terms in the first sum describe p-p (and h-h) correlations while those in the second sum p-h correlations. Since these terms contain $K_{\alpha\beta\gamma:\alpha'}$, they describe the coupling to collective p-p, h-h, and p-h correlations. The terms in $G_{\alpha\beta\gamma:\alpha'}$ come from

$$\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle = \langle\Phi(t)|a_\delta a_\gamma|\Phi(t)\rangle\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\beta a_\alpha|\Phi(t)\rangle + \cdots: \tag{A14}$$

$$\begin{aligned}G_{\alpha\beta\gamma:\alpha'} = \sum_\lambda(\Delta_{\alpha\lambda}\mathcal{C}_{\beta\gamma\alpha'\lambda} - \Delta_{\beta\lambda}\mathcal{C}_{\alpha\gamma\alpha'\lambda} + \Delta_{\gamma\lambda}\mathcal{C}_{\alpha\beta\alpha'\lambda}) - \sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A\big[&\big(\delta_{\alpha\lambda_1}\kappa_{\beta\lambda_3} - \delta_{\beta\lambda_1}\kappa_{\alpha\lambda_3}\big)\mathcal{C}_{\gamma\lambda_4\alpha'\lambda_2}\\ &+ \big(\delta_{\beta\lambda_1}\kappa_{\gamma\lambda_3} - \delta_{\gamma\lambda_1}\kappa_{\beta\lambda_3}\big)\mathcal{C}_{\alpha\lambda_4\alpha'\lambda_2} - \big(\delta_{\alpha\lambda_1}\kappa_{\gamma\lambda_3} - \delta_{\gamma\lambda_1}\kappa_{\alpha\lambda_3}\big)\mathcal{C}_{\beta\lambda_4\alpha'\lambda_2}\big].\end{aligned} \tag{A15}$$

These terms describe the coupling to $\mathcal{C}_{\alpha\beta\alpha'\beta'}$. In the above derivation of Eq. (9) the genuine correlated matrices $\langle\Phi(t)|a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle$ and $\langle\Phi(t)|a_\delta a_\gamma a_\beta a_\alpha|\Phi(t)\rangle$ are neglected.

APPENDIX B

We consider the Gorkov Green's function

$$\mathcal{G}_{\alpha\beta}(t,t') = \begin{pmatrix} G_{\alpha\beta}(t,t') & F_{\alpha\beta}(t,t') \\ -F^*_{\alpha\beta}(t,t') & -G^*_{\alpha\beta}(t,t')\end{pmatrix}, \tag{B1}$$

where $iG_{\alpha\beta}(t,t') = \langle0|T(a_\alpha(t)a^\dagger_\beta(t'))|0\rangle$ and $iF_{\alpha\beta}(t,t') = \langle0|T(a_\alpha(t)a_\beta(t'))|0\rangle$ with $a_\alpha(t) = \exp[i(H-\mu\hat{N})t/\hbar]a_\alpha\exp[-i(H-\mu\hat{N})t/\hbar]$. The Green's functions are written in terms of the transition amplitudes $x^\mu_\alpha = \langle\mu|a_\alpha|0\rangle$ and $y^\mu_\alpha = \langle\mu|a^\dagger_\alpha|0\rangle$ as

$$\begin{aligned}iG_{\alpha\beta}(t,t') = \theta(t-t')\langle0|a_\alpha(t)a^\dagger_\beta(t')|0\rangle - \theta(t'-t)\langle0|a^\dagger_\beta(t')a_\alpha(t)|0\rangle = \sum_\mu[&\theta(t-t')\langle0|a_\alpha|\mu\rangle\langle\mu|a^\dagger_\beta|0\rangle e^{-i\omega_\mu(t-t')/\hbar}\\ &- \theta(t'-t)\langle0|a^\dagger_\beta|\mu\rangle\langle\mu|a_\alpha|0\rangle e^{-i\omega_\mu(t'-t)/\hbar}] = \sum_\mu[\theta(t-t')(y^\mu_\alpha)^*y^\mu_\beta e^{-i\omega_\mu(t-t')/\hbar} - \theta(t'-t)(x^\mu_\beta)^*x^\mu_\alpha e^{-i\omega_\mu(t'-t)/\hbar}],\end{aligned} \tag{B2}$$

$$i F_{\alpha\beta}(t,t') = \theta(t-t')\langle 0|a_\alpha(t)a_\beta(t')|0\rangle - \theta(t'-t)\langle 0|a_\beta(t')a_\alpha(t)|0\rangle = \sum_\mu [\theta(t-t')\langle 0|a_\alpha|\mu\rangle\langle\mu|a_\beta|0\rangle e^{-i\omega_\mu(t-t')/\hbar}$$
$$- \theta(t'-t)\langle 0|a_\beta|\mu\rangle\langle\mu|a_\alpha|0\rangle e^{-i\omega_\mu(t'-t)/\hbar}] = \sum_\mu [\theta(t-t')(y^\mu_\alpha)^* x^\mu_\beta e^{-i\omega_\mu(t-t')/\hbar} - \theta(t'-t)\left(y^\mu_\beta\right)^* x^\mu_\alpha e^{-i\omega_\mu(t'-t)/\hbar}]. \tag{B3}$$

The equations of motion for the Green's functions can be formulated using the equations of motion for the transition amplitudes x^μ_α and y^μ_α [13]. First we derive the perturbative expressions for the self-energies of the Green's function $G_{\alpha\beta}(t,t')$ which are related to corrections to the pairing potential and the mean-field potential. The equation motion for x^μ_α is written as

$$\omega_\mu x^\mu_\alpha = \langle\mu|[H-\mu\hat{N},a_\alpha]|0\rangle = -\tilde{\epsilon}_\alpha x^\mu_\alpha - \Delta_\alpha y^\mu_{\bar{\alpha}} - \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3}\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A X^\mu_{\lambda_2\lambda_3:\lambda_1}, \tag{B4}$$

where $X^\mu_{\alpha\beta:\alpha'} = \langle\mu|a^\dagger_{\alpha'}a_\beta a_\alpha|0\rangle$. We assume that $\epsilon_{\alpha\alpha'} = \epsilon_\alpha\delta_{\alpha\alpha'}$, $n_{\alpha\alpha'} = n_\alpha\delta_{\alpha\alpha'}$ and $\Delta_{\alpha\beta} = \Delta_\alpha\delta_{\beta\bar{\alpha}}$. The equation of motion for $X^\mu_{\alpha\beta:\alpha'}$ contains the terms proportional to y^μ_α and x^μ_α

$$\omega_\mu X^\mu_{\alpha\beta:\alpha'} = \langle\mu|[H-\mu\hat{N},a^\dagger_{\alpha'}a_\beta a_\alpha]|0\rangle = (\tilde{\epsilon}_{\alpha'} - \tilde{\epsilon}_\alpha - \tilde{\epsilon}_\beta)X^\mu_{\alpha\beta:\alpha'} + \sum_\lambda[\langle\lambda\alpha|v|\alpha'\bar{\beta}\rangle_A(n_\alpha - n_{\alpha'})\kappa_\beta$$
$$- \langle\lambda\beta|v|\alpha'\bar{\alpha}\rangle_A(n_\beta - n_{\alpha'})\kappa_\alpha]y^\mu_\lambda + \sum_\lambda\langle\alpha\beta|v|\alpha'\lambda\rangle_A(\bar{n}_\alpha\bar{n}_\beta n_{\alpha'} + n_\alpha n_\beta\bar{n}_{\alpha'})x^\mu_\lambda + \text{ more terms with } X^\mu_{\alpha\beta:\alpha'}. \tag{B5}$$

Inserting $X^\mu_{\alpha\beta:\alpha'}$ into Eq. (B4), we obtain

$$\omega_\mu x^\mu_\alpha = -\tilde{\epsilon}_\alpha x^\mu_\alpha - \Delta_\alpha y^\mu_{\bar{\alpha}} - \sum_{\lambda\lambda_1\lambda_2\lambda_3}\left[\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\frac{n_{\lambda_3}-n_{\lambda_1}}{\omega_\mu+\tilde{\epsilon}_{\lambda_2}+\tilde{\epsilon}_{\lambda_3}-\tilde{\epsilon}_{\lambda_1}}\langle\lambda\lambda_3|v|\bar{\lambda}_2\lambda_1\rangle_A\kappa_{\lambda_2}\right]y^\mu_\lambda$$
$$+\frac{1}{2}\sum_{\lambda\lambda_1\lambda_2\lambda_3}\left[\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\frac{\bar{n}_{\lambda_2}\bar{n}_{\lambda_3}n_{\lambda_1}+n_{\lambda_2}n_{\lambda_3}\bar{n}_{\lambda_1}}{\omega_\mu+\tilde{\epsilon}_{\lambda_2}+\tilde{\epsilon}_{\lambda_3}-\tilde{\epsilon}_{\lambda_1}}\langle\lambda_2\lambda_3|v|\lambda\lambda_1\rangle_A\right]x^\mu_\lambda. \tag{B6}$$

The third term is the perturbative expression of the self-energy describing a correction to the pairing potential Δ_α and the last term a correction to the mean-field potential. The diagonal part of the third term $\Sigma_{1\alpha}$ is given as

$$\Sigma_{1\alpha} = \sum_{\lambda_1\lambda_2\lambda_3}\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\frac{n_{\lambda_3}-n_{\lambda_1}}{\omega_\mu+\tilde{\epsilon}_{\lambda_2}+\tilde{\epsilon}_{\lambda_3}-\tilde{\epsilon}_{\lambda_1}}\langle\bar{\alpha}\lambda_3|v|\bar{\lambda}_2\lambda_1\rangle_A\kappa_{\lambda_2}. \tag{B7}$$

Similarly, the self-energy $\Sigma_{2\alpha}$ for the last term of Eq. (B6) is given by

$$\Sigma_{2\alpha} = -\frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3}\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\frac{\bar{n}_{\lambda_2}\bar{n}_{\lambda_3}n_{\lambda_1}+n_{\lambda_2}n_{\lambda_3}\bar{n}_{\lambda_1}}{\omega_\mu+\tilde{\epsilon}_{\lambda_2}+\tilde{\epsilon}_{\lambda_3}-\tilde{\epsilon}_{\lambda_1}}\langle\lambda_2\lambda_3|v|\alpha\lambda_1\rangle_A. \tag{B8}$$

Next we show that the equation for the pairing tensor [Eq. (8)] is derived from that for $F_{\alpha\beta}(t,t')$. This is because the pairing tensor is given as the equal-time limit of $F_{\alpha\beta}(t,t')$ as

$$\lim_{t'\to t+0}(-i)F_{\alpha\beta}(t,t') = \kappa_{\alpha\beta} = \sum_\mu\left(y^\mu_\beta\right)^* x^\mu_\alpha. \tag{B9}$$

The equation motion for y^μ_α is written as

$$\omega_\mu y^\mu_\alpha = \langle\mu|[H-\mu\hat{N},a^\dagger_\alpha]|0\rangle = \tilde{\epsilon}_\alpha y^\mu_\alpha + \Delta^*_\alpha x^\mu_{\bar{\alpha}} + \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3}\langle\lambda_1\lambda_2|v|\alpha\lambda_3\rangle_A Y^\mu_{\lambda_3:\lambda_1\lambda_2}, \tag{B10}$$

where $Y^\mu_{\alpha':\alpha\beta} = \langle\mu|a^\dagger_\alpha a^\dagger_\beta a_{\alpha'}|0\rangle$. Using Eq. (B4) and the complex conjugate of Eq. (B10) (we assume ω_μ is real), we calculate $\sum_\mu[\omega_\mu(y^\mu_{\bar{\alpha}})^* x^\mu_\alpha - (y^\mu_{\bar{\alpha}})^*\omega_\mu x^\mu_\alpha]$ and obtain

$$0 = 2\tilde{\epsilon}_\alpha\sum_\mu\left(y^\mu_{\bar{\alpha}}\right)^* x^\mu_\alpha + \Delta_\alpha\sum_\mu\left(y^\mu_{\bar{\alpha}}\right)^* y^\mu_{\bar{\alpha}} - \Delta_\alpha\sum_\mu\left(x^\mu_\alpha\right)^* x^\mu_\alpha + \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3}\langle\alpha\lambda_1|v|\lambda_2\lambda_3\rangle_A\sum_\mu\left(y^\mu_{\bar{\alpha}}\right)^* X^\mu_{\lambda_2\lambda_3:\lambda_1}$$
$$+\frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_3}\langle\bar{\alpha}\lambda_1|v|\lambda_2\lambda_3\rangle_A\sum_\mu\left(Y^\mu_{\lambda_1:\lambda_2\lambda_3}\right)^* x^\mu_\alpha. \tag{B11}$$

When the replacements $\sum_\mu (y^\mu_{\bar\alpha})^* x^\mu_\alpha = \kappa_\alpha$, $\sum_\mu (y^\mu_{\bar\alpha})^* y^\mu_{\bar\alpha} = 1 - n_\alpha$, $\sum_\mu (x^\mu_\alpha)^* x^\mu_\alpha = n_\alpha$, and $\sum_\mu (y^\mu_{\bar\alpha})^* X^\mu_{\lambda_2\lambda_3:\lambda_1} = -\sum_\mu (Y^\mu_{\lambda_1:\lambda_2\lambda_3})^* x^\mu_\alpha = -K_{\alpha\lambda_2\lambda_3:\lambda_1}$ are made, the above equation is of the same form as Eq. (8) for a stationary solution. From the equations of motion for x^μ_α, y^μ_α, $X^\mu_{\alpha\beta:\alpha'}$, and $Y^\mu_{\alpha':\alpha\beta}$, we can derive the pertubative expression for κ_α [Eq. (20)]. Let us discuss this point in some more detail. Considering $\sum_\mu [\omega_\mu (y^\mu_\gamma)^* X^\mu_{\alpha\beta:\alpha'} - (y^\mu_\gamma)^* \omega_\mu X^\mu_{\alpha\beta:\alpha'}]$, we show that the term $\sum_\mu (y^\mu_\gamma)^* X^\mu_{\alpha\beta:\alpha}$ on the right-hand side of Eq. (B11) is reduced to $-K_{\alpha\beta\gamma:\alpha'}$ given in Eq. (19). From the equations of motion for y^μ_γ and $X^\mu_{\alpha\beta:\alpha'}$ we obtain

$$0 = (\tilde\epsilon_\alpha + \tilde\epsilon_\beta + \tilde\epsilon_\gamma - \tilde\epsilon_{\alpha'}) \sum_\mu \left(y^\mu_\gamma\right)^* X^\mu_{\alpha\beta:\alpha'} - \sum_{\mu\lambda} [\langle\lambda\alpha|v|\alpha'\bar\beta\rangle_A (n_\alpha - n_{\alpha'})\kappa_\beta - \langle\lambda\beta|v|\alpha'\bar\alpha\rangle_A (n_\beta - n_{\alpha'})\kappa_\alpha] \left(y^\mu_\gamma\right)^* y^\mu_\lambda$$

$$- \sum_{\mu\lambda} \langle\alpha\beta|v|\alpha'\lambda\rangle_A (\bar n_\alpha \bar n_\beta n_{\alpha'} + n_\alpha n_\beta \bar n_{\alpha'}) \left(y^\mu_\gamma\right)^* x^\mu_\lambda + \frac{1}{2} \sum_{\mu\lambda_1\lambda_2\lambda_3} \langle\gamma\lambda_3|v|\lambda_1\lambda_2\rangle_A \left(Y^\mu_{\lambda_3:\lambda_1\lambda_2}\right)^* X^\mu_{\alpha\beta:\alpha'}. \tag{B12}$$

If we use $\sum_\mu (y^\mu_\beta)^* x^\mu_\alpha = \delta_{\beta\bar\alpha}\kappa_\alpha$, $\sum_\mu (y^\mu_\alpha)^* y^\mu_\beta = \delta_{\alpha\beta}(1 - n_\alpha)$, and the additional relation

$$\sum_\mu \left(Y^\mu_{\alpha':\alpha\beta}\right)^* X^\mu_{\sigma\rho:\sigma'} = \sum_\mu \langle 0|a^\dagger_{\alpha'} a_\beta a_\alpha |\mu\rangle\langle\mu|a^\dagger_{\sigma'} a_\rho a_\sigma|0\rangle \approx \delta_{\sigma'\alpha}(\delta_{\sigma\bar\beta}\delta_{\rho\alpha'} - \delta_{\rho\bar\beta}\delta_{\sigma\alpha'})\bar n_\alpha n_{\alpha'}\kappa_\beta - \delta_{\sigma'\beta}(\delta_{\sigma\bar\alpha}\delta_{\rho\alpha'} - \delta_{\rho\bar\alpha}\delta_{\sigma\alpha'})\bar n_\beta n_{\alpha'}\kappa_\alpha, \tag{B13}$$

the right-hand side of Eq. (B12) becomes that of Eq. (19). In a similar way it can be shown that the sum $\sum_\mu (Y^\mu_{\lambda_1:\lambda_2\lambda_3})^* x^\mu_\alpha$ on the right-hand side of Eq. (B11) becomes $K_{\alpha\lambda_2\lambda_3:\lambda_1}$ given by Eq. (19). The equations for $n_{\alpha\alpha'}$ and $\mathcal{C}_{\alpha\beta\alpha'\beta'}$ are also related to those for x^μ_α, y^μ_α, $X^\mu_{\alpha\beta:\alpha'}$, and $Y^\mu_{\alpha':\alpha\beta}$.

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