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Spurious modes in Extended RPA theories

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Abstract. The necessary conditions that the spurious state associated with the translational motion and its double-phonon state have zero excitation energy in Extended RPA (ERPA) theories which include both one-body and two-body amplitudes are investigated using the small-amplitude limit of the time-dependent density-matrix theory (STDDM). STDDM provides us with a quite general form of ERPA, as compared with other similar theories, in the sense that all components of one-body and two-body amplitudes are taken into account. Two conditions are found necessary to guarantee the above property of the single and double spurious states: The first is that no truncation in the single-particle space should be made. This condition is necessary for the closure relation to be used and is common for the single and double spurious states. The second depends on the mode. For the single spurious state all components of the one-body amplitudes must be included, and for the double spurious state all components of one-body and two-body amplitudes have to be included. It is also shown that the Kohn theorem and the continuity equations for transition densities and currents hold under the same conditions as the spurious states. ERPA theories formulated using the Hartree-Fock ground state have a non-hermiticity problem. A method for formulating ERPA with hermiticity is also proposed using the time-dependent density-matrix formalism.

PACS. 21.60.Jz Hartree-Fock and random-phase approximations

1 Introduction

The double-phonon states of giant resonances have become the subject of a number of recent experimental and theoretical investigations [1,2]. In the case of giant resonances (single-phonon states), the Random Phase Approximation (RPA) has extensively been used as a standard microscopic theory to study basic properties of giant resonances [3]. It is guaranteed in RPA that physical states do not couple to spurious states such as that associated with the translational motion because RPA in the Hartree-Fock (HF) basis gives zero excitation energy to spurious states [4]. For a microscopic study of the double-phonon states of giant resonances, we need to extend RPA to deal with two-body amplitudes as well as one-body amplitudes. One of such an Extended RPA theory (ERPA) may be the Second RPA (SRPA) [5] which has also extensively been used to study decay properties of giant resonances [6,7]. When the double-phonon states are studied in ERPA, it should be guaranteed that both spurious states and their double-phonon states are decoupled from physical states. The aim of this paper is to investigate the necessary conditions that the spurious state associated with the translational motion and its double-phonon state, *i.e.* the single and double spurious modes, have zero excitation energy in ERPA. We use the small-amplitude limit of the time-dependent density-matrix theory (STDDM) [8]. The reason why STDDM is used is that, containing all components of one-body and two-body amplitudes, STDDM constitutes a more general framework of ERPA than SRPA. It will be shown that keeping all components of the one-body and two-body amplitudes in ERPA is essential in bringing the spurious states to zero excitation energy. We would like to point out that to our knowledge the issue of the double spurious mode in ERPAs has never been addressed before in the literature. Any ERPA including STDDM, which is formulated using an approximate ground state, inherently has asymmetry and non-hermiticity. A method for recovering symmetry and hermiticity in the framework of the time-dependent density-matrix formalism is also proposed in this paper. The paper is organized as follows: STDDM is presented and its relation to other ERPA formulations is discussed in sect. 2. The necessary conditions to give zero excitation energy to the spurious state associated with the translational motion and its double-phonon state are discussed in sect. 3. The Kohn theorem [9–11] and the continuity equations for transition densities and

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currents are also discussed as related subjects in sect. 3. In sect. 4 a method for formulating ERPA with hermiticity is proposed and sect. 5 is devoted to a summary.

2 Extended RPA formalism

2.1 Small-amplitude limit of the time-dependent density-matrix theory

The time-dependent density-matrix theory (TDDM) gives the time evolution of a one-body density-matrix $\rho(1,1')$ and the correlated part $C(12,1'2')$ of a two-body density-matrix [12], where numbers denote space, spin, and isospin coordinates. Linearizing the equations of motion for ρ and C with respect to $\delta\rho$ and δC, where $\delta\rho$ and δC denote deviations from the ground-state values ρ_0 and C_0, *i.e.* $\delta\rho = \rho - \rho_0$ and $\delta C = C - C_0$, respectively, we obtain STDDM [8]. Expanding $\delta\rho$ and δC with single-particle states ψ_α as

$$\delta\rho(11',t) = \sum_{\alpha\alpha'} x_{\alpha\alpha'}(t)\psi_\alpha(1,t)\psi^*_{\alpha'}(1',t), \tag{1}$$

$$\delta C(121'2',t) = \sum_{\alpha\beta\alpha'\beta'} X_{\alpha\beta\alpha'\beta'}(t) \times\psi_\alpha(1,t)\psi_\beta(2,t)\psi^*_{\alpha'}(1',t)\psi^*_{\beta'}(2',t), \tag{2}$$

and assuming the HF ground state, that is, ρ_0 is the one-body density-matrix in HF approximation and $C_0 = 0$, we obtain the following equations of STDDM for the Fourier components of $x_{\alpha\alpha'}(t)$ and $X_{\alpha\beta\alpha'\beta'}(t)$ [8]:

$$\begin{aligned}(\omega - \epsilon_\alpha + \epsilon_{\alpha'})x_{\alpha\alpha'} = {}& (f_{\alpha'} - f_\alpha)\sum_{\lambda\lambda'}\langle\alpha\lambda|v|\alpha'\lambda'\rangle_A x_{\lambda'\lambda} \\ &+ \sum_{\lambda\lambda'\lambda''}[X_{\lambda\lambda'\alpha'\lambda''}\langle\alpha\lambda''|v|\lambda\lambda'\rangle \\ &-X_{\alpha\lambda'\lambda\lambda''}\langle\lambda\lambda''|v|\alpha'\lambda'\rangle],\end{aligned} \tag{3}$$

$$\begin{aligned}&(\omega - \epsilon_\alpha - \epsilon_\beta + \epsilon_{\alpha'} + \epsilon_{\beta'})X_{\alpha\beta\alpha'\beta'} = \\ &\quad -\sum_\lambda[(\bar f_\beta f_{\alpha'} f_{\beta'} + f_\beta \bar f_{\alpha'}\bar f_{\beta'})\langle\lambda\beta|v|\alpha'\beta'\rangle_A x_{\alpha\lambda} \\ &\quad +(\bar f_\alpha f_{\alpha'} f_{\beta'} + f_\alpha \bar f_{\alpha'}\bar f_{\beta'})\langle\alpha\lambda|v|\alpha'\beta'\rangle_A x_{\beta\lambda} \\ &\quad -(\bar f_\alpha \bar f_\beta f_{\beta'} + f_\alpha f_\beta \bar f_{\beta'})\langle\alpha\beta|v|\lambda\beta'\rangle_A x_{\lambda\alpha'} \\ &\quad -(\bar f_\alpha \bar f_\beta f_{\alpha'} + f_\alpha f_\beta \bar f_{\alpha'})\langle\alpha\beta|v|\alpha'\lambda\rangle_A x_{\lambda\beta'}] \\ &\quad +\sum_{\lambda\lambda'}[(1 - f_\alpha - f_\beta)\langle\alpha\beta|v|\lambda\lambda'\rangle X_{\lambda\lambda'\alpha'\beta'} \\ &\quad -(1 - f_{\alpha'} - f_{\beta'})\langle\lambda\lambda'|v|\alpha'\beta'\rangle X_{\alpha\beta\lambda\lambda'}] \\ &\quad +\sum_{\lambda\lambda'}[(f_{\alpha'} - f_\alpha)\langle\alpha\lambda|v|\alpha'\lambda'\rangle_A X_{\lambda'\beta\lambda\beta'} \\ &\quad -(f_{\beta'} - f_\alpha)\langle\alpha\lambda|v|\lambda'\beta'\rangle_A X_{\lambda'\beta\alpha'\lambda} \\ &\quad +(f_{\beta'} - f_\beta)\langle\lambda\beta|v|\lambda'\beta'\rangle_A X_{\alpha\lambda'\alpha'\lambda} \\ &\quad -(f_{\alpha'} - f_\beta)\langle\lambda\beta|v|\alpha'\lambda'\rangle_A X_{\alpha\lambda'\lambda\beta'}],\end{aligned} \tag{4}$$

where ϵ_α is the HF single-particle energy, $f_\alpha = 1(0)$ for occupied (unoccupied) single-particle states and $\bar f_\alpha = 1 - f_\alpha$, and the subscript A indicates that the corresponding matrix element is antisymmetrized. Let us mention that eqs. (3) and (4) may also be obtained from the following equations of motion:

$$\langle\Phi_0|[a^+_{\alpha'}a_\alpha, H]|\Phi\rangle = \omega\langle\Phi_0|a^+_{\alpha'}a_\alpha|\Phi\rangle, \tag{5}$$

$$\langle\Phi_0|[a^+_{\alpha'}a^+_{\beta'}a_\beta a_\alpha, H]|\Phi\rangle = \omega\langle\Phi_0|a^+_{\alpha'}a^+_{\beta'}a_\beta a_\alpha|\Phi\rangle, \tag{6}$$

where [ ] is the commutation relation, H the total Hamiltonian consisting of the kinetic energy term and a two-body interaction, $|\Phi_0\rangle$ the ground-state wave function and $|\Phi\rangle$ the wave function for an excited state with excitation energy ω. Linearizing eqs. (5) and (6) with respect to $x_{\alpha\alpha'} = \langle\Phi_0|a^+_{\alpha'}a_\alpha|\Phi\rangle$ and $X_{\alpha\beta\alpha'\beta'} = \langle\Phi_0|a^+_{\alpha'}a^+_{\beta'}a_\beta a_\alpha|\Phi\rangle$, and assuming the HF ground state for $|\Phi_0\rangle$ when expectation values for the ground state are evaluated such as $\langle\Phi_0|a^+_\alpha a_{\alpha'}|\Phi_0\rangle \approx \delta_{\alpha\alpha'}f_\alpha$, we obtain eqs. (3) and (4).

In the following, we discuss some relations of STDDM with RPA and other versions of ERPA. When the coupling to the two-body amplitudes $X_{\alpha\beta\alpha'\beta'}$ is neglected in eq. (3), the equation for the one-body amplitudes becomes

$$(\omega - \epsilon_\alpha + \epsilon_{\alpha'})x_{\alpha\alpha'} = (f_{\alpha'} - f_\alpha)\sum_{\lambda\lambda'}\langle\alpha\lambda|v|\alpha'\lambda'\rangle_A x_{\lambda'\lambda}. \tag{7}$$

When f_α is the Fermi-Dirac distribution, eq. (7) is equivalent to the finite-temperature RPA [13,14]. Hereafter, single-particle indices p and h are used to refer to unoccupied and occupied single-particle states, respectively. Since the sums on the right-hand sides of the equations for x_{ph} and x_{hp} are unrestricted, x_{ph} and x_{hp} can couple to $x_{pp'}$ and $x_{hh'}$. Such a coupling scheme of eq. (7) may be better understood in matrix form

see equation (8) *on the next page*

where obvious summation symbols and Kronecker's δ's are omitted for simplicity. Since the Hamiltonian matrix is non-Hermitian, $x_{\alpha\alpha'}$ is orthogonal not to $x_{\alpha\alpha'}$ but to a left-hand-side eigenvector $\tilde x_{\alpha\alpha'}$ which satisfies

$$\begin{aligned}(\omega - \epsilon_\alpha + \epsilon_{\alpha'})\tilde x^*_{\alpha\alpha'} &= \sum_{\lambda\lambda'}(f_{\lambda'} - f_\lambda)\langle\lambda\alpha'|v|\lambda'\alpha\rangle_A \tilde x^*_{\lambda\lambda'} \\ &= \sum_{ph}(\langle p\alpha'|v|h\alpha\rangle_A \tilde x^*_{ph} - \langle h\alpha'|v|p\alpha\rangle_A \tilde x^*_{hp}) \\ &\quad \text{(at temperature } T = 0).\end{aligned} \tag{9}$$

The matrix form of eq. (9) becomes

see equation (10) *on the next page.*

The orthonormal condition is written as

$$\langle\tilde\lambda|\lambda'\rangle = \sum_{\alpha\alpha'}\tilde x^*_{\alpha\alpha'}(\lambda)x_{\alpha\alpha'}(\lambda') = \delta_{\lambda\lambda'}, \tag{11}$$

where $|\lambda\rangle$ represents an eigenvector $x_{\alpha\alpha'}$ with the eigenvalue ω_λ, and $|\tilde\lambda\rangle$ the left-hand-side eigenvector of the

$$\begin{pmatrix} \epsilon_p-\epsilon_h+\langle ph'|v|hp'\rangle_A & \langle pp'|v|hh'\rangle_A & \langle pp'|v|hp''\rangle_A & \langle ph'|v|hh''\rangle_A \\ -\langle hh'|v|pp'\rangle_A & \epsilon_h-\epsilon_p-\langle hp'|v|ph'\rangle_A & -\langle hp'|v|pp''\rangle_A & -\langle hh'|v|ph''\rangle_A \\ 0 & 0 & \epsilon_p-\epsilon_{p'} & 0 \\ 0 & 0 & 0 & \epsilon_h-\epsilon_{h'} \end{pmatrix} \begin{pmatrix} x_{p'h'} \\ x_{h'p'} \\ x_{p''p'} \\ x_{h''h'} \end{pmatrix} = \omega \begin{pmatrix} x_{ph} \\ x_{hp} \\ x_{pp'} \\ x_{hh'} \end{pmatrix}, \quad (8)$$

$$(\tilde{x}^*_{p''h''}, \tilde{x}^*_{h''p''}, \tilde{x}^*_{pp'}, \tilde{x}^*_{hh'}) \begin{pmatrix} \epsilon_p-\epsilon_h+\langle p''h|v|h''p\rangle_A & \langle p''p|v|h''h\rangle_A & \langle p''p|v|h''p'\rangle_A & \langle p''h|v|h''h'\rangle_A \\ -\langle h''h|v|p''p\rangle_A & \epsilon_h-\epsilon_p-\langle h''p|v|p''h\rangle_A & -\langle h''p|v|p''p'\rangle_A & -\langle h''h|v|p''h'\rangle_A \\ 0 & 0 & \epsilon_p-\epsilon_{p'} & 0 \\ 0 & 0 & 0 & \epsilon_h-\epsilon_{h'} \end{pmatrix}$$
$$= \omega\left(\tilde{x}^*_{ph}, \tilde{x}^*_{hp}, \tilde{x}^*_{pp'}, \tilde{x}^*_{hh'}\right). \quad (10)$$

Hamiltonian matrix with the eigenvalue ω_λ. The completeness relation becomes

$$\sum_\lambda |\lambda\rangle\langle\tilde{\lambda}| = \sum_\lambda x_{\alpha\alpha'}(\lambda)\tilde{x}^*_{\beta\beta'}(\lambda) = I, \quad (12)$$

where I is the unit matrix. These orthonormal and completeness relations are generalizations of the RPA ones. Due to the occupation factor $f_\alpha - f_{\alpha'}$, the one-body amplitudes $x_{pp'}$ and $x_{hh'}$ vanish unless $\omega = \epsilon_\alpha - \epsilon_{\alpha'}$ (see eq. (7)), whereas $\tilde{x}_{\alpha\alpha'}$ always have all components as seen from eq. (9): $\tilde{x}_{\alpha\alpha'}$ corresponds to the generalized RPA amplitude which appears in the Landau's expression for the damping width of zero sound [15,16]. If the particle (p)-particle (p) and hole (h)-hole (h) components of $x_{\alpha\alpha'}$ are neglected, eq. (7) is reduced to the RPA equations,

$$(\omega-\epsilon_p+\epsilon_h)x_{ph} = \sum_{p'h'}[\langle ph'|v|hp'\rangle_A x_{p'h'} + \langle pp'|v|hh'\rangle_A x_{h'p'}], \quad (13)$$

$$(\omega-\epsilon_h+\epsilon_p)x_{hp} = -\sum_{p'h'}[\langle hh'|v|pp'\rangle_A x_{p'h'} + \langle hp'|v|ph'\rangle_A x_{h'p'}]. \quad (14)$$

When the coupling to the one-body amplitudes is neglected in eq. (4), the equation for the two-body amplitudes becomes

$$\begin{aligned}(\omega-\epsilon_\alpha-\epsilon_\beta+\epsilon_{\alpha'}+\epsilon_{\beta'})X_{\alpha\beta\alpha'\beta'} = &\sum_{\lambda\lambda'}[(1-f_\alpha-f_\beta)\langle\alpha\beta|v|\lambda\lambda'\rangle X_{\lambda\lambda'\alpha'\beta'} \\ &-(1-f_{\alpha'}-f_{\beta'})\langle\lambda\lambda'|v|\alpha'\beta'\rangle X_{\alpha\beta\lambda\lambda'}] \\ &+\sum_{\lambda\lambda'}[(f_{\alpha'}-f_\alpha)\langle\alpha\lambda|v|\alpha'\lambda'\rangle_A X_{\lambda'\beta\lambda\beta'} \\ &-(f_{\beta'}-f_\alpha)\langle\alpha\lambda|v|\lambda'\beta'\rangle_A X_{\lambda'\beta\alpha'\lambda} \\ &+(f_{\beta'}-f_\beta)\langle\lambda\beta|v|\lambda'\beta'\rangle_A X_{\alpha\lambda'\alpha'\lambda} \\ &-(f_{\alpha'}-f_\beta)\langle\lambda\beta|v|\alpha'\lambda'\rangle_A X_{\alpha\lambda'\lambda\beta'}]. \end{aligned} \quad (15)$$

This equation is equivalent to the formula given in ref. [17] for the two-body space. Keeping only the 2p-2h, 2h-2p and 1p1h-1p1h components of $X_{\alpha\beta\alpha'\beta'}$ in eq. (15) leads to the version of ERPA for low-lying two-phonon states [18]. It has been pointed out [18] that the 1p1h-1p1h components of $X_{\alpha\beta\alpha'\beta'}$ are important to reproduce collectivity of low-lying double-phonon states. A time-dependent version of eq. (15) has been applied to the double-phonon states of giant dipole and quadrupole resonances in ^{40}Ca using a realistic Skyrme-type interaction for both the mean-field potential and the residual interaction, and it was found that the 2p-2h, 2h-2p and 1p1h-1p1h components are the most important two-body amplitudes for these double-phonon states [19]. In eqs. (3) and (4) the one-body amplitude $x_{\alpha\alpha'}$ and the two-body amplitude $X_{\alpha\beta\alpha'\beta'}$ have all components: For example, $x_{\alpha\alpha'}$ has 1p-1h, 1h-1p, 1p-1p and 1h-1h components. On the other hand, only the 1p-1h and 1h-1p components of $x_{\alpha\alpha'}$ and the 2p-2h and 2h-2p components of $X_{\alpha\beta\alpha'\beta'}$ are taken into account in SRPA [5] and the SRPA equations are obtained from eqs. (3) and (4) by keeping only these amplitudes.

Equations (3) and (4) have asymmetric couplings between the $x_{\alpha\alpha'}$ and $X_{\alpha\beta\alpha'\beta'}$ amplitudes: In eq. (3) $x_{\alpha\alpha'}$ couples to all components of $X_{\alpha\beta\alpha'\beta'}$, while in eq. (4) only the 2p-2h, 1p-3h and 1h-3p components of $X_{\alpha\beta\alpha'\beta'}$ (and their complex conjugates) couple to $x_{\alpha\alpha'}$ due to the occupation factors ($\bar{f}_\beta f_{\alpha'} f_{\beta'}$ etc.). Equations (7) and (15) which have no coupling between one-body and two-body amplitudes are also non-Hermitian due to occupation factors such as $f_{\alpha'} - f_\alpha$. The asymmetry and non-hermiticity originate from the structure of the equations for the reduced density matrices (see eqs. (5) and (6)). For a non-Hermitian Hamiltonian matrix, the left-hand-side eigenvectors of the Hamiltonian matrix constitute a basis which is orthogonal to $(x_{\alpha\alpha'}, X_{\alpha\beta\alpha'\beta'})$, and the orthonormal condition is written as

$$\langle\tilde{\lambda}|\lambda'\rangle = \sum_{\alpha\alpha'}\tilde{x}^*_{\alpha\alpha'}(\lambda)x_{\alpha\alpha'}(\lambda') + \sum_{\alpha\beta\alpha'\beta'}\tilde{X}^*_{\alpha\beta\alpha'\beta'}(\lambda)X_{\alpha\beta\alpha'\beta'}(\lambda') = \delta_{\lambda\lambda'}, \quad (16)$$

where $|\lambda\rangle$ represents an eigenvector $(x_{\alpha\alpha'}, X_{\alpha\beta\alpha'\beta'})$ with the eigenvalue ω_λ, and $|\tilde{\lambda}\rangle$ the left-hand-side eigenvector of the Hamiltonian matrix with the same eigenvalue. The completeness relation is written as

$$\sum_{\lambda}\begin{pmatrix} x_{\alpha\alpha'}(\lambda) \\ X_{\alpha\beta\alpha'\beta'}(\lambda)\end{pmatrix}(\tilde{x}^*_{\beta\beta'}(\lambda)\ \tilde{X}^*_{\beta\gamma\beta'\gamma'}(\lambda)) = I. \quad (17)$$

The asymmetry and non-hermiticity in eqs. (3) and (4) are necessary to prove the properties of the spurious states and the Kohn theorems as will be discussed below. However, due to the non-hermiticity of the problem, some of the eigenvalues may become complex. Our exploratory numerical calculations for the oxygen isotopes ^{22,24}O using the neutron $2s$ and $1d$ states and a pairing-type residual interaction which had been used in the calculations of quadrupole states in these nuclei [20] show that the non-hermiticity of STDDM is quite moderate: Only a small fraction (about 10%) of the eigenstates have complex energies, whose imaginary parts are less than 0.1 MeV. The results of these numerical calculations will be discussed elsewhere. On the other hand, we will show in sect. 4 that there is a prescription for constructing ERPA with symmetry and hermiticity using a correlated ground state in TDDM.

3 Single and double spurious states

3.1 One-body and two-body operators for the translational motion

We consider the following one-body and two-body operators associated with the translational motion:

$$\boldsymbol{P} = \sum_{\alpha\beta}\langle\alpha| - i\nabla|\beta\rangle a^+_\alpha a_\beta \quad (18)$$

and

$$\boldsymbol{P}\cdot\boldsymbol{P} = \sum_{\alpha\alpha'}\langle\alpha| - \nabla^2|\alpha'\rangle a^+_\alpha a_{\alpha'} + \sum_{\alpha\beta\alpha'\beta'}\langle\alpha| - i\nabla|\alpha'\rangle\cdot\langle\beta| - i\nabla|\beta'\rangle a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'}. \quad (19)$$

Since the Hamiltonian H has translational invariance, these operators commute with H, that is, $[H,\boldsymbol{P}] = [H,\boldsymbol{P}\cdot\boldsymbol{P}] = 0$. We will evaluate $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle$ and $\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle$, where $|\Phi_1\rangle$ and $|\Phi_2\rangle$ are the spurious states excited with $\boldsymbol{P}$ and $\boldsymbol{P}\cdot\boldsymbol{P}$, respectively, and show that these states have zero excitation energy in STDDM. The evaluation of $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle$ and $\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle$ using the equations of motion for the transition amplitudes is equivalent to that of $\langle\Phi_0|[\boldsymbol{P},H]|\Phi_1\rangle$ and $\langle\Phi_0|[\boldsymbol{P}\cdot\boldsymbol{P},H]|\Phi_2\rangle$, provided that $\langle\Phi_0|[\boldsymbol{P},H]|\Phi_1\rangle$ and $\langle\Phi_0|[\boldsymbol{P}\cdot\boldsymbol{P},H]|\Phi_2\rangle$ are calculated in the same way as used to derive the equations of motion for the transition amplitudes. In the case of the exact problem, it is, with eqs. (5) and (6), trivial to see that $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle$ and $\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle$ are identical to zero because the left-hand sides of eqs. (5) and (6) are reduced to the commutation relations between the Hamiltonian and these translational operators. Since the linearization and the HF assumption are made in the derivation of STDDM, it is not trivial to show the above properties of the spurious states. However, the linearization should be valid in the weak-coupling limit and therefore we can anticipate that the Goldstone theorem also holds in this case, provided that the linearization procedure is correctly performed.

3.2 Spurious states in RPA

As is well known, RPA gives zero excitation energy to the spurious state $|\Phi_1\rangle$ excited with $\boldsymbol{P}$, although only the 1p-1h and 1h-1p components of the one-body amplitudes are taken into account in spite of the fact that $\boldsymbol{P}$ also contains in addition 1p-1p and 1h-1h components. To illustrate our approach for the problem of the spurious states, we begin with proving $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle = 0$ in RPA. Using the relation $\langle\Phi_0|a^+_{\alpha'}a_\alpha|\Phi_1\rangle = x_{\alpha\alpha'}$ and eqs. (13) and (14) for x_{ph} and x_{hp}, we modify $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle$ as

$$\begin{aligned}\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle &= \omega\sum_{ph}[\langle h|\nabla|p\rangle x_{ph} + \langle p|\nabla|h\rangle x_{hp}] \\ &= \sum_{ph}[\langle h|\nabla|p\rangle(\epsilon_p - \epsilon_h)x_{ph} + \langle p|\nabla|h\rangle(\epsilon_h - \epsilon_p)x_{hp}] \\ &+ \sum_{php'h'}[\langle h|\nabla|p\rangle(\langle ph'|v|hp'\rangle_A x_{p'h'} + \langle pp'|v|hh'\rangle_A x_{h'p'}) \\ &-\langle p|\nabla|h\rangle(\langle hp'|v|ph'\rangle_A x_{h'p'} + \langle hh'|v|pp'\rangle_A)x_{p'h'}]. \quad (20)\end{aligned}$$

A further modification is made using $h_0\psi_\alpha = \epsilon_\alpha\psi_\alpha$, where h_0 is the HF single-particle Hamiltonian, and the closure relation $\sum_p \psi_p(\boldsymbol{r})\psi^*_p(\boldsymbol{r}') = \delta^3(\boldsymbol{r}-\boldsymbol{r}') - \sum_h \psi_h(\boldsymbol{r})\psi^*_h(\boldsymbol{r}')$:

$$\begin{aligned}\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle &= \sum_{ph}[\langle h|[\nabla,h_0]|p\rangle x_{ph} + \langle p|[\nabla,h_0]|h\rangle x_{hp}] \\ &+\sum_{hph'}[(\langle hh'|\nabla_1 v|hp\rangle_A - \langle hh'|v\nabla_1|hp\rangle + \langle hh'|v\nabla_2|ph\rangle)x_{ph'} \\ &+(\langle hp|\nabla_1 v|hh'\rangle_A - \langle hp|v\nabla_1|hh'\rangle + \langle hp|v\nabla_2|h'h\rangle)x_{h'p})]. \quad (21)\end{aligned}$$

The first term on the right-hand side of the above equation can be written in terms of v using

$$\begin{aligned}\langle\alpha'|[\nabla,h_0]|\alpha\rangle &= \sum_h[\langle\alpha' h|(\nabla_1 v)|\alpha h\rangle_A \\ &-\langle\alpha' h|v\nabla_1|h\alpha\rangle + \langle\alpha' h|v\nabla_2|h\alpha\rangle]. \quad (22)\end{aligned}$$

Finally eq. (21) becomes

$$\begin{aligned}\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle &= \sum_{phh'}[(\langle hh'|(\nabla_1 v)|ph'\rangle_A - \langle hh'|v\nabla_1|h'p\rangle \\ &+\langle hh'|v\nabla_2|h'p\rangle)x_{ph} + (\langle ph'|(\nabla_1 v)|hh'\rangle_A \\ &-\langle ph'|v\nabla_1|h'h\rangle + \langle ph'|v\nabla_2|h'h\rangle)x_{hp}] \\ &+\sum_{phh'}[(\langle h'h|(\nabla_1 v)|h'p\rangle_A - \langle h'h|v\nabla_1|ph'\rangle \\ &+\langle h'h|v\nabla_2|ph'\rangle)x_{ph} + (\langle h'p|(\nabla_1 v)|h'h\rangle_A \\ &-\langle h'p|v\nabla_1|hh'\rangle + \langle h'p|v\nabla_2|hh'\rangle)x_{hp})], \quad (23)\end{aligned}$$

where $(\nabla_1 v)$ means that ∇_1 acts only on v. Since v has translational invariance, the sum of the following two terms on the right-hand side of eq. (23) becomes zero:

$$\langle hh'|(\nabla_1 v)|ph'\rangle_A + \langle h'h|(\nabla_1 v)|h'p\rangle_A = \langle hh'|(\nabla_1 v) + (\nabla_2 v)|ph'\rangle_A = 0. \tag{24}$$

Another sum of the two terms also vanishes

$$-\langle hh'|v\nabla_1|h'p\rangle + \langle h'h|v\nabla_2|ph'\rangle = \langle h'h| - v\nabla_2 + v\nabla_2|ph'\rangle = 0. \tag{25}$$

Similarly, all other terms on the right-hand side of eq. (23) cancel out. This means $\omega = 0$. As shown above, both the inclusion of the backward amplitude x_{hp} and the unrestricted sum over unoccupied single-particle states are essential in RPA to give zero excitation energy to the spurious state [4]. A detailed numerical investigation for the elimination of spurious-state mixing in the case of RPA has recently been carried out by Agrawal *et al.* [21].

3.3 Spurious state in STDDM

Along the lines illustrated above, we then show that $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle = 0$ in STDDM. Using the equation for $x_{\alpha\alpha'}$ (eq. (3)), we modify $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle$ as

$$\begin{aligned}\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle &= \sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle\omega x_{\alpha\alpha'} \\ &= \sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle\{(\epsilon_\alpha - \epsilon_{\alpha'})x_{\alpha\alpha'} \\ &\quad +(f_{\alpha'} - f_\alpha)\sum_{\lambda\lambda'}\langle\alpha\lambda|v|\alpha'\lambda'\rangle_A x_{\lambda'\lambda} \\ &\quad + \sum_{\lambda\lambda'\lambda''}[X_{\lambda\lambda'\alpha'\lambda''}\langle\alpha\lambda''|v|\lambda\lambda'\rangle \\ &\quad -X_{\alpha\lambda'\lambda\lambda''}\langle\lambda\lambda''|v|\alpha'\lambda'\rangle]\},\end{aligned} \tag{26}$$

where the sums are over both occupied and unoccupied single-particle states. Using $h_0\psi_\alpha = \epsilon_\alpha\psi_\alpha$ and the closure relation $\sum_\alpha \psi(\boldsymbol{r})\psi^*_\alpha(\boldsymbol{r}') = \delta^3(\boldsymbol{r} - \boldsymbol{r}')$, we further modify eq. (26) as

$$\begin{aligned}\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle &= \sum_{\alpha\alpha'}\langle\alpha'|[\nabla, h_0]|\alpha\rangle x_{\alpha\alpha'} \\ &+ \sum_{\lambda\lambda'h}[\langle h\lambda|\nabla_1 v|h\lambda'\rangle_A - (\langle h\lambda|v\nabla_1|h\lambda'\rangle \\ &-\langle h\lambda|v\nabla_2|\lambda' h\rangle)]x_{\lambda'\lambda} + \sum_{\alpha\alpha'\lambda\lambda'\lambda''}[X_{\lambda\lambda'\alpha'\lambda''}\langle\alpha'\lambda''|\nabla_1 v|\lambda\lambda'\rangle \\ &-X_{\alpha\lambda'\lambda\lambda''}\langle\lambda\lambda''|v\nabla_1|\alpha\lambda'\rangle].\end{aligned} \tag{27}$$

Using eq. (22) and changing summation indices, we obtain

$$\begin{aligned}\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle &= \sum_{\alpha\alpha' h}[\langle\alpha' h|(\nabla_1 v)|\alpha h\rangle_A - \langle\alpha' h|v\nabla_1|h\alpha\rangle \\ &+\langle\alpha' h|v\nabla_2|h\alpha\rangle + \langle h\alpha'|(\nabla_1 v)|h\alpha\rangle_A - \langle h\alpha'|v\nabla_1|\alpha h\rangle \\ &+\langle h\alpha'|v\nabla_2|\alpha h\rangle)]x_{\alpha\alpha'} + \sum_{\alpha\beta\alpha'\beta'}X_{\alpha\beta\alpha'\beta'}\langle\alpha'\beta'|(\nabla_1 v)|\alpha\beta\rangle.\end{aligned} \tag{28}$$

The first sum on the right-hand side of the above equation which includes terms proportional to $x_{\alpha\alpha'}$ is a generalization of eq. (23) and vanishes for an interaction v with translational invariance. The second term on the right-hand side of eq. (28) can be expressed as

$$\begin{aligned}&\sum_{\alpha\beta\alpha'\beta'}X_{\alpha\beta\alpha'\beta'}\langle\alpha'\beta'|(\nabla_1 v)|\alpha\beta\rangle \\ &= \frac{1}{2}\sum_{\alpha\beta\alpha'\beta'}X_{\alpha\beta\alpha'\beta'}(\langle\alpha'\beta'|(\nabla_1 v)|\alpha\beta\rangle + \langle\beta'\alpha'|(\nabla_1 v)|\beta\alpha\rangle) \\ &= \frac{1}{2}\sum_{\alpha\beta\alpha'\beta'}X_{\alpha\beta\alpha'\beta'}\langle\alpha'\beta'|(\nabla_1 v) + (\nabla_2 v)|\alpha\beta\rangle.\end{aligned} \tag{29}$$

Since v has translational invariance, $(\nabla_1 v) + (\nabla_2 v) = 0$. Thus, again $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle = 0$ is proven. As shown above, unrestricted summation over the single-particle indices α and α' in eq. (26) is essential to derive the last term on the right-hand side of eq. (27). This means that, contrary to the standard RPA where only ph and hp components of $\boldsymbol{P}$ are needed, any ERPA formalisms with restricted one-body amplitudes *cannot* give zero excitation energy to the spurious state associated with the translational motion. However, this does not depend on approximations for two-body amplitudes as long as the symmetry property is respected as seen in eq. (29).

3.4 Double spurious state in STDDM

In a way similar to the above, we show that $\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle = 0$, where $|\Phi_2\rangle$ is the double spurious state. The term $\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle$ contains both the one-body and two-body contributions,

$$\begin{aligned}&-\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle = \\ &\quad\omega\Big\{\sum_{\alpha\alpha'}(\langle\alpha'|\nabla^2|\alpha\rangle - \sum_h 2\langle\alpha'|\nabla|h\rangle\cdot\langle h|\nabla|\alpha\rangle)x_{\alpha\alpha'} \\ &\quad+ \sum_{\alpha\beta\alpha'\beta'}\langle\alpha'|\nabla|\alpha\rangle\cdot\langle\beta'|\nabla|\beta\rangle X_{\alpha\beta\alpha'\beta'}\Big\}.\end{aligned} \tag{30}$$

Using eqs. (3) and (4) for $x_{\alpha\alpha'}$ and $X_{\alpha\beta\alpha'\beta'}$, $h_0\psi_\alpha = \epsilon_\alpha\psi_\alpha$ and the closure relation $\sum_\alpha \psi(\boldsymbol{r})\psi^*_\alpha(\boldsymbol{r}') = \delta^3(\boldsymbol{r} - \boldsymbol{r}')$, we modify the right-hand side of the above equation. After some lengthy manipulations, the terms containing $x_{\alpha\alpha'}$ and one summation index over occupied single-particle states become

$$\begin{aligned}&2\sum_{\alpha\alpha' h}[\langle\alpha' h|(\nabla_1^2 v)|\alpha h\rangle_A + \langle\alpha' h|(\nabla_1 v)\cdot\nabla_1|\alpha h\rangle \\ &\quad-\langle\alpha' h|(\nabla_1 v)\cdot\nabla_1|h\alpha\rangle + \langle h\alpha'|(\nabla_1 v)\cdot\nabla_1|h\alpha\rangle \\ &\quad-\langle h\alpha'|(\nabla_1 v)\cdot\nabla_1|\alpha h\rangle]x_{\alpha\alpha'} \\ &\quad+2\sum_{\alpha\alpha' h}[\langle\alpha' h|(\nabla_1\cdot\nabla_2 v)|\alpha h\rangle_A + \langle\alpha' h|(\nabla_1 v)\cdot\nabla_2|\alpha h\rangle \\ &\quad-\langle\alpha' h|(\nabla_1 v)\cdot\nabla_2|h\alpha\rangle + \langle\alpha' h|(\nabla_2 v)\cdot\nabla_1|\alpha h\rangle \\ &\quad-\langle\alpha' h|(\nabla_2 v)\cdot\nabla_1|h\alpha\rangle]x_{\alpha\alpha'},\end{aligned} \tag{31}$$

where the first sum comes from the terms with $x_{\alpha\alpha'}$ on the right-hand side of eq. (30) and the second sum from the term with $X_{\alpha\beta\alpha'\beta'}$. Since v has translational invariance, $(\nabla_1^2 v)+(\nabla_1\cdot\nabla_2 v)=0$. Therefore, the sum of the following two terms in eq. (31) becomes $\langle\alpha' h|(\nabla_1^2 v)|\alpha h\rangle_A+\langle\alpha' h|(\nabla_1\cdot\nabla_2 v)|\alpha h\rangle_A=0$. All other terms vanish for similar reasons. In addition to the terms shown in eq. (31), there appear terms with $x_{\alpha\alpha'}$ and two summation indices over occupied single-particle states, and also terms with $X_{\alpha\beta\alpha'\beta'}$ in the modification process of eq. (30). It is straightforward, though lengthy, to show that these terms also vanish for a translationally invariant interaction. Thus $\omega\langle\Phi_0|\boldsymbol{P}\cdot\boldsymbol{P}|\Phi_2\rangle=0$, that is, $\omega=0$. As mentioned above, unrestricted summation over single-particle states is again essential to obtain this conclusion. This means that only ERPAs with all one-body and two-body amplitudes, that is, $x_{ph}, x_{hp}, x_{pp'}, x_{hh'}, X_{pp'hh'}, X_{hh'pp'}, X_{php'h'}, X_{phh'h''}, X_{h'h''ph}, X_{pp'hp''}, X_{hp''pp'}, X_{pp'p''p'''}$ and $X_{hh'h''h'''}$, give zero excitation energy to the double-phonon state corresponding to the spurious mode associated with the translational motion. Let us also point out that in taking into account *all* amplitudes of x and X may seem trivial that the Goldstone modes are restored. We should not forget, however, that in the derivation of STDDM we have made quite drastic approximations which make it necessary to show explicitly that the invariances are fulfilled. Since STDDM and the ERPA with hermiticity, which will be given in sect. 4, are formulated using all one-body and two-body amplitudes, they may have zero-energy solutions. These zero-energy solutions presumably couple to the spurious modes if they have the same quantum numbers as the spurious modes. However, as long as these ERPAs are applied to study collective states such as giant resonances, the coupling of the spurious modes to the zero-energy solutions cannot be a serious problem. Indeed, in a subsequent paper with numerical applications, we will show that zero-energy solutions cause no problem.

3.5 Single and double Kohn modes

When a system is confined to a harmonic potential $U=\frac{1}{2}m\omega_0^2r^2$, the spurious mode associated with the translational motion has an eigenvalue of $\hbar\omega_0$, independently of the translationally invariant two-body interaction. This property is known as the Kohn theorem [9–11]. In this section we show that our ERPA equations satisfy the Kohn theorem and also that the eigenvalue of the double Kohn mode becomes $2\hbar\omega_0$. Due to the presence of the harmonic potential the single-particle states are chosen to be eigenstates of the modified Hamiltonian, $h'\psi_\alpha=\epsilon_\alpha\psi_\alpha$, where $h'=h_0+\frac{1}{2}m\omega_0^2r^2$. In a way similar to the spurious mode, we evaluate $\omega\langle\Phi_0|\boldsymbol{P}|\Phi_1\rangle$ using the equations of motion in STDDM. Since the two-body interaction has translational invariance, terms with the two-body interaction vanish and

$$\omega\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle=-\sum_{\alpha\alpha'}\langle\alpha|m\omega_0^2\boldsymbol{r}|\alpha'\rangle x_{\alpha'\alpha}=-m\omega_0^2\langle\Phi_0|\boldsymbol{Q}|\Phi_1\rangle \tag{32}$$

holds, where $\boldsymbol{Q}=\sum\langle\alpha|\boldsymbol{r}|\alpha'\rangle a^+_\alpha a_{\alpha'}$. Similarly, a non-vanishing contribution to $\omega\langle\Phi_0|\boldsymbol{Q}|\Phi_1\rangle$ comes only from the kinetic energy term, and we obtain

$$\omega\langle\Phi_0|\boldsymbol{Q}|\Phi_1\rangle=-\frac{\hbar^2}{m}\langle\Phi_0|i\boldsymbol{P}|\Phi_1\rangle. \tag{33}$$

As for the spurious mode in the case of translational invariance, subsect. 3.3, it is essential to keep all components of the one-body amplitudes to obtain the above expressions. From eqs. (32) and (33), we get $\omega=\pm\hbar\omega_0$.

In the case of the double Kohn mode, expectation values of three operators couple in the following way:

$$\omega\langle\Phi_0|i\boldsymbol{P}\cdot i\boldsymbol{P}|\Phi_2\rangle=2m\omega_0^2\langle\Phi_0|\boldsymbol{Q}\cdot i\boldsymbol{P}|\Phi_2\rangle, \tag{34}$$

$$\omega\langle\Phi_0|\boldsymbol{Q}\cdot i\boldsymbol{P}|\Phi_2\rangle=\frac{\hbar^2}{m}\langle\Phi_0|i\boldsymbol{P}\cdot i\boldsymbol{P}|\Phi_2\rangle+m\omega_0^2\langle\Phi_0|\boldsymbol{Q}\cdot\boldsymbol{Q}|\Phi_2\rangle, \tag{35}$$

$$\omega\langle\Phi_0|\boldsymbol{Q}\cdot\boldsymbol{Q}|\Phi_2\rangle=2\frac{\hbar^2}{m}\langle\Phi_0|\boldsymbol{Q}\cdot i\boldsymbol{P}|\Phi_2\rangle. \tag{36}$$

The right-hand side of eq. (34) comes from the harmonic potential. Both the kinetic energy term and the harmonic potential contribute to the right-hand side of eq. (35), and the kinetic energy term becomes non-vanishing on the right-hand side of eq. (36). All terms with the two-body interaction vanish due to translational invariance. It is essential to keep all components of the one-body and two-body amplitudes to derive eqs. (34)-(36) as in the case of the double spurious mode discussed in sect. 3.4. From the above equations we get $\omega=\pm 2\hbar\omega_0$.

3.6 Continuity equations

We end this section by showing that our ERPA equations satisfy continuity equations. In a way similar to the single spurious mode we evaluate $\omega_\lambda\langle\Phi_0|\hat\rho(\boldsymbol{r})|\Phi_\lambda\rangle$, where $\hat\rho$ is the density operator $\hat\rho(\boldsymbol{r})=\sum\psi^*_\alpha(\boldsymbol{r})\psi_{\alpha'}(\boldsymbol{r})a^+_\alpha a_{\alpha'}$, and obtain

$$\omega_\lambda\langle\Phi_0|\hat\rho(\boldsymbol{r})|\Phi_\lambda\rangle=-\nabla\cdot\langle\Phi_0|\boldsymbol{j}(\boldsymbol{r})|\Phi_\lambda\rangle, \tag{37}$$

where the current operator $\boldsymbol{j}$ is given by

$$\boldsymbol{j}(\boldsymbol{r})=\frac{\hbar^2}{2m}\sum[\psi^*_\alpha(\boldsymbol{r})\nabla\psi_{\alpha'}(\boldsymbol{r})-(\nabla\psi^*_\alpha(\boldsymbol{r}))\psi_{\alpha'}(\boldsymbol{r})]a^+_\alpha a_{\alpha'} \tag{38}$$

for a momentum-independent two-body interaction. Thus, the continuity equation for the one-body transition density and current is satisfied. Keeping all components of the one-body amplitudes is essential to obtain the continuity equation.

Similarly, the transition amplitude for the two-body density operator $\hat\rho_2(\boldsymbol{r},\boldsymbol{r}')$ defined by

$$\hat\rho_2(\boldsymbol{r},\boldsymbol{r}')=\sum_{\alpha\beta\alpha'\beta'}\psi^*_\alpha(\boldsymbol{r})\psi^*_\beta(\boldsymbol{r}')\psi_{\beta'}(\boldsymbol{r}')\psi_{\alpha'}(\boldsymbol{r})a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'} \tag{39}$$

satisfies the continuity equation

$$\omega_\lambda\langle\Phi_0|\hat\rho_2(\boldsymbol{r},\boldsymbol{r}')|\Phi_\lambda\rangle=-(\nabla_r\cdot\langle\Phi_0|\boldsymbol{j}_2(\boldsymbol{r},\boldsymbol{r}')|\Phi_\lambda\rangle+\nabla_{r'}\cdot\langle\Phi_0|\boldsymbol{j}_2(\boldsymbol{r}',\boldsymbol{r})|\Phi_\lambda\rangle), \tag{40}$$

where the two-body current operator $\boldsymbol{j}_2$ for a momentum-independent two-body interaction is given by

$$\boldsymbol{j}_2(\boldsymbol{r},\boldsymbol{r}') = \frac{\hbar^2}{2m}\sum[\psi^*_\alpha(\boldsymbol{r})(\nabla\psi_{\alpha'}(\boldsymbol{r})) -(\nabla\psi^*_\alpha(\boldsymbol{r}))\psi_{\alpha'}(\boldsymbol{r}))]\psi^*_\beta(\boldsymbol{r}')\psi_{\beta'}(\boldsymbol{r}')a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'}. \quad (41)$$

In the derivation of eq. (40) it is again essential to keep all components of the one-body and two-body amplitudes.

4 ERPA with hermiticity

The equations of STDDM (eqs. (3) and (4)) show asymmetry and non-hermiticity, although this causes no problem in conserving various physical properties as discussed above. In the following we show that ERPA with symmetry and hermiticity can be formulated using the equation-of-motion approach [22] and the correlated ground state in TDDM. We have pointed out [23], in deriving Landau's expression for the spreading width of a collective state, that it is important to include ground-state correlations to remove the asymmetry in STDDM. It is well known [22] that the asymmetry problem always appears in the equation-of-motion approach when the ground state is replaced by an approximate one. Before presenting the formulation of our ERPA, therefore, we summarize the origin of the asymmetry in the equation-of-motion approach. When $|\Phi_0\rangle$ is the exact ground state of the Hamiltonian, there exists an identity involving a one-body operator $A = a^+_\alpha a_{\alpha'}$ and a two-body operator $B = a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'}$:

$$\langle\Phi_0|[[B,H],A]|\Phi_0\rangle - \langle\Phi_0|[[A,H],B]|\Phi_0\rangle = \langle\Phi_0|[H,[A,B]]|\Phi_0\rangle = 0. \quad (42)$$

When $|\Phi_0\rangle$ is approximated by the HF ground state, the above identity is violated, that is,

$$\langle\Phi_0|[H,[A,B]]|\Phi_0\rangle \neq 0 \quad (43)$$

and, consequently,

$$\langle\Phi_0|[[B,H],A]|\Phi_0\rangle \neq \langle\Phi_0|[A,H],B]|\Phi_0\rangle. \quad (44)$$

Since the left-hand side of the above equation describes the coupling of the one-body amplitudes to the two-body ones, and the right-hand side that of the two-body amplitudes to the one-body ones, the resulting ERPA has asymmetric couplings. In order to avoid the difficulty of eq. (44), Rowe introduced a symmetrized double commutator [22]. However, it was pointed out [16] that there is an ambiguity in the choice of such a double commutator.

Now we proceed to the presentation of our ERPA with ground-state correlations. The ground state $|\Phi_0\rangle$ in TDDM is constructed so that

$$\langle\Phi_0|[H,a^+_\alpha a_{\alpha'}]|\Phi_0\rangle = 0 \quad (45)$$

and

$$\langle\Phi_0|[H,a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'}]|\Phi_0\rangle = 0 \quad (46)$$

are satisfied for any single-particle indices [8]. In other words the occupation matrix $n^0_{\alpha\alpha'}$ and the correlation matrix $C^0_{\alpha\beta\alpha'\beta'}$, the expansion coefficients of ρ_0 and C_0, respectively, are determined in TDDM so that the above two equations are satisfied. The explicit expression for eqs. (45) and (46) depends on the single-particle state ψ_α. The equations for $n^0_{\alpha\alpha'}$ and $C^0_{\alpha'\beta'\alpha\beta}$ shown in appendix A are obtained when ψ_α is chosen to be an eigenstate of the mean-field Hamiltonian $h_0(\rho_0)$, that is,

$$h_0(\rho_0)\psi_\alpha(1) = -\frac{\hbar^2\nabla^2}{2m}\psi_\alpha(1) +\int d2v(1,2)[\rho_0(2,2)\psi_\alpha(1)-\rho_0(1,2)\psi_\alpha(2)] = \epsilon_\alpha\psi_\alpha(1), \quad (47)$$

where

$$\rho_0(11') = \sum_{\alpha\alpha'} n^0_{\alpha\alpha'}\psi_\alpha(1)\psi^*_{\alpha'}(1'). \quad (48)$$

Although it is not evident to find an analytic solution of eqs. (45) and (46) [24], a method for obtaining $n^0_{\alpha\alpha'}$ and $C^0_{\alpha\beta\alpha'\beta'}$ numerically has been proposed [25] and already been tested for realistic nuclei in the study of giant resonances built on the correlated ground state [26,27]. Since the commutation relation $[A,B] = [a^+_\alpha a_{\alpha'}, a^+_\beta a^+_\gamma a_{\gamma'}a_{\beta'}]$ in eq. (42) becomes a sum of two-body operators, we find

$$\langle\Phi_0|[H,[a^+_\alpha a_{\alpha'}, a^+_\beta a^+_\gamma a_{\gamma'}a_{\beta'}]]|\Phi_0\rangle = 0 \quad (49)$$

which holds due to eq. (46). This means that the coupling matrices are symmetric, that is,

$$\langle\Phi_0|[[a^+_\beta a^+_\gamma a_{\gamma'}a_{\beta'},H],a^+_\alpha a_{\alpha'}]|\Phi_0\rangle = \langle\Phi_0|[[a^+_\alpha a_{\alpha'},H],a^+_\beta a^+_\gamma a_{\gamma'}a_{\beta'}]|\Phi_0\rangle \quad (50)$$

for the correlated ground state in TDDM. The ERPA equations based on the TDDM ground state are formulated using the equation of motion approach [22] as

$$\langle\Psi_0|[[a^+_\alpha a_{\alpha'},H],Q^+]|\Psi_0\rangle = \omega\langle\Psi_0|[a^+_\alpha a_{\alpha'},Q^+]|\Psi_0\rangle\,, \quad (51)$$

$$\langle\Psi_0|[[:a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'}:,H],Q^+]|\Psi_0\rangle = \omega\langle\Psi_0|[:a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'}:,Q^+]|\Psi_0\rangle, \quad (52)$$

where the operator Q^+ is defined by

$$Q^+ = \sum(x_{\lambda\lambda'}a^+_\lambda a_{\lambda'} + X_{\lambda_1\lambda_2\lambda'_1\lambda'_2} : a^+_{\lambda_1}a^+_{\lambda_2}a_{\lambda'_2}a_{\lambda'_1}:) \quad (53)$$

and $|\Psi_0\rangle$ is assumed to have the following properties:

$$Q^+|\Psi_0\rangle = |\Psi\rangle\,, \quad (54)$$

$$Q|\Psi_0\rangle = 0\,. \quad (55)$$

In eqs. (52) and (53), : : stands for $:a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'} := a^+_\alpha a^+_\beta a_{\beta'}a_{\alpha'} - \mathcal{A}(a^+_\alpha a_{\alpha'}\ \langle\Psi_0|a^+_\beta a_{\beta'}|\Psi_0\rangle + a^+_\beta a_{\beta'}\ \langle\Psi_0|a^+_\alpha a_{\alpha'}|\Psi_0\rangle)$, where $\mathcal{A}$ is an antisymmetrization operator. The above equation can be written in matrix form

$$\begin{pmatrix} A & C \\ B & D\end{pmatrix}\begin{pmatrix} x \\ X\end{pmatrix} = \omega\begin{pmatrix} S_1 & T_1 \\ T_2 & S_2\end{pmatrix}\begin{pmatrix} x \\ X\end{pmatrix}, \quad (56)$$

where each matrix element is given by

$$S_1(\alpha'\alpha:\lambda\lambda') = \langle\Psi_0|[a^+_\alpha a_{\alpha'}, a^+_\lambda a_{\lambda'}]|\Psi_0\rangle, \quad (57)$$

$$S_2(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle\Psi_0|[:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:, :a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}:]|\Psi_0\rangle, \quad (58)$$

$$T_1(\alpha'\alpha:\lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle\Psi_0|[a^+_\alpha a_{\alpha'}, :a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}:]|\Psi_0\rangle, \quad (59)$$

$$T_2(\alpha'\beta'\alpha\beta:\lambda\lambda') = \langle\Psi_0|[:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:, a^+_\lambda a_{\lambda'}]|\Psi_0\rangle, \quad (60)$$

$$A(\alpha'\alpha:\lambda\lambda') = \langle\Psi_0|[[a^+_\alpha a_{\alpha'}, H], a^+_\lambda a_{\lambda'}]|\Psi_0\rangle, \quad (61)$$

$$B(\alpha'\beta'\alpha\beta:\lambda\lambda') = \langle\Psi_0|[[:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:, H], a^+_\lambda a_{\lambda'}]|\Psi_0\rangle, \quad (62)$$

$$C(\alpha'\alpha:\lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle\Psi_0|[[a^+_\alpha a_{\alpha'}, H], :a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}:]|\Psi_0\rangle, \quad (63)$$

$$D(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle\Psi_0|[[:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:, H], :a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}:]|\Psi_0\rangle. \quad (64)$$

When the above matrices are evaluated, the ground state $|\Psi_0\rangle$ is replaced by $|\Phi_0\rangle$ in TDDM. Then all matrices in the above are written in terms of $n^0_{\alpha\alpha'}$ and $C^0_{\alpha\beta\alpha'\beta'}$, which are shown in appendix B. Due to eqs. (45) and (46), the above matrices have the following symmetries:

$$A(\alpha'\alpha:\lambda\lambda') = A(\lambda'\lambda:\alpha\alpha') = A(\lambda\lambda':\alpha'\alpha)^*, \quad (65)$$

$$B(\alpha'\beta'\alpha\beta:\lambda\lambda') = C(\lambda'\lambda:\alpha\beta\alpha'\beta') = C(\lambda\lambda':\alpha'\beta'\alpha\beta)^*. \quad (66)$$

This version of ERPA gives zero excitation energy to spurious modes associated with operators $\mathcal{O}$ which commute with H and consist of one-body and (or) two-body operators. This is because $\omega\langle\Psi_0|\mathcal{O}|\Psi\rangle = \langle\Psi_0|[H,\mathcal{O}]|\Psi\rangle = 0$ holds due to eqs. (51) and (52). Although the coupling matrix between the one-body and two-body amplitudes is symmetric, the Hamiltonian matrix on the left-hand side of eq. (56) is not yet Hermitian because $D = D^+$ does not hold. This originates in the fact that $\langle\Phi_0|[H, [:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:, :a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}:]]|\Phi_0\rangle \neq 0$. In order to obtain a Hermitian Hamiltonian matrix without any truncation of the two-body amplitudes, we need to impose

$$\langle\Phi_0|[H, a^+_\alpha a^+_\beta a^+_\gamma a_{\gamma'} a_{\beta'} a_{\alpha'}]|\Phi_0\rangle = 0 \quad (67)$$

in addition to eqs. (45) and (46). This condition guarantees $\langle\Phi_0|[H,[:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:, :a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}:]]|\Phi_0\rangle = 0$, and thereby

$$D(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) = D(\lambda'_1\lambda'_2\lambda_1\lambda_2:\alpha\beta\alpha'\beta') = D(\lambda_1\lambda_2\lambda'_1\lambda'_2:\alpha'\beta'\alpha\beta)^*. \quad (68)$$

Equation (67) is explicitly shown in appendix B. For a Hermitian Hamiltonian matrix the orthonormal condition is given by [28]

$$(x^*_{\mu'} X^*_{\mu'}) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x_\mu \\ X_\mu \end{pmatrix} = \delta_{\mu\mu'}, \quad (69)$$

where x_μ and X_μ constitute an eigenstate of eq. (56) with $\omega = \omega_\mu$. The completeness relation becomes

$$\sum_\mu \begin{pmatrix} x_\mu \\ X_\mu \end{pmatrix} (x^*_\mu X^*_\mu) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} = I. \quad (70)$$

The transition amplitudes for one-body and two-body operators, $z = \langle\Psi_0|a^+_\alpha a_{\alpha'}|\Psi\rangle$ and $Z = \langle\Psi_0|:a^+_\alpha a^+_\beta a_{\beta'} a_{\alpha'}:|\Psi\rangle$, respectively, are calculated as follows:

$$\begin{pmatrix} z \\ Z \end{pmatrix} = \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix}. \quad (71)$$

Equation (56) has a certain similarity with the so-called Self-Consistent RPA (SCRPA) equations [22,29,30], extended to include higher configurations. In case the $X_{\lambda_1\lambda_2\lambda'_1\lambda'_2}$ amplitudes are dropped in eq. (53), eq. (56) reduces to something similar to what has become known as renormalized RPA (r-RPA) [31]. The main difference seems to come from the fact that here eq. (45) serves to determine the occupation matrix $n^0_{\alpha\alpha'}$, whereas in r-RPA eq. (45) is used to establish the single-particle basis. It should be interesting to investigate this relation more in detail in the future.

5 Summary

The necessary conditions that the spurious state associated with the translational motion and the double spurious mode have zero excitation energy in Extended ERPA (ERPA) were investigated using the small-amplitude limit of the time-dependent density-matrix theory (STDDM). The reason why STDDM was used is that it has a quite general form of the ERPA kind based on the HF ground state. In the case of the single spurious state it is found that ERPA, which keeps all components of the one-body amplitudes, gives the spurious state at zero excitation energy. This does not depend on approximations for the two-body amplitudes as long as they are properly antisymmetrized. For example, ERPA with only the 2p-2h and 2h-2p components of the two-body amplitudes preserves this property of the single spurious state. In the case of the double spurious state, all components of the one-body and two-body amplitudes, if they couple, are found necessary to yield the mode at zero excitation energy. Of course, no truncation in single-particle space should be made in both cases. The Kohn theorem for the single and double Kohn modes and the continuity equations for transition densities and currents were also investigated and found to hold under the same conditions as those necessary for the spurious states. It was pointed out that STDDM inherently has asymmetry and non-hermiticity, although it conserves various physical properties as mentioned above. A formulation of ERPA with hermiticity was also presented using TDDM, in which it was discussed that a three-body correlation matrix needs to be included in the description of ground-state correlations. The investigations in this work were performed for the spurious translational motion. It seems, however, clear that analogous considerations can be made for any spontaneously broken symmetry. An interesting case could be the coupling of quark-antiquark to the four-quark sector using, *e.g.* the Nambu–Jona-Lasinio model [32]. In this case one knows that chiral symmetry is spontaneously broken [32] and therefore in the chiral limit a double Goldstone mode (two pions) should appear. In the case of finite current quark masses analogous equations to those yielding the Kohn modes considered here should exist, actually well known as the Gell-Mann–Oakes–Renner relation [33]. To our knowledge the issue of the double spurious mode in ERPAs is taken up for the first time in this work.

Appendix A.

When ψ_α is chosen to be an eigenstate of the mean-field Hamiltonian (eq. (47)), eqs. (45) and (46) become [8]

$$(\epsilon_{\alpha'}-\epsilon_\alpha)n^0_{\alpha\alpha'}=\sum_{\lambda_1\lambda_2\lambda_3}(C^0_{\lambda_1\lambda_2\alpha'\lambda_3}\langle\alpha\lambda_3|v|\lambda_1\lambda_2\rangle \\ -C^0_{\alpha\lambda_3\lambda_1\lambda_2}\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle), \tag{A.1}$$

$$(\epsilon_{\alpha'}+\epsilon_{\beta'}-\epsilon_\alpha-\epsilon_\beta)C^0_{\alpha\beta\alpha'\beta'}= \\ B^0_{\alpha\beta\alpha'\beta'}+P^0_{\alpha\beta\alpha'\beta'}+H^0_{\alpha\beta\alpha'\beta'}, \tag{A.2}$$

where

$$B^0_{\alpha\beta\alpha'\beta'}=\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \\ \times[(\delta_{\alpha\lambda_1}-n^0_{\alpha\lambda_1})(\delta_{\beta\lambda_2}-n^0_{\beta\lambda_2})n^0_{\lambda_3\alpha'}n^0_{\lambda_4\beta'} \\ -n^0_{\alpha\lambda_1}n^0_{\beta\lambda_2}(\delta_{\lambda_3\alpha'}-n^0_{\lambda_3\alpha'})(\delta_{\lambda_4\beta'}-n^0_{\lambda_4\beta'})], \tag{A.3}$$

$$P^0_{\alpha\beta\alpha'\beta'}=\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle \\ \times[(\delta_{\alpha\lambda_1}\delta_{\beta\lambda_2}-\delta_{\alpha\lambda_1}n^0_{\beta\lambda_2}-n^0_{\alpha\lambda_1}\delta_{\beta\lambda_2})C^0_{\lambda_3\lambda_4\alpha'\beta'} \\ -(\delta_{\lambda_3\alpha'}\delta_{\lambda_4\beta'}-\delta_{\lambda_3\alpha'}n^0_{\lambda_4\beta'}-n^0_{\lambda_3\alpha'}\delta_{\lambda_4\beta'})C^0_{\alpha\beta\lambda_1\lambda_2}], \tag{A.4}$$

$$H^0_{\alpha\beta\alpha'\beta'}=\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\langle\lambda_1\lambda_2|v|\lambda_3\lambda_4\rangle_A \\ \times[\delta_{\alpha\lambda_1}(n^0_{\lambda_3\alpha'}C^0_{\lambda_4\beta\lambda_2\beta'}-n^0_{\lambda_3\beta'}C^0_{\lambda_4\beta\lambda_2\alpha'}+C^0_{\lambda_3\lambda_4\beta\alpha'\lambda_2\beta'}) \\ +\delta_{\beta\lambda_2}(n^0_{\lambda_4\beta'}C^0_{\lambda_3\alpha\lambda_1\alpha'}-n^0_{\lambda_4\alpha'}C^0_{\lambda_3\alpha\lambda_1\beta'}+C^0_{\lambda_4\lambda_3\alpha\beta'\lambda_1\alpha'}) \\ -\delta_{\alpha'\lambda_3}(n^0_{\alpha\lambda_1}C^0_{\lambda_4\beta\lambda_2\beta'}-n^0_{\beta\lambda_1}C^0_{\lambda_4\alpha\lambda_2\beta'}+C^0_{\alpha\lambda_4\beta\lambda_1\lambda_2\beta'}) \\ -\delta_{\beta'\lambda_4}(n^0_{\beta\lambda_2}C^0_{\lambda_3\alpha\lambda_1\alpha'}-n^0_{\alpha\lambda_2}C^0_{\lambda_3\beta\lambda_1\alpha'}+C^0_{\beta\lambda_3\alpha\lambda_2\lambda_1\alpha'})]. \tag{A.5}$$

The three-body correlation matrix $C^0_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ is also included in eq. (A.5). The equation for $C^0_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ is obtained by neglecting the four-body amplitudes and becomes

$$(\epsilon_{\alpha'}+\epsilon_{\beta'}+\epsilon_{\gamma'}-\epsilon_\alpha-\epsilon_\beta-\epsilon_\gamma)C^0_{\alpha\beta\gamma\alpha'\beta'\gamma'}= \\ U_{\alpha\beta\gamma\alpha'\beta'\gamma'}+U_{\alpha\beta\gamma\beta'\gamma'\alpha'}-U_{\alpha\beta\gamma\alpha'\gamma'\beta'} \\ -U^*_{\alpha'\beta'\gamma'\alpha\beta\gamma}-U^*_{\alpha'\beta'\gamma'\beta\gamma\alpha}+U^*_{\alpha'\beta'\gamma'\alpha\gamma\beta} \\ +V_{\alpha\beta\gamma\alpha'\beta'\gamma'}+V_{\alpha\beta\gamma\beta'\gamma'\alpha'}-V_{\alpha\beta\gamma\alpha'\gamma'\beta'} \\ -V^*_{\alpha'\beta'\gamma'\alpha\beta\gamma}-V^*_{\alpha'\beta'\gamma'\beta\gamma\alpha}+V^*_{\alpha'\beta'\gamma'\alpha\gamma\beta}, \tag{A.6}$$

where

$$U_{\alpha\beta\gamma\alpha'\beta'\gamma'}=-\sum_{\lambda_1\lambda_2}[\langle\lambda_1\lambda_2|v|\alpha'\beta'\rangle_A(n^0_{\gamma\lambda_1}C^0_{\alpha\beta\lambda_2\gamma'} \\ -n^0_{\beta\lambda_1}C^0_{\alpha\gamma\lambda_2\gamma'}+n^0_{\alpha\lambda_1}C^0_{\beta\gamma\lambda_2\gamma'}) \\ +\langle\lambda_1\lambda_2|v|\alpha'\beta'\rangle C^0_{\alpha\beta\gamma\lambda_1\lambda_2\gamma'}], \tag{A.7}$$

$$V_{\alpha\beta\gamma\alpha'\beta'\gamma'}=-\sum_{\lambda_1\lambda_2\lambda_3}\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle(-n^0_{\lambda_3\gamma'}n^0_{\gamma\lambda_2}C^0_{\alpha\beta\lambda_1\beta'} \\ +n^0_{\lambda_3\gamma'}C^0_{\alpha\beta\gamma\lambda_1\lambda_2\beta'} \\ +C^0_{\alpha\beta\lambda_1\lambda_2}C^0_{\gamma\lambda_3\beta'\gamma'}-C^0_{\alpha\beta\lambda_1\beta'}C^0_{\gamma\lambda_3\lambda_2\gamma'} \\ +\text{all other exchange terms}). \tag{A.8}$$

Equations for correlation matrices of higher ranks may be formulated according to the truncation rules given in ref. [12].

Appendix B.

The matrix elements of eqs. (57)-(60) are explicitly shown below:

$$S_1(\alpha'\alpha:\lambda\lambda')=n^0_{\lambda'\alpha}\delta_{\alpha'\lambda}-n^0_{\alpha'\lambda}\delta_{\alpha\lambda'}, \tag{B.1}$$

$$T_1(\alpha'\alpha:\lambda_1\lambda_2\lambda'_1\lambda'_2)=C^0_{\lambda'_1\lambda'_2\alpha\lambda_2}\delta_{\alpha'\lambda_1}+C^0_{\alpha'\lambda'_1\lambda_1\lambda_2}\delta_{\alpha\lambda'_2} \\ -C^0_{\alpha'\lambda'_2\lambda_1\lambda_2}\delta_{\alpha\lambda'_1}-C^0_{\lambda'_1\lambda'_2\alpha\lambda_1}\delta_{\alpha'\lambda_2}, \tag{B.2}$$

$$T_2(\alpha'\beta'\alpha\beta:\lambda\lambda')=C^0_{\lambda'\beta'\alpha\beta}\delta_{\alpha'\lambda}+C^0_{\alpha'\beta'\lambda\alpha}\delta_{\beta\lambda'} \\ -C^0_{\alpha'\beta'\lambda\beta}\delta_{\alpha\lambda'}-C^0_{\lambda'\alpha'\alpha\beta}\delta_{\beta'\lambda} \tag{B.3}$$

$$S_2(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)= \\ \mathcal{A}(\delta_{\alpha'\lambda_1}\delta_{\beta'\lambda_2})(\mathcal{A}(n^0_{\lambda'_1\alpha}n^0_{\lambda'_2\beta})+C^0_{\lambda'_1\lambda'_2\alpha\beta}) \\ -\mathcal{A}(\delta_{\alpha\lambda'_1}\delta_{\beta\lambda'_2})(\mathcal{A}(n^0_{\alpha'\lambda_1}n^0_{\beta'\lambda_2})+C^0_{\alpha'\beta'\lambda_1\lambda_2}) \\ +F(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)-F(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_2\lambda'_1) \\ -F(\alpha'\beta'\beta\alpha:\lambda_1\lambda_2\lambda'_1\lambda'_2)+F(\alpha'\beta'\beta\alpha:\lambda_1\lambda_2\lambda'_2\lambda'_1) \\ -F(\lambda'_1\lambda'_2\lambda_1\lambda_2:\alpha\beta\alpha'\beta')+F(\lambda'_1\lambda'_2\lambda_2\lambda_1:\alpha\beta\alpha'\beta') \\ +F(\lambda'_1\lambda'_2\lambda_1\lambda_2:\alpha\beta\beta'\alpha')-F(\lambda'_1\lambda'_2\lambda_2\lambda_1:\alpha\beta\beta'\alpha'), \tag{B.4}$$

where

$$F(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)=\delta_{\alpha\lambda'_1}[\mathcal{A}(n^0_{\alpha'\lambda_1}n^0_{\beta'\lambda_2})n^0_{\lambda'_2\beta} \\ +n^0_{\lambda'_2\beta}C^0_{\alpha'\beta'\lambda_1\lambda_2}+n^0_{\alpha'\lambda_1}C^0_{\beta'\lambda'_2\lambda_2\beta}-n^0_{\beta'\lambda_1}C^0_{\alpha'\lambda'_2\lambda_2\beta} \\ -n^0_{\alpha'\lambda_2}C^0_{\beta'\lambda'_2\lambda_1\beta}+n^0_{\beta'\lambda_2}C^0_{\alpha'\lambda'_2\lambda_1\beta}+C^0_{\alpha'\beta'\lambda'_2\lambda_1\lambda_2\beta}]. \tag{B.5}$$

The three-body correlation matrix is also included in eq. (B.5). The matrix elements A, B, C, and D are given in the following. For simplicity, terms containing $C^0_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ are not shown. They appear in B, C, and D: Wherever there is a term containing $n^0_{\alpha\alpha'}C^0_{\beta\gamma\beta'\gamma'}$, there exists a corresponding term with $C^0_{\alpha\beta\gamma\alpha'\beta'\gamma'}$. The expressions for A, B, C, and D are not unique and their symmetry properties are not necessarily apparent. Equations (45), (46), and (67) allow us to take other expressions and guarantee symmetry properties:

$$
\begin{aligned}
&A(\alpha'\alpha:\lambda\lambda') = (\epsilon_{\alpha'}-\epsilon_{\alpha})(\delta_{\lambda\alpha'}n^0_{\lambda'\alpha}-\delta_{\lambda'\alpha}n^0_{\alpha'\lambda})\\
&+\sum_{\gamma\delta}[\langle\gamma\delta|v|\alpha\lambda\rangle(\mathcal{A}(n^0_{\lambda'\gamma}n^0_{\alpha'\delta})+C^0_{\lambda'\alpha'\gamma\delta})\\
&+\langle\lambda'\alpha'|v|\delta\gamma\rangle(\mathcal{A}(n^0_{\gamma\lambda}n^0_{\delta\alpha})+C^0_{\delta\gamma\alpha\lambda})\\
&-\langle\lambda'\delta|v|\alpha\gamma\rangle_A(n^0_{\gamma\lambda}n^0_{\alpha'\delta}+C^0_{\alpha'\gamma\delta\lambda})\\
&-\langle\gamma\alpha'|v|\delta\lambda\rangle_A(n^0_{\lambda'\gamma}n^0_{\delta\alpha}+C^0_{\lambda'\delta\gamma\alpha})]\\
&-\sum_{\gamma\delta\gamma'}(\langle\alpha'\gamma|v|\delta\gamma'\rangle\delta_{\lambda'\alpha}C^0_{\delta\gamma'\lambda\gamma}+\langle\gamma\delta|v|\alpha\gamma'\rangle\delta_{\lambda\alpha'}C^0_{\lambda'\gamma'\gamma\delta}),
\end{aligned}
\tag{B.6}
$$

$$
\begin{aligned}
&B(\alpha'\beta'\alpha\beta:\lambda\lambda') =\\
&\quad\sum_{\gamma}\{\langle\lambda'\gamma|v|\alpha\beta\rangle_A[\mathcal{A}(n^0_{\alpha'\lambda}n^0_{\beta'\gamma})+C^0_{\alpha'\beta'\lambda\gamma}]\\
&\quad+\langle\alpha'\beta'|v|\lambda\gamma\rangle_A[\mathcal{A}(n^0_{\lambda'\alpha}n^0_{\gamma\beta})+C^0_{\lambda'\gamma\alpha\beta}]\}\\
&\quad+H(\alpha'\beta'\alpha\beta:\lambda\lambda')-H(\beta'\alpha'\alpha\beta:\lambda\lambda')\\
&\quad+H^*(\alpha\beta\alpha'\beta':\lambda'\lambda)-H^*(\beta\alpha\alpha'\beta':\lambda'\lambda)\\
&\quad+I(\alpha'\beta'\alpha\beta:\lambda\lambda')-I(\alpha'\beta'\beta\alpha:\lambda\lambda')\\
&\quad+I^*(\alpha\beta\alpha'\beta':\lambda'\lambda)-I^*(\alpha\beta\beta'\alpha':\lambda'\lambda),
\end{aligned}
\tag{B.7}
$$

$$
C(\alpha'\alpha:\lambda_1\lambda_2\lambda'_1\lambda'_2)=B(\lambda'_1\lambda'_2\lambda_1\lambda_2:\alpha\alpha'),
\tag{B.8}
$$

where

$$
\begin{aligned}
&H(\alpha'\beta'\alpha\beta:\lambda\lambda') = -\delta_{\lambda\alpha'}\{(\epsilon_\alpha+\epsilon_\beta-\epsilon_{\alpha'}-\epsilon_{\beta'})C^0_{\lambda'\beta'\alpha\beta}\\
&+\sum_{\gamma\delta}(\langle\gamma\delta|v|\alpha\beta\rangle(\mathcal{A}(n^0_{\lambda'\gamma}n^0_{\beta'\delta})+C^0_{\lambda'\beta'\gamma\delta})\\
&-\sum_{\gamma\delta\gamma'}[\langle\gamma\delta|v|\alpha\gamma'\rangle_A(n^0_{\lambda'\gamma}n^0_{\beta'\delta}n^0_{\gamma'\beta}+n^0_{\lambda'\gamma}C^0_{\beta'\gamma'\delta\beta}\\
&-n^0_{\beta'\gamma}C^0_{\lambda'\gamma'\delta\beta})+\langle\gamma\delta|v|\alpha\gamma'\rangle n^0_{\gamma'\beta}C^0_{\lambda'\beta'\gamma\delta}\\
&-\langle\gamma\delta|v|\beta\gamma'\rangle_A(n^0_{\lambda'\gamma}n^0_{\beta'\delta}n^0_{\gamma'\alpha}+n^0_{\lambda'\gamma}C^0_{\beta'\gamma'\delta\alpha}\\
&-n^0_{\beta'\gamma}C^0_{\lambda'\gamma'\delta\alpha})-\langle\gamma\delta|v|\beta\gamma'\rangle n^0_{\gamma'\alpha}C^0_{\lambda'\beta'\gamma\delta}\\
&+\langle\beta'\gamma|v|\delta\gamma'\rangle_A(n^0_{\lambda'\gamma}n^0_{\delta\beta}n^0_{\gamma'\alpha}+n^0_{\gamma'\alpha}C^0_{\delta\lambda'\beta\gamma}\\
&-n^0_{\gamma'\beta}C^0_{\delta\lambda'\alpha\gamma})+\langle\beta'\gamma|v|\delta\gamma'\rangle n^0_{\lambda'\gamma}C^0_{\gamma'\delta\alpha\beta}]\},
\end{aligned}
\tag{B.9}
$$

$$
\begin{aligned}
&I(\alpha'\beta'\alpha\beta:\lambda\lambda') = \sum_{\gamma\delta}\{[\langle\gamma\delta|v|\alpha\lambda\rangle_A(n^0_{\alpha'\gamma}n^0_{\beta'\delta}n^0_{\lambda'\beta}\\
&+n^0_{\alpha'\gamma}C^0_{\beta'\lambda'\delta\beta}-n^0_{\beta'\gamma}C^0_{\alpha'\lambda'\delta\beta})\\
&+\langle\gamma\delta|v|\alpha\lambda\rangle(n^0_{\lambda'\beta}C^0_{\alpha'\beta'\gamma\delta}+n^0_{\lambda'\gamma}C^0_{\alpha'\beta'\delta\beta})]\\
&-\langle\lambda'\gamma|v|\alpha\delta\rangle_A[\mathcal{A}(n^0_{\alpha'\lambda}n^0_{\beta'\gamma})n^0_{\delta\beta}+n^0_{\delta\lambda}C^0_{\alpha'\beta'\gamma\beta}\\
&+n^0_{\delta\beta}C^0_{\alpha'\beta'\lambda\gamma}+n^0_{\alpha'\lambda}C^0_{\beta'\delta\gamma\beta}-n^0_{\beta'\lambda}C^0_{\alpha'\delta\gamma\beta}\\
&-n^0_{\alpha'\gamma}C^0_{\beta'\delta\lambda\beta}+n^0_{\beta'\gamma}C^0_{\alpha'\delta\lambda\beta}]\}.
\end{aligned}
\tag{B.10}
$$

The matrix D is given as

$$
\begin{aligned}
&D(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) =\\
&\quad(\epsilon_{\alpha'}+\epsilon_{\beta'}-\epsilon_\alpha-\epsilon_\beta)S_2(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)\\
&\quad+\langle\lambda'_1\lambda'_2|v|\alpha\beta\rangle_A(\mathcal{A}(n^0_{\alpha'\lambda_1}n^0_{\beta'\lambda_2})+C^0_{\alpha'\beta'\lambda_1\lambda_2})\\
&\quad+\langle\alpha'\beta'|v|\lambda_1\lambda_2\rangle_A(\mathcal{A}(n^0_{\lambda'_1\alpha}n^0_{\lambda'_2\beta})+C^0_{\lambda'_1\lambda'_2\alpha\beta})\\
&\quad+J(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)+J^*(\alpha\beta\alpha'\beta':\lambda'_1\lambda'_2\lambda_1\lambda_2)\\
&\quad+K(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)+L(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2)\\
&\quad+\text{all other exchange terms of } K \text{ and } L,
\end{aligned}
\tag{B.11}
$$

where

$$
\begin{aligned}
&J(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) = -\mathcal{A}(\delta_{\lambda_1\alpha'}\delta_{\lambda_2\beta'})\Big\{\sum_{\gamma\delta}[\langle\gamma\delta|v|\alpha\beta\rangle\\
&-\sum_{\gamma'}(\langle\gamma\delta|v|\alpha\gamma'\rangle n^0_{\gamma'\beta}-\langle\gamma\delta|v|\beta\gamma'\rangle n^0_{\gamma'\alpha}))]\\
&(\mathcal{A}(n^0_{\lambda'_1\gamma}n^0_{\lambda'_2\delta})+C^0_{\lambda'_1\lambda'_2\gamma\delta})+\sum_{\gamma\delta\gamma'}[\langle\gamma\delta|v|\alpha\gamma'\rangle(n^0_{\lambda'_1\beta}C^0_{\gamma'\lambda'_2\gamma\delta}\\
&-n^0_{\lambda'_2\beta}C^0_{\gamma'\lambda'_1\gamma\delta}-n^0_{\lambda'_1\gamma}C^0_{\gamma'\lambda'_2\beta\delta}+n^0_{\lambda'_2\gamma}C^0_{\gamma'\lambda'_1\beta\delta})\\
&-\langle\gamma\delta|v|\beta\gamma'\rangle(n^0_{\lambda'_1\alpha}C^0_{\gamma'\lambda'_2\gamma\delta}-n^0_{\lambda'_2\alpha}C^0_{\gamma'\lambda'_1\gamma\delta}\\
&-n^0_{\lambda'_1\gamma}C^0_{\gamma'\lambda'_2\alpha\delta}+n^0_{\lambda'_2\gamma}C^0_{\gamma'\lambda'_1\alpha\delta})]\Big\},
\end{aligned}
\tag{B.12}
$$

$$
\begin{aligned}
&K(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) =\\
&\delta_{\lambda_1\alpha'}\Big\{\sum_{\gamma\delta}[\langle\gamma\delta|v|\alpha\beta\rangle_A(n^0_{\lambda'_1\gamma}n^0_{\lambda'_2\delta}n^0_{\beta'\lambda_2}+n^0_{\lambda'_1\gamma}C^0_{\lambda'_2\beta'\delta\lambda_2})\\
&+\langle\gamma\delta|v|\alpha\lambda_2\rangle_A(n^0_{\lambda'_1\gamma}n^0_{\lambda'_2\beta}n^0_{\beta'\delta}+n^0_{\lambda'_1\gamma}C^0_{\lambda'_2\beta'\beta\delta})\\
&+\langle\gamma\beta'|v|\lambda_2\delta\rangle_A(n^0_{\delta\beta}n^0_{\lambda'_1\alpha}n^0_{\lambda'_2\gamma}+n^0_{\delta\beta}C^0_{\lambda'_1\lambda'_2\alpha\gamma})\\
&+\text{all other exchange terms}]\\
&-\sum_{\gamma\delta\gamma'}[\langle\gamma\delta|v|\alpha\gamma'\rangle_A(n^0_{\lambda'_1\gamma}n^0_{\beta'\delta}n^0_{\lambda'_2\beta}n^0_{\gamma'\lambda_2}+n^0_{\lambda'_1\gamma}n^0_{\beta'\delta}C^0_{\lambda'_2\gamma'\beta\lambda_2}\\
&+C^0_{\lambda'_1\beta'\gamma\delta}C^0_{\lambda'_2\gamma'\beta\lambda_2})-\langle\gamma\beta'|v|\gamma'\delta\rangle_A(n^0_{\lambda'_1\alpha}n^0_{\lambda'_2\gamma}n^0_{\gamma'\beta}n^0_{\delta\lambda_2}\\
&+n^0_{\gamma'\beta}n^0_{\lambda'_1\alpha}C^0_{\lambda'_2\delta\gamma\lambda_2}+C^0_{\lambda'_2\gamma'\alpha\beta}C^0_{\lambda'_1\delta\gamma\lambda_2})\\
&+\text{all other exchange terms}]\Big\},
\end{aligned}
\tag{B.13}
$$

$$
\begin{aligned}
&L(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda'_1\lambda'_2) =\\
&-\sum_{\gamma}[\langle\alpha'\gamma|v|\lambda_1\lambda_2\rangle(n^0_{\beta'\gamma}n^0_{\lambda'_1\alpha}n^0_{\lambda'_2\beta}+n^0_{\beta'\gamma}C^0_{\lambda'_1\lambda'_2\alpha\beta})\\
&+\text{all other exchange terms}]\\
&+\sum_{\gamma\delta}[\langle\alpha'\gamma|v|\lambda_1\delta\rangle_A(n^0_{\delta\beta}n^0_{\lambda'_1\alpha}n^0_{\lambda'_2\gamma}n^0_{\beta'\lambda_2}\\
&+n^0_{\beta'\lambda_2}n^0_{\delta\beta}C^0_{\lambda'_1\lambda'_2\alpha\gamma}+C^0_{\beta'\delta\lambda_2\beta}C^0_{\lambda'_1\lambda'_2\alpha\gamma})\\
&+\text{all other exchange terms}].
\end{aligned}
\tag{B.14}
$$

Finally, we discuss a relation between eq. (56) and a set of the STDDM equations (eqs. (3) and (4)). When the ground state is approximated by the HF one, eqs. (B.1)-(B.4) become

$$S_1(\alpha'\alpha:\lambda\lambda') = (f_\alpha - f_{\alpha'})\delta_{\alpha\lambda'}\delta_{\alpha'\lambda}, \quad \text{(B.15)}$$
$$S_2(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda_1'\lambda_2') = \mathcal{A}(\delta_{\alpha\lambda_1'}\delta_{\beta\lambda_2'})\mathcal{A}(\delta_{\alpha'\lambda_1}\delta_{\beta'\lambda_2})F^0_{\alpha'\beta'\alpha\beta}, \quad \text{(B.16)}$$
$$T_1(\alpha'\alpha:\lambda_1\lambda_2\lambda_1'\lambda_2') = T_2(\alpha'\beta'\alpha\beta:\lambda\lambda') = 0, \quad \text{(B.17)}$$

where

$$F^0_{\alpha'\beta'\alpha\beta} = f_\alpha f_\beta \bar{f}_{\alpha'}\bar{f}_{\beta'} - \bar{f}_\alpha \bar{f}_\beta f_{\alpha'} f_{\beta'}. \quad \text{(B.18)}$$

Equations (B.6)-(B.8) and (B.11) become the following:

$$A(\alpha'\alpha:\lambda\lambda') = [(\epsilon_{\alpha'} - \epsilon_\alpha)\delta_{\alpha\lambda'}\delta_{\alpha'\lambda} + \langle\lambda'\alpha'|v|\alpha\lambda\rangle_A(f_{\alpha'} - f_\alpha)](f_{\lambda'} - f_\lambda), \quad \text{(B.19)}$$

$$\begin{aligned}B(\alpha'\beta'\alpha\beta:\lambda\lambda') =& \\ -[(\bar{f}_\alpha\bar{f}_\beta f_{\beta'} + f_\alpha f_\beta \bar{f}_{\beta'})\langle\lambda'\beta'|v|\alpha\beta\rangle_A\delta_{\alpha'\lambda}& \\ -(\bar{f}_\alpha\bar{f}_\beta f_{\alpha'} + f_\alpha f_\beta \bar{f}_{\alpha'})\langle\lambda'\alpha'|v|\alpha\beta\rangle_A\delta_{\beta'\lambda}& \\ -(\bar{f}_\beta f_{\alpha'} f_{\beta'} + f_\beta \bar{f}_{\alpha'}\bar{f}_{\beta'})\langle\alpha'\beta'|v|\lambda\beta\rangle_A\delta_{\alpha\lambda'}& \\ +(\bar{f}_\alpha f_{\alpha'} f_{\beta'} + f_\alpha \bar{f}_{\alpha'}\bar{f}_{\beta'})\langle\alpha'\beta'|v|\lambda\alpha\rangle_A\delta_{\beta\lambda'}](f_{\lambda'} - f_\lambda),& \quad \text{(B.20)}\end{aligned}$$

$$C(\alpha'\alpha:\lambda_1\lambda_2\lambda_1'\lambda_2') = B(\lambda_1'\lambda_2'\lambda_1\lambda_2:\alpha\alpha'), \quad \text{(B.21)}$$

$$\begin{aligned}D(\alpha'\beta'\alpha\beta:\lambda_1\lambda_2\lambda_1'\lambda_2') =& F^0_{\lambda_1\lambda_2\lambda_1'\lambda_2'} \\ \times\Big\{&(\epsilon_{\alpha'} + \epsilon_{\beta'} - \epsilon_\alpha - \epsilon_\beta)\mathcal{A}(\delta_{\alpha\lambda_1'}\delta_{\beta\lambda_2'})\mathcal{A}(\delta_{\alpha'\lambda_1}\delta_{\beta'\lambda_2}) \\ &+(1 - f_{\alpha'} - f_{\beta'})\langle\alpha'\beta'|v|\lambda_1\lambda_2\rangle_A\mathcal{A}(\delta_{\alpha\lambda_1'}\delta_{\beta\lambda_2'}) \\ &-(1 - f_\alpha - f_\beta)\langle\lambda_1'\lambda_2'|v|\alpha\beta\rangle_A\mathcal{A}(\delta_{\alpha'\lambda_1}\delta_{\beta'\lambda_2}) \\ &+(f_\alpha - f_{\alpha'})[\langle\alpha'\lambda_1'|v|\alpha\lambda_1\rangle_A\delta_{\beta'\lambda_2}\delta_{\beta\lambda_2'} \\ &+\langle\alpha'\lambda_2'|v|\alpha\lambda_2\rangle_A\delta_{\beta'\lambda_1}\delta_{\beta\lambda_1'} \\ &-\langle\alpha'\lambda_1'|v|\alpha\lambda_2\rangle_A\delta_{\beta'\lambda_1}\delta_{\beta\lambda_2'} - \langle\alpha'\lambda_2'|v|\alpha\lambda_1\rangle_A\delta_{\beta'\lambda_2}\delta_{\beta\lambda_1'}] \\ &+(f_\beta - f_{\beta'})[\langle\beta'\lambda_1'|v|\beta\lambda_1\rangle_A\delta_{\alpha'\lambda_2}\delta_{\alpha\lambda_2'} \\ &+\langle\beta'\lambda_2'|v|\beta\lambda_2\rangle_A\delta_{\alpha'\lambda_1}\delta_{\alpha\lambda_1'} \\ &-\langle\beta'\lambda_1'|v|\beta\lambda_2\rangle_A\delta_{\alpha'\lambda_1}\delta_{\alpha\lambda_2'} - \langle\beta'\lambda_2'|v|\beta\lambda_1\rangle_A\delta_{\alpha'\lambda_2}\delta_{\alpha\lambda_1'}] \\ &-(f_\alpha - f_{\beta'})[\langle\beta'\lambda_1'|v|\alpha\lambda_1\rangle_A\delta_{\alpha'\lambda_2}\delta_{\beta\lambda_2'} \\ &+\langle\beta'\lambda_2'|v|\alpha\lambda_2\rangle_A\delta_{\alpha'\lambda_1}\delta_{\beta\lambda_1'} \\ &-\langle\beta'\lambda_1'|v|\alpha\lambda_2\rangle_A\delta_{\alpha'\lambda_1}\delta_{\beta\lambda_2'} - \langle\beta'\lambda_2'|v|\alpha\lambda_1\rangle_A\delta_{\alpha'\lambda_2}\delta_{\beta\lambda_1'}] \\ &-(f_\alpha - f_{\beta'})[\langle\beta'\lambda_1'|v|\alpha\lambda_1\rangle_A\delta_{\alpha'\lambda_2}\delta_{\beta\lambda_2'} \\ &+\langle\beta'\lambda_2'|v|\alpha\lambda_2\rangle_A\delta_{\alpha'\lambda_1}\delta_{\beta\lambda_1'} \\ &-\langle\beta'\lambda_1'|v|\alpha\lambda_2\rangle_A\delta_{\alpha'\lambda_1}\delta_{\beta\lambda_2'} - \langle\beta'\lambda_2'|v|\alpha\lambda_1\rangle_A\delta_{\alpha'\lambda_2}\delta_{\beta\lambda_1'}]\Big\}. \quad \text{(B.22)}\end{aligned}$$

If S_1x and S_2X which appear in the equation for X, that is, $Bx + DX = \omega S_2 X$, are replaced by x and X, respectively, the equation for X is equivalent to eq. (4). However, the replacement $S_1x \to x$ and $S_2X \to X$ in $Ax + CX = \omega S_1 x$ cannot give eq. (3) because of the symmetric coupling between x and X. Since the expression for C (eq. (B.8)) is not unique as mentioned above, we can always take an expression for C which leads to the same coupling matrix as in eq. (3) in the HF limit. Such an expression for C is the following:

$$\begin{aligned}C(\alpha'\alpha:\lambda_1\lambda_2\lambda_1'\lambda_2') =& \\ F^0_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(\langle\alpha'\lambda_2'|v|\lambda_1\lambda_2\rangle_A\delta_{\lambda_1'\alpha} &- \langle\alpha'\lambda_1'|v|\lambda_1\lambda_2\rangle_A\delta_{\lambda_2'\alpha} \\ -\langle\lambda_1'\lambda_2'|v|\alpha\lambda_2\rangle_A\delta_{\lambda_1\alpha'} &+ \langle\lambda_1'\lambda_2'|v|\alpha\lambda_1\rangle_A\delta_{\lambda_2\alpha'}). \quad \text{(B.23)}\end{aligned}$$

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