Spurious states in extended RPA theories, part II

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Abstract. Using an extended RPA theory (ERPA) which contains the effects of ground-state correlations and preserves hermiticity, conditions that spurious modes have zero-energy solutions in extended RPA theories are investigated from a general point of view. The single and double excitations of translational motion are considered as illustrative examples.

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

1 Introduction

It is well-known that in the case of spontaneously broken continuous symmetries the random-phase approximation (RPA) in a fully self-consistent form gives zero-energy solutions for spurious or Goldstone modes associated with one-body operators which commute with the total hamiltonian [1,2]. [1] Thus, spurious states are decoupled from physical states in RPA. For a microscopic description of collective states associated with two-body operators such as double-phonon states [3,4], we need to use extended theories of RPA which enable us to calculate two-body transition amplitudes in addition to one-body transition amplitudes. One of such extended RPA theories is the second RPA (SRPA) [5] which has been used for the study of decay properties of giant resonances [6]. However, the problem of spurious states in extended RPA theories has not thoroughly been investigated. In our previous work [7] we studied the conditions for extended RPA theories to have zero-energy solutions for the single and double excitations of translational motion. We pointed out that all components of one-body and two-body transition amplitudes must be included in extended RPA theories. However, the extended RPA theory used in the study was not completely general because the effects of ground-state correlations were neglected, and the derivation of the conditions was also specific to the extended RPA theory used. In this paper we reinvestigate the problem of spurious states using a more general approach than used in ref.[7] and a more elaborate extended RPA theory which meets the requirement of hermiticity [7]. The paper is organized as follows: In sect. 2 our extended RPA theory (ERPA) is presented and some properties of ERPA which have not been investigated in previous publications [7,8] are discussed. In sect. 3 it is shown in a transparent way that ERPA has zero-energy solutions for spurious modes. The relation of ERPA and the small amplitude limit of the time-dependent density-matrix theory (STDDM) [9] which has been used for realistic calculations [10] is discussed also in sect. 3 and it is pointed out that STDDM also gives zero excitation energy to spurious modes. The single and double excitations of translational motion are considered in sect. 4 as illustrative examples, and sect. 5 is devoted to the summary.

2 Extended RPA

We consider the Hamiltonian

$$\hat{H} = \sum_{\lambda\lambda'} \langle\lambda|t|\lambda'\rangle a^+_\lambda a_{\lambda'} + \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda'_1\lambda'_2} \langle\lambda_1\lambda_2|v|\lambda'_1\lambda'_2\rangle a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1}, \tag{1}$$

where t is the kinetic energy operator, v is a two-body interaction and $a^+_\lambda(a_\lambda)$ the creation (annihilation) operator of a nucleon in a single-particle state λ.

2.1 Ground state

First we discuss the ground state $|0\rangle$ which is used to evaluate various matrices in ERPA. The ground state is given by the stationary conditions of the occupation matrix $n_{\alpha\alpha'}$, the two-body correlation matrix $C_{\alpha\beta\alpha'\beta'}$ and the three-body correlation matrix $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ defined as

$$n_{\alpha\alpha'} = \langle 0|a^+_{\alpha'} a_\alpha|0\rangle \tag{2}$$
$$C_{\alpha\beta\alpha'\beta'} = \langle 0|a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha|0\rangle - \mathcal{A}(n_{\alpha\alpha'} n_{\beta\beta'}) \tag{3}$$
$$C_{\alpha\beta\gamma\alpha'\beta'\gamma'} = \langle 0|a^+_{\alpha'} a^+_{\beta'} a^+_{\gamma'} a_\gamma a_\beta a_\alpha|0\rangle - \mathcal{A}(n_{\alpha\alpha'} n_{\beta\beta'} n_{\gamma\gamma'} + \mathcal{S}(n_{\alpha\alpha'} C_{\beta\gamma\beta'\gamma'})), \tag{4}$$

where $\mathcal{A}$ and $\mathcal{S}$ mean that the products in the parentheses are properly antisymmetrized and symmetrized under the exchange of single-particle indices [11]. The stationary conditions are written as

$$\langle 0|[a^+_{\alpha'} a_\alpha, \hat{H}]|0\rangle = 0 \tag{5}$$
$$\langle 0|[a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha, \hat{H}]|0\rangle = 0 \tag{6}$$
$$\langle 0|[a^+_{\alpha'} a^+_{\beta'} a^+_{\gamma'} a_\gamma a_\beta a_\alpha, \hat{H}]|0\rangle = 0. \tag{7}$$

[1] In nuclear physics it has become customary to call those zero energy solutions of RPA 'spurious modes'. In reality they are not really 'spurious'. For example in the case of rotation the 'spurious' mode is just the band head of the rotational band. Nonetheless we will keep the expression 'spurious' mode in this paper.

The expectation values of four-body operators in Eq.(7) are approximated by the products of $n_{\alpha\alpha'}$, $C_{\alpha\beta\alpha'\beta'}$ and $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$: the four-body correlation matrix is neglected. Eqs.(5)-(7) are explicitly given in ref.[7], where the single-particle states which satisfy Hartree-Fock (HF)-like equation

$$t\phi_\alpha(1) + \int d2[\rho(2,2)v(1,2)\phi_\alpha(1) - \rho(1,2)v(1,2)\phi_\alpha(2)] = h\phi_\alpha(1) = \epsilon_\alpha\phi_\alpha(1), \tag{8}$$

are used. Here, ρ is the one-body density matrix given by $\rho(1,1') = \sum_{\alpha\alpha'} n_{\alpha\alpha'}\phi_\alpha(1)\phi^*_\alpha(1')$ and numbers indicate spatial, spin and isospin coordinates. The solutions for Eqs.(5)-(7) may be obtained using iterative gradient method which has been used to solve Eqs.(5) and (6) in ref. [12]. In this gradient method a matrix derived form the functional derivatives Eqs. (5) and (6) with respect to $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$ is used. This matrix is the same as the hamiltonian matrix of ERPA used in Ref. [12]. This implies that the ground state in our approach is not independent of the excited states of the corresponding ERPA equation. The three-body correlation matrix $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ is necessary to make ERPA hermitian as will be discussed below.

2.2 ERPA equation

We consider an excitation operator consisting of one-body and two-body operators

$$\hat{Q}^+_\mu = \sum_{\lambda\lambda'} x^\mu_{\lambda\lambda'} : a^+_\lambda a_{\lambda'} : + \sum_{\lambda_1\lambda_2\lambda'_1\lambda'_2} X^\mu_{\lambda_1\lambda_2\lambda'_1\lambda'_2} : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} : \tag{9}$$

which satisfies

$$\hat{Q}^+_\mu|\Psi_0\rangle = |\mu\rangle, \tag{10}$$

$$\hat{Q}_\mu|\Psi_0\rangle = 0. \tag{11}$$

Here, $|\Psi_0\rangle$ is the ground state in ERPA, $|\mu\rangle$ is an excited state and : : implies that uncorrelated parts consisting of lower-level operators are to be subtracted; for example,

$$: a^+_{\alpha'} a_\alpha : = a^+_{\alpha'} a_\alpha - n_{\alpha\alpha'} \tag{12}$$

$$\begin{aligned} : a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha : &= a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha - \mathcal{AS}(n_{\alpha\alpha'} : a^+_{\beta'} a_\beta :) \\ &- [\mathcal{A}(n_{\alpha\alpha'} n_{\beta\beta'}) + C_{\alpha\beta\alpha'\beta'}]. \end{aligned} \tag{13}$$

The ERPA equations are derived from the following equations of motion [13]

$$\langle\Psi_0|[[: a^+_{\alpha'} a_\alpha :, \hat{H}], \hat{Q}^+_\mu]|\Psi_0\rangle = \omega_\mu \langle\Psi_0|[: a^+_{\alpha'} a_\alpha :, \hat{Q}^+_\mu]|\Psi_0\rangle \tag{14}$$

$$\langle\Psi_0|[[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{H}], \hat{Q}^+_\mu]|\Psi_0\rangle = \omega_\mu \langle\Psi_0|[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{Q}^+_\mu]|\Psi_0\rangle, \tag{15}$$

where ω_μ is the excitation energy of $|\mu\rangle$. In the evaluation of the matrix elements in the above equations, we will not use the relation Eq. (11) which defines the ground state $|\Psi_0\rangle$ within the present approach. This is done in the so-called Self-Consistent RPA (SCRPA) which so far mostly has been investigated only on the one-body level of Eq. (9) [13, 14,15,16]. This leads to a non-linear theory because $|\Psi_0\rangle$ depends on the amplitudes $x^\mu_{\alpha\alpha'}$ (and $X^\mu_{\alpha\beta\alpha'\beta'}$). We here want to simplify the theory and linearize Eqs. (14) and (15). This is achieved in determining the ground state via Eqs. (5)-(8). If we only retain the one-body part in Eq. (9) and $n_{\alpha\alpha'}$ in the ground state, only Eq. (5) enters the game and it is solved with the well-known Hartree-Fock ground state. However, if in Eq. (9) also the two-body part is kept, then we have in addition to consider the relations Eqs. (6) and (7). This stems from the fact that $\langle\Psi_0|[\hat{H}, \hat{Q}^+_\mu]|\Psi_0\rangle = 0$ is one of the equations of motion in the exact case [2]. These extra relations also assure that the ensuing extended RPA equations are of the canonical form of coupled harmonic oscillators (see section 2.3 below). Equations (5)-(7) can be solved for the one, two and three-body density matrices as has been shown in ref. [12] and then the approximate ground state $|0\rangle$ is implicitly determined. Explicitly the ERPA equations are written as

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix}, \tag{16}$$

where the matrix elements are given by

$$A(\alpha\alpha' : \lambda\lambda') = \langle 0|[[: a^+_{\alpha'} a_\alpha :, \hat{H}], : a^+_\lambda a_{\lambda'} :]|0\rangle \tag{17}$$

$$B(\alpha\beta\alpha'\beta' : \lambda\lambda') = \langle 0|[[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{H}], : a^+_\lambda a_{\lambda'} :]|0\rangle \tag{18}$$
$$C(\alpha\alpha' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle 0|[[: a^+_{\alpha'} a_\alpha :, \hat{H}], : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :]|0\rangle \tag{19}$$
$$D(\alpha\beta\alpha'\beta' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle 0|[[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{H}], : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :]|0\rangle \tag{20}$$

$$S_1(\alpha\alpha' : \lambda\lambda') = \langle 0|[: a^+_{\alpha'} a_\alpha :, : a^+_\lambda a_{\lambda'} :]|0\rangle \tag{21}$$
$$T_1(\alpha\alpha' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle 0|[: a^+_{\alpha'} a_\alpha :, : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :]|0\rangle \tag{22}$$
$$T_2(\alpha\beta\alpha'\beta' : \lambda\lambda') = \langle 0|[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, : a^+_\lambda a_{\lambda'} :]|0\rangle \tag{23}$$
$$S_2(\alpha\beta\alpha'\beta' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = \langle 0|[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :]|0\rangle. \tag{24}$$

When the ground-state correlations are neglected, the one-body section of Eq. (16), $Ax^\mu = \omega_\mu S_1 x^\mu$, is equivalent to the RPA equation.

2.3 Hermiticity of ERPA matrix

The hamiltonian matrix on the left hand side of Eq.(16) is hermitian. This is because the following operator identity for $\hat{A}$ and $\hat{B}$, which are either $: a^+_{\alpha'} a_\alpha :$ or $: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :$,

$$\langle 0|[[\hat{B}, \hat{H}], \hat{A}]|0\rangle - \langle 0|[[\hat{A}, \hat{H}], \hat{B}]|0\rangle = \langle 0|[\hat{H}, [\hat{A}, \hat{B}]]|0\rangle = 0 \tag{25}$$

is satisfied due to the ground-state conditions Eqs.(5)-(7). We show this explicitly for the matrix D in Eq. (20) where $\hat{A}$ and $\hat{B}$ are both two-body operators $: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :$ and $: a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :$, respectively. Since $[\hat{A}, \hat{B}]$ consists of at most three-body operators, Eq.(25) holds because of Eqs.(5)-(7). This means

$$D(\alpha\beta\alpha'\beta' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = D(\lambda'_1\lambda'_2\lambda_1\lambda_2 : \alpha'\beta'\alpha\beta). \tag{26}$$

From its definition (Eq.(20)) the hermitian conjugate of D is

$$D(\lambda_1\lambda_2\lambda'_1\lambda'_2 : \alpha\beta\alpha'\beta')^* = D(\lambda'_1\lambda'_2\lambda_1\lambda_2 : \alpha'\beta'\alpha\beta). \tag{27}$$

Eqs.(26) and (27) imply that D is hermitian, namely,

$$D(\alpha\beta\alpha'\beta' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = D(\lambda_1\lambda_2\lambda'_1\lambda'_2 : \alpha\beta\alpha'\beta')^*. \tag{28}$$

The following symmetries of other matrices A, B and C are shown in a similar way:

$$A(\alpha\alpha' : \lambda\lambda') = A(\lambda'\lambda : \alpha'\alpha) = A(\lambda\lambda' : \alpha\alpha')^*, \tag{29}$$
$$C(\alpha\alpha' : \lambda_1\lambda_2\lambda'_1\lambda'_2) = B(\lambda'_1\lambda'_2\lambda_1\lambda_2 : \alpha'\alpha) = B(\lambda_1\lambda_2\lambda'_1\lambda'_2 : \alpha\alpha')^*. \tag{30}$$

Therefore the hamiltonian matrix in Eq. (16)

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix}$$

is hermitian. The three-body correlation matrix is necessary for Eq.(28), whereas Eqs.(29) and (30) hold without it. The matrices S_1, T_1, T_2 and S_2 have the following properties

$$S_1(\alpha\alpha' : \lambda\lambda')^* = S_1(\lambda\lambda' : \alpha\alpha') = -S_1(\alpha'\alpha : \lambda'\lambda) \tag{31}$$
$$T_1(\alpha\alpha' : \lambda_1\lambda_2\lambda'_1\lambda'_2)^* = T_2(\lambda_1\lambda_2\lambda'_1\lambda'_2 : \alpha\alpha') = -T_1(\alpha'\alpha : \lambda'_1\lambda'_2\lambda_1\lambda_2) \tag{32}$$
$$T_2(\alpha\beta\alpha'\beta' : \lambda\lambda')^* = T_1(\lambda\lambda' : \alpha\beta\alpha'\beta') = -T_2(\alpha'\beta'\alpha\beta : \lambda'\lambda) \tag{33}$$
$$S_2(\alpha\beta\alpha'\beta' : \lambda_1\lambda_2\lambda'_1\lambda'_2)^* = S_2(\lambda_1\lambda_2\lambda'_1\lambda'_2 : \alpha\beta\alpha'\beta') = -S_2(\alpha'\beta'\alpha\beta : \lambda'_1\lambda'_2\lambda_1\lambda_2). \tag{34}$$

Therefore also the matrix in Eq. (16)

$$\begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix}$$

is hermitian. However, the total matrix problem is non-hermitian because of the metric involved in the above equation. Taking hermitian conjugate of Eq.(16) and using the above symmetries, we can show that when

$$\begin{pmatrix} x^{\mu}_{\alpha\alpha'} \\ X^{\mu}_{\alpha\beta\alpha'\beta'} \end{pmatrix}$$

is a positive energy solution with $\omega_\mu (> 0)$,

$$\begin{pmatrix} {x^{\mu}_{\alpha'\alpha}}^* \\ {X^{\mu}_{\alpha'\beta'\alpha\beta}}^* \end{pmatrix}$$

is a negative energy solution with $-\omega_\mu$ as in other extended RPA theories [6].

2.4 Orthonormal condition

For a hermitian hamiltonian matrix the orthogonal condition is given as [17]

$$(x^{\mu *} \quad X^{\mu *}) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^{\mu'} \\ X^{\mu'} \end{pmatrix} = 0 \qquad \text{for} \;\; \omega_\mu \neq \omega_{\mu'}. \tag{35}$$

The normalization of a positive energy solution may be

$$(x^{\mu *} \quad X^{\mu *}) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix} = 1. \tag{36}$$

Since

$$\begin{pmatrix} {x^{\mu}_{\alpha'\alpha}}^* \\ {X^{\mu}_{\alpha'\beta'\alpha\beta}}^* \end{pmatrix}$$

is a solution with $-\omega_\mu (\omega_\mu > 0)$, the normalization condition for a negative energy solution is given by

$$\begin{pmatrix} x^{\mu}_{\alpha'\alpha} & X^{\mu}_{\alpha'\beta'\alpha\beta} \end{pmatrix} \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} {x^{\mu}_{\alpha'\alpha}}^* \\ {X^{\mu}_{\alpha'\beta'\alpha\beta}}^* \end{pmatrix} = -1. \tag{37}$$

Accordingly, the closure relation is written as

$$\sum_{\omega_\mu > 0} \begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix} (x^{\mu *} \; X^{\mu *}) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} - \sum_{\omega_\mu > 0} \begin{pmatrix} {x^{\mu}_{\alpha'\alpha}}^* \\ {X^{\mu}_{\alpha'\beta'\alpha\beta}}^* \end{pmatrix} \begin{pmatrix} x^{\mu}_{\alpha'\alpha} \; X^{\mu}_{\alpha'\beta'\alpha\beta} \end{pmatrix} \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} = I, \tag{38}$$

where I is the unit matrix.

2.5 Energy-weighted sum rule

Finally we discuss the energy-weighted sum rule and show that the Thouless theorem [1] is satisfied. We consider a hermitian operator

$$\hat{F} = F_0 + \sum_{\lambda\lambda'} f_{\lambda\lambda'} : a^+_\lambda a_{\lambda'} : + \sum_{\lambda_1\lambda_2\lambda'_1\lambda'_2} F_{\lambda_1\lambda_2\lambda'_1\lambda'_2} : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :, \tag{39}$$

where F_0 is $\langle 0|\hat{F}|0\rangle$. Since the one-body and two-body transition amplitudes $z^{\mu}_{\alpha\alpha'} = \langle 0| : a^+_{\alpha'} a_\alpha : |\mu\rangle$ and $Z^{\mu}_{\alpha\beta\alpha'\beta'} = \langle 0| : a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha : |\mu\rangle$ are given by

$$\begin{pmatrix} z^{\mu} \\ Z^{\mu} \end{pmatrix} = \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix}, \tag{40}$$

the energy-weighted strength S is written as

$$S = \sum_{\omega_\mu>0} \omega_\mu |\langle 0|\hat{F}|\mu\rangle|^2 = \sum_{\omega_\mu>0} \omega_\mu \,(f \;\; F) \begin{pmatrix} z^\mu \\ Z^\mu \end{pmatrix} (z^{\mu *} \;\; Z^{\mu *}) \begin{pmatrix} f \\ F \end{pmatrix}. \quad (41)$$

Taking into account the contribution of the negative energy solutions, we have

$$\begin{aligned} S &= \frac{1}{2}\sum_{\omega_\mu>0} \omega_\mu \,(f \;\; F) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix} (x^{\mu *} \;\; X^{\mu *}) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} f \\ F \end{pmatrix} \\ &+ \frac{1}{2}\sum_{\omega_\mu>0} \omega_\mu \,(f \;\; F) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} {x^\mu_{\alpha'\alpha}}^* \\ {X^\mu_{\alpha'\beta'\alpha\beta}}^* \end{pmatrix} \left(x^\mu_{\alpha'\alpha} \;\; X^\mu_{\alpha'\beta'\alpha\beta}\right) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} f \\ F \end{pmatrix} \\ &= \frac{1}{2}\sum_{\omega_\mu>0} (f \;\; F) \begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix} (x^{\mu *} \;\; X^{\mu *}) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} f \\ F \end{pmatrix} \\ &- \frac{1}{2}\sum_{\omega_\mu>0} (f \;\; F) \begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} {x^\mu_{\alpha'\alpha}}^* \\ {X^\mu_{\alpha'\beta'\alpha\beta}}^* \end{pmatrix} \left(x^\mu_{\alpha'\alpha} \;\; X^\mu_{\alpha'\beta'\alpha\beta}\right) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} f \\ F \end{pmatrix} \\ &= \frac{1}{2}(f \;\; F) \begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} f \\ F \end{pmatrix} \\ &= \frac{1}{2}\langle 0|[[\hat{F},\hat{H}],\hat{F}]|0\rangle. \end{aligned} \quad (42)$$

Here we used the closure relation Eq.(38). Thus it is shown that the Thouless theorem holds.

3 Spurious modes in ERPA

We discuss conditions that ERPA gives zero excitation energy to spurious modes associated with operators which commute with the hamiltonian. This actually holds for situations for which the ground state determined by Eqs. (5)-(8) has a spontaneously broken symmetry.

3.1 Hamiltonian matrix of ERPA

We rewrite the hamiltonian matrix in ERPA in a different way using the commutation relations between the hamiltonian and one-body and two-body operators, which are written as

$$[: a^+_{\alpha'} a_\alpha :, \hat{H}] = \sum_{\gamma\gamma'} a(\alpha\alpha' : \gamma\gamma') : a^+_{\gamma'} a_\gamma : + \sum_{\gamma_1\gamma_2\gamma_1'\gamma_2'} c(\alpha\alpha' : \gamma_1\gamma_2\gamma_1'\gamma_2') : a^+_{\gamma_1'} a^+_{\gamma_2'} a_{\gamma_2} a_{\gamma_1} : \quad (43)$$

$$\begin{aligned} [: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{H}] &= \sum_{\gamma\gamma'} b(\alpha\beta\alpha'\beta' : \gamma\gamma') : a^+_{\gamma'} a_\gamma : \\ &+ \sum_{\gamma_1\gamma_2\gamma_1'\gamma_2'} d(\alpha\beta\alpha'\beta' : \gamma_1\gamma_2\gamma_1'\gamma_2') : a^+_{\gamma_1'} a^+_{\gamma_2'} a_{\gamma_2} a_{\gamma_1} : \\ &+ \sum_{\gamma_1\gamma_2\gamma_3\gamma_1'\gamma_2'\gamma_3'} e(\alpha\beta\alpha'\beta' : \gamma_1\gamma_2\gamma_3\gamma_1'\gamma_2'\gamma_3') : a^+_{\gamma_1'} a^+_{\gamma_2'} a^+_{\gamma_3'} a_{\gamma_3} a_{\gamma_2} a_{\gamma_1} : . \end{aligned} \quad (44)$$

The matrices a, b, c, d and e are explicitly given in the Appendix. The ground-state conditions Eqs.(5), (6) and (8) are employed in the derivation of these matrices. Using a, b, c, d and e, the matrices A, B, C and D in ERPA are written as

$$A = \langle 0|[[: a^+_{\alpha'} a_\alpha :, \hat{H}], : a^+_\lambda a_{\lambda'} :]|0\rangle = aS_1 + cT_2 \quad (45)$$

$$B = \langle 0|[[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{H}], : a^+_\lambda a_{\lambda'} :]|0\rangle = bS_1 + dT_2 + eT_{31} \quad (46)$$

$$C = \langle 0|[[: a^+_{\alpha'} a_\alpha :, \hat{H}], : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda_2'} a_{\lambda_1'} :]|0\rangle = aT_1 + cS_2 \quad (47)$$

$$D = \langle 0|[[: a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha :, \hat{H}], : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda_2'} a_{\lambda_1'} :]|0\rangle = bT_1 + dS_2 + eT_{32}, \quad (48)$$

where

$$T_{31} = \langle 0|[: a^+_{\alpha'} a^+_{\beta'} a^+_{\gamma'} a_\gamma a_\beta a_\alpha :, : a^+_\lambda a_{\lambda'} :]|0\rangle, \tag{49}$$

$$T_{32} = \langle 0|[: a^+_{\alpha'} a^+_{\beta'} a^+_{\gamma'} a_\gamma a_\beta a_\alpha :, : a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda'_2} a_{\lambda'_1} :]|0\rangle. \tag{50}$$

Since a four-body correlation matrix is not considered, expectation values of four-body operators in T_{32} are approximated by the products of $n_{\alpha\alpha'}$, $C_{\alpha\beta\alpha'\beta'}$ and $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$.

3.2 Operator for a spurious mode

Let us consider an operator

$$\hat{F} = F_0 + \sum_{\alpha\alpha'} f_{\alpha'\alpha} : a^+_{\alpha'} a_\alpha : + \sum_{\alpha\beta\alpha'\beta'} F_{\alpha'\beta'\alpha\beta} : a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha : \tag{51}$$

which commutes with $\hat{H}$. Using Eqs.(43) and (44), the commutation relation $[\hat{F}, \hat{H}]$ is written as

$$\begin{aligned}
[\hat{F}, \hat{H}] = & \sum_{\alpha\alpha'\gamma\gamma'} f_{\alpha'\alpha} \times a(\alpha\alpha' : \gamma\gamma') : a^+_{\gamma'} a_\gamma : \\
& + \sum_{\alpha\alpha'\gamma_1\gamma_2\gamma'_1\gamma'_2} f_{\alpha'\alpha} \times c(\alpha\alpha' : \gamma_1\gamma_2\gamma'_1\gamma'_2) : a^+_{\gamma'_1} a^+_{\gamma'_2} a_{\gamma_2} a_{\gamma_1} : \\
& + \sum_{\alpha\beta\alpha'\beta'\gamma\gamma'} F_{\alpha'\beta'\alpha\beta} \times b(\alpha\beta\alpha'\beta' : \gamma\gamma') : a^+_{\gamma'} a_\gamma : \\
& + \sum_{\alpha\beta\alpha'\beta'\gamma_1\gamma_2\gamma'_1\gamma'_2} F_{\alpha'\beta'\alpha\beta} \times d(\alpha\beta\alpha'\beta' : \gamma_1\gamma_2\gamma'_1\gamma'_2) : a^+_{\gamma'_1} a^+_{\gamma'_2} a_{\gamma_2} a_{\gamma_1} : \\
& + \sum_{\alpha\beta\alpha'\beta'\gamma_1\gamma_2\gamma_3\gamma'_1\gamma'_2\gamma'_3} F_{\alpha'\beta'\alpha\beta} \times e(\alpha\beta\alpha'\beta' : \gamma_1\gamma_2\gamma_3\gamma'_1\gamma'_2\gamma'_3) : a^+_{\gamma'_1} a^+_{\gamma'_2} a^+_{\gamma'_3} a_{\gamma_3} a_{\gamma_2} a_{\gamma_1} : .
\end{aligned} \tag{52}$$

The condition $[\hat{F}, \hat{H}] = 0$ implies that all terms on the right-hand side of the above equation vanish when symmetrization and antisymmetrization are properly considered, namely,

$$\sum_{\alpha\alpha'} f_{\alpha'\alpha} \times a(\alpha\alpha' : \gamma\gamma') + \sum_{\alpha\beta\alpha'\beta'} F_{\alpha'\beta'\alpha\beta} \times b(\alpha\beta\alpha'\beta' : \gamma\gamma') = 0 \tag{53}$$

$$\sum_{\alpha\alpha'} f_{\alpha'\alpha} \times c'(\alpha\alpha' : \gamma_1\gamma_2\gamma'_1\gamma'_2) + \sum_{\alpha\beta\alpha'\beta'} F_{\alpha'\beta'\alpha\beta} \times d'(\alpha\beta\alpha'\beta' : \gamma_1\gamma_2\gamma'_1\gamma'_2) = 0 \tag{54}$$

$$\sum_{\alpha\beta\alpha'\beta'} F_{\alpha'\beta'\alpha\beta} \times e'(\alpha\beta\alpha'\beta' : \gamma_1\gamma_2\gamma_3\gamma'_1\gamma'_2\gamma'_3) = 0, \tag{55}$$

where c', d' and e' mean that symmetrization and antisymmetrization have been performed on the corresponding unprimed quantities. For example

$$\begin{aligned}
c'(\alpha\alpha' : \gamma_1\gamma_2\gamma'_1\gamma'_2) = & \frac{1}{4}[c(\alpha\alpha' : \gamma_1\gamma_2\gamma'_1\gamma'_2) + c(\alpha\alpha' : \gamma_2\gamma_1\gamma'_2\gamma'_1) \\
& - c(\alpha\alpha' : \gamma_2\gamma_1\gamma'_1\gamma'_2) - c(\alpha\alpha' : \gamma_1\gamma_2\gamma'_2\gamma'_1)].
\end{aligned} \tag{56}$$

Since the matrices a, b and d include $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$, the conditions Eqs.(53)-(55) must be supplemented with the ground-state conditions Eqs.(5)-(8) if necessary.

3.3 Zero excitation energy for spurious mode

Now we show that in the case of a spontaneous broken symmetry the spurious state associated with a corresponding symmetry operator which commutes with H has zero excitation energy in ERPA. We consider $\omega_\mu\langle 0|\hat{F}|\mu\rangle$, where

$\langle 0|\hat{F}|\mu\rangle \neq 0$ because the ground state has a broken symmetry. Using Eqs.(45)-(48), we obtain

$$\begin{aligned}\omega_\mu\langle 0|\hat{F}|\mu\rangle &= \omega_\mu\,(f \quad F)\begin{pmatrix} S_1 & T_1 \\ T_2 & S_2\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} = (f \quad F)\begin{pmatrix} A & C \\ B & D\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} \\ &= (f \quad F)\begin{pmatrix} aS_1 + cT_2 & aT_1 + cS_2 \\ bS_1 + dT_2 + eT_{31} & bT_1 + dS_2 + eT_{32}\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} \\ &= ((fa + Fb)S_1 + (fc' + Fd')T_2 + Fe'T_{31})\,x^\mu \\ &+ ((fa + Fb)T_1 + (fc' + Fd')S_2 + Fe'T_{32})\,X^\mu. \end{aligned} \tag{57}$$

The right-hand side of the above equation vanishes due to Eqs.(53)-(55). This implies $\omega_\mu = 0$ for spurious modes. From the above discussion it is clear that keeping all components of the matrices a, b, c and d is essential for ERPA to give zero energy solutions to spurious modes associated with one-body and (or) two-body operators. Equation (57) also implies that the transition amplitudes of the symmetry operator $\hat{F}$ vanish for physical excited states because $\omega_\mu \neq 0$ in such cases.

3.4 Approximate form of ERPA

So far the application of ERPA has been made using an approximate form of ERPA, which is derived as the small amplitude limit of the time-dependent density-matrix theory (STDDM) [9,10]. In this subsection we point out that STDDM preserves the property of ERPA for spurious modes. In STDDM, the three-body correlation matrix $C_{\alpha\beta\gamma\alpha'\beta'\gamma'}$ and the matrix e are neglected. Then the ERPA equations in this approximation are written as

$$\begin{pmatrix} A & C' \\ B' & D'\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} = \omega_\mu\begin{pmatrix} S_1 & T_1 \\ T_2 & S'_2\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix}, \tag{58}$$

where S'_2 does not have the three-body correlation matrix, and B', C' and D' are given by $B' = bS_1 + dT_2$, $C' = aT_1 + cS'_2$ and $D' = bT_1 + dS'_2$, respectively. Other matrices in Eq.(58) are the same as those in ERPA. Contrary to Eq. (16) the hermiticity of

$$\begin{pmatrix} A & C' \\ B' & D'\end{pmatrix}$$

is lost.

Equation (58) can be written in a different form as

$$\begin{aligned}\begin{pmatrix} A & C' \\ B' & D'\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} &= \begin{pmatrix} aS_1 + cT_2 & aT_1 + cS'_2 \\ bS_1 + dT_2 & bT_1 + dS'_2\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} \\ &= \begin{pmatrix} a & c \\ b & d\end{pmatrix}\begin{pmatrix} S_1 & T_1 \\ T_2 & S'_2\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix} = \omega_\mu\begin{pmatrix} S_1 & T_1 \\ T_2 & S'_2\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix}.\end{aligned} \tag{59}$$

Using the transition amplitude

$$\begin{pmatrix} z^\mu \\ Z^\mu\end{pmatrix} = \begin{pmatrix} S_1 & T_1 \\ T_2 & S'_2\end{pmatrix}\begin{pmatrix} x^\mu \\ X^\mu\end{pmatrix}, \tag{60}$$

Eq.(58) is written as

$$\begin{pmatrix} a & c \\ b & d\end{pmatrix}\begin{pmatrix} z^\mu \\ Z^\mu\end{pmatrix} = \omega_\mu\begin{pmatrix} z^\mu \\ Z^\mu\end{pmatrix}. \tag{61}$$

This is the form derived as the small amplitude limit of TDDM. STDDM also gives zero excitation energy to spurious modes associated with one-body and two-body operators. This is because Eqs.(53) and (54) are satisfied. The effects of ground-state correlations are included in STDDM because the matrices a, b and d in Eq. (61) contain $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$ (see the Appendix). A simplified version of STDDM where the effects of ground-state correlations were entirely neglected was used in ref.[7] to find the conditions that extended RPA theories have zero energy solutions for spurious modes.

4 Translational motion

In this section we explicitly evaluate Eqs.(53) and (54) for translational motion. As is the case of the HF ground state, the ground state determined by Eqs. (5)-(8) exhibits spontaneously broken translational invariance.

4.1 Single spurious mode

We consider the operator

$$i\boldsymbol{P}=\sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle:a^+_{\alpha'}a_\alpha:, \tag{62}$$

where $\langle 0|i\boldsymbol{P}|0\rangle=0$ is assumed. In this case $f_{\alpha'\alpha}$ in Eq.(51) is $\langle\alpha'|\nabla|\alpha\rangle$ and $F_{\alpha'\beta'\alpha\beta}=0$. Using the expression for a (Eq.(80)), we write the first term on the left-hand side of Eq.(53) as

$$\begin{aligned}\sum_{\alpha\alpha'}f_{\alpha'\alpha}a(\alpha\alpha':\gamma\gamma')&=\sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle((\epsilon_\alpha-\epsilon_{\alpha'})\delta_{\alpha\gamma}\delta_{\alpha'\gamma'}\\&+\sum_\lambda(\langle\alpha\gamma'|v|\lambda\gamma\rangle_A n_{\lambda\alpha'}-\langle\lambda\gamma'|v|\alpha'\gamma\rangle_A n_{\alpha\lambda}))\\&=\langle\gamma'|[\nabla,h]|\gamma\rangle+\sum_{\lambda\lambda'}(\langle\lambda'\gamma'|\nabla_1 v|\lambda\gamma\rangle_A\\&-\langle\lambda'\gamma'|v\nabla_1|\lambda\gamma\rangle+\langle\lambda'\gamma'|v\nabla_2|\gamma\lambda\rangle)n_{\lambda\lambda'},\end{aligned} \tag{63}$$

where $\epsilon_\alpha|\alpha\rangle$ is replaced by $h|\alpha\rangle$ and the closure relation $\sum_\alpha\phi_\alpha(\boldsymbol{r}_1)\phi^*_\alpha(\boldsymbol{r}_2)=\delta^3(\boldsymbol{r}_1-\boldsymbol{r}_2)$ is used for the summation over α and α'. Since ∇ commutes with t, only the mean-field potential contributes to $[\nabla,h]$:

$$\begin{aligned}\langle\alpha'|[\nabla,h]|\alpha\rangle&=\sum_{\lambda\lambda'}(\langle\alpha'\lambda'|(\nabla_1 v)|\alpha\lambda\rangle_A\\&-\langle\alpha'\lambda'|v\nabla_1|\lambda\alpha\rangle+\langle\alpha'\lambda'|v\nabla_2|\lambda\alpha\rangle)n_{\lambda\lambda'},\end{aligned} \tag{64}$$

where $(\nabla_1 v)$ means that ∇_1 acts only on v. Then,

$$\begin{aligned}\sum_{\alpha\alpha'}f_{\alpha'\alpha}a(\alpha\alpha':\gamma\gamma')&=\sum_{\lambda\lambda'}(\langle\gamma'\lambda'|(\nabla_1 v)|\gamma\lambda\rangle_A-\langle\gamma'\lambda'|v\nabla_1|\lambda\gamma\rangle+\langle\gamma'\lambda'|v\nabla_2|\lambda\gamma\rangle\\&+\langle\lambda'\gamma'|(\nabla_1 v)|\lambda\gamma\rangle_A-\langle\lambda'\gamma'|v\nabla_1|\gamma\lambda\rangle+\langle\lambda'\gamma'|v\nabla_2|\gamma\lambda\rangle)n_{\lambda\lambda'}\\&=\sum_{\lambda\lambda'}\left(\langle\gamma'\lambda'|(\nabla_1 v)+(\nabla_2 v)|\gamma\lambda\rangle_A\right)n_{\lambda\lambda'},\end{aligned} \tag{65}$$

where symmetries, $\langle\alpha\beta|(\nabla_1 v)|\alpha'\beta'\rangle=\langle\beta\alpha|(\nabla_2 v)|\beta'\alpha'\rangle$ and $\langle\alpha\beta|v\nabla_1|\alpha'\beta'\rangle=\langle\beta\alpha|v\nabla_2|\beta'\alpha'\rangle$, are used. The last line of Eq.(65) vanishes because of translational invariance of v: $\nabla_1 v(\boldsymbol{r}_1-\boldsymbol{r}_2)+\nabla_2 v(\boldsymbol{r}_1-\boldsymbol{r}_2)=0$. Similarly, the first term on the left-hand side of Eq.(54) becomes, using the expression for c (Eq.(82)),

$$\begin{aligned}\sum_{\alpha\alpha'}f_{\alpha'\alpha}c(\alpha\alpha':\gamma_1\gamma_2\gamma_1'\gamma_2')&=\sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle(\langle\alpha\gamma_2'|v|\gamma_1\gamma_2\rangle\delta_{\alpha'\gamma_1'}-\langle\gamma_1'\gamma_2'|v|\alpha'\gamma_2\rangle\delta_{\alpha\gamma_1})\\&=\langle\gamma_1'\gamma_2'|\nabla_1 v|\gamma_1\gamma_2\rangle-\langle\gamma_1'\gamma_2'|v\nabla_1|\gamma_1\gamma_2\rangle\\&=\langle\gamma_1'\gamma_2'|(\nabla_1 v)|\gamma_1\gamma_2\rangle.\end{aligned} \tag{66}$$

Therefore,

$$\begin{aligned}\sum_{\alpha\alpha'}f_{\alpha'\alpha}c'(\alpha\alpha':\gamma_1\gamma_2\gamma_1'\gamma_2')&=\frac{1}{4}\sum_{\alpha\alpha'}f_{\alpha'\alpha}(c(\alpha\alpha':\gamma_1\gamma_2\gamma_1'\gamma_2')+c(\alpha\alpha':\gamma_2\gamma_1\gamma_2'\gamma_1')\\&-c(\alpha\alpha':\gamma_1\gamma_2\gamma_2'\gamma_1')-c(\alpha\alpha':\gamma_2\gamma_1\gamma_1'\gamma_2'))\\&=\frac{1}{4}(\langle\gamma_1'\gamma_2'|(\nabla_1 v)+(\nabla_2 v)|\gamma_1\gamma_2\rangle\\&-\langle\gamma_1'\gamma_2'|(\nabla_1 v)+(\nabla_2 v)|\gamma_2\gamma_1\rangle)=0.\end{aligned} \tag{67}$$

Thus, it is shown that Eqs.(53) and (54) hold. As shown above, unrestricted summation over the single-particle indices α and α' and the symmetries over $\gamma_1\gamma_2\gamma_1'\gamma_2'$ are essential to obtain Eq.(67). The above discussions imply that any extended RPA theories having all components of the one-body amplitudes and proper symmetries of the two-body amplitudes give zero energy solutions to the spurious modes associated with one-body operators. This conclusion does not depend on approximations for the two-body transition amplitudes as long as the symmetry property is respected.

In RPA, the matrix a does not have all components: $\alpha\alpha'$ and $\gamma\gamma'$ in a are restricted to either 1 particle - 1 hole states or 1 hole - 1 particle states and, therefore, the closure relation associated with the sum over α or α' in Eq.(63) is modified to

$$\sum_{\epsilon_\alpha>\epsilon_F}\phi_\alpha(\boldsymbol{r}_1)\phi_\alpha^*(\boldsymbol{r}_2)=\sum_\alpha\phi_\alpha(\boldsymbol{r}_1)\phi_\alpha^*(\boldsymbol{r}_1)-\sum_{\epsilon_\alpha<\epsilon_F}\phi_\alpha(\boldsymbol{r}_1)\phi_\alpha^*(\boldsymbol{r}_2)+\delta^3(\boldsymbol{r}_1-\boldsymbol{r}_2), \tag{68}$$

where ϵ_F is the Fermi energy. However, due to cancellation among the matrix elements of v originating from the second term on the right-hand side of Eq.(68), an expression similar to Eq.(65) is obtained and Eq.(53) holds in RPA. 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. [18].

4.2 Double spurious state

As an example of spurious modes associated with two-body operators, we consider the double excitation of translational motion. The corresponding operator is $i\boldsymbol{P}\cdot i\boldsymbol{P}$ which consist of both one-body and two-body operators

$$\begin{aligned}
i\boldsymbol{P}\cdot i\boldsymbol{P}&=\left(\sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle a^+_{\alpha'}a_\alpha\right)^2=\sum_{\alpha\beta\alpha'\beta'}\langle\alpha'|\nabla|\alpha\rangle\cdot\langle\beta'|\nabla|\beta\rangle a^+_{\alpha'}a_\alpha a^+_{\beta'}a_\beta\\
&=\sum_{\alpha\alpha'}\langle\alpha'|\nabla^2|\alpha\rangle a^+_{\alpha'}a_\alpha+\sum_{\alpha\beta\alpha'\beta'}\langle\alpha'|\nabla|\alpha\rangle\cdot\langle\beta'|\nabla|\beta\rangle a^+_{\alpha'}a^+_{\beta'}a_\beta a_\alpha\\
&=\sum_{\alpha\alpha'}\langle\alpha'|\nabla^2|\alpha\rangle n_{\alpha\alpha'}+\sum_{\alpha\beta\alpha'\beta'}\langle\alpha'|\nabla|\beta\rangle\cdot\langle\beta'|\nabla|\alpha\rangle(C_{\beta\alpha\alpha'\beta'}-n_{\alpha\alpha'}n_{\beta\beta'})\\
&+\sum_{\alpha\alpha'}(\langle\alpha'|\nabla^2|\alpha\rangle-2\sum_{\beta\beta'}\langle\alpha'|\nabla|\beta\rangle\cdot\langle\beta'|\nabla|\alpha\rangle n_{\beta\beta'}):a^+_{\alpha'}a_\alpha:\\
&+\sum_{\alpha\beta\alpha'\beta'}\langle\alpha'|\nabla|\alpha\rangle\cdot\langle\beta'|\nabla|\beta\rangle:a^+_{\alpha'}a^+_{\beta'}a_\beta a_\alpha:,
\end{aligned}\tag{69}$$

where $\sum_{\alpha\alpha'}\langle\alpha'|\nabla|\alpha\rangle n_{\alpha\alpha'}=0$ is assumed. From the above expression, $f_{\alpha'\alpha}$ and $F_{\alpha'\beta'\alpha\beta}$ in Eq.(51) for $i\boldsymbol{P}\cdot i\boldsymbol{P}$ are given by

$$f_{\alpha'\alpha}=\langle\alpha'|\nabla^2|\alpha\rangle-2\sum_{\beta\beta'}\langle\alpha'|\nabla|\beta\rangle\cdot\langle\beta'|\nabla|\alpha\rangle n_{\beta\beta'} \tag{70}$$

$$F_{\alpha'\beta'\alpha\beta}=\langle\alpha'|\nabla|\alpha\rangle\cdot\langle\beta'|\nabla|\beta\rangle. \tag{71}$$

Since the evaluation of all relations Eqs.(53)-(55) is quite involved, we do not show the full proof. Instead, we only demonstrate Eq.(54) as an example. Using Eq.(82) and the closure relation for single-particle states, the first term on the left-hand side of Eq.(54) is expressed as

$$\begin{aligned}
\sum_{\alpha\alpha'}f_{\alpha'\alpha}c(\alpha\alpha':\gamma_1\gamma_2\gamma_1'\gamma_2')&=\sum_{\alpha\alpha'}(\langle\alpha'|\nabla^2|\alpha\rangle-2\sum_{\beta\beta'}\langle\alpha'|\nabla|\beta\rangle\cdot\langle\beta'|\nabla|\alpha\rangle n_{\beta\beta'})\\
&\times(\langle\alpha\gamma_2'|v|\gamma_1\gamma_2\rangle\delta_{\alpha'\gamma_1'}-\langle\gamma_1'\gamma_2'|v|\alpha'\gamma_2\rangle\delta_{\alpha\gamma_1})\\
&=\langle\gamma_1'\gamma_2'|\nabla_1^2v|\gamma_1\gamma_2\rangle-\langle\gamma_1'\gamma_2'|v\nabla_1^2|\gamma_1\gamma_2\rangle\\
&-2\sum_{\alpha\lambda}((\langle\alpha\gamma_2'|\nabla_1v|\gamma_1\gamma_2\rangle\cdot\langle\gamma_1'|\nabla|\lambda\rangle\\
&-\langle\gamma_1'\gamma_2'|v\nabla_1|\lambda\gamma_2\rangle\cdot\langle\alpha|\nabla|\gamma_1\rangle)n_{\lambda\alpha}.
\end{aligned}\tag{72}$$

The second term on the left-hand side of Eq.(54) becomes, using the expression for d (Eq.(83)),

$$\sum_{\alpha\beta\alpha'\beta'}F_{\alpha'\beta'\alpha\beta}d(\alpha\beta\alpha'\beta'\ :\ \gamma_1\gamma_2\gamma_1'\gamma_2')=\sum_{\alpha\beta\alpha'\beta'}\langle\alpha'|\nabla|\alpha\rangle\cdot\langle\beta'|\nabla|\beta\rangle$$

$$\times\ ((\epsilon_\alpha+\epsilon_\beta-\epsilon_{\alpha'}-\epsilon_{\beta'})\delta_{\alpha\gamma_1}\delta_{\beta\gamma_2}\delta_{\alpha'\gamma_1'}\delta_{\beta'\gamma_2'}$$
$$+\ \delta_{\alpha'\gamma_1'}\delta_{\beta'\gamma_2'}\sum_{\lambda\lambda'}(\delta_{\alpha\lambda}\delta_{\beta\lambda'}-\delta_{\beta\lambda'}n_{\alpha\lambda}-\delta_{\alpha\lambda}n_{\beta\lambda'})\langle\lambda\lambda'|v|\gamma_1\gamma_2\rangle$$
$$-\ \delta_{\alpha\gamma_1}\delta_{\beta\gamma_2}\sum_{\lambda\lambda'}(\delta_{\alpha'\lambda}\delta_{\beta'\lambda'}-\delta_{\beta'\lambda'}n_{\lambda\alpha'}-\delta_{\alpha'\lambda}n_{\lambda'\beta'})\langle\gamma_1'\gamma_2'|v|\lambda\lambda'\rangle$$
$$+\ \delta_{\beta\gamma_2}\delta_{\beta'\gamma_2'}\sum_{\lambda}(\langle\alpha\gamma_1'|v|\lambda\gamma_1\rangle_A n_{\lambda\alpha'}-\langle\lambda\gamma_1'|v|\alpha'\gamma_1\rangle_A n_{\alpha\lambda})$$
$$+\ \delta_{\beta\gamma_2}\delta_{\alpha'\gamma_1'}\sum_{\lambda}(\langle\alpha\gamma_2'|v|\lambda\gamma_1\rangle_A n_{\lambda\beta'}-\langle\lambda\gamma_2'|v|\beta'\gamma_1\rangle_A n_{\alpha\lambda})$$
$$+\ \delta_{\alpha\gamma_1}\delta_{\alpha'\gamma_1'}\sum_{\lambda}(\langle\beta\gamma_2'|v|\lambda\gamma_2\rangle_A n_{\lambda\beta'}-\langle\lambda\gamma_2'|v|\beta'\gamma_2\rangle_A n_{\beta\lambda})$$
$$+\ \delta_{\alpha\gamma_1}\delta_{\beta'\gamma_2'}\sum_{\lambda}(\langle\beta\gamma_1'|v|\lambda\gamma_2\rangle_A n_{\lambda\alpha'}-\langle\lambda\gamma_1'|v|\alpha'\gamma_2\rangle_A n_{\beta\lambda}))$$
$$=\langle\gamma_1'|[\nabla,h]|\gamma_1\rangle\cdot\langle\gamma_2'|\nabla|\gamma_2\rangle+\langle\gamma_2'|[\nabla,h]|\gamma_2\rangle\cdot\langle\gamma_1'|\nabla|\gamma_1\rangle$$
$$+\ \langle\gamma_1'\gamma_2'|\nabla_1\cdot\nabla_2 v|\gamma_1\gamma_2\rangle-\sum_{\alpha\lambda}\langle\gamma_1'|\nabla|\lambda\rangle\cdot\langle\alpha\gamma_2'|\nabla_2 v|\gamma_1\gamma_2\rangle n_{\lambda\alpha}$$
$$-\sum_{\alpha\lambda}\langle\gamma_2'|\nabla|\lambda\rangle\cdot\langle\gamma_1'\alpha|\nabla_1 v|\gamma_1\gamma_2\rangle n_{\lambda\alpha}$$
$$-\ \langle\gamma_1'\gamma_2'|v\nabla_1\cdot\nabla_2|\gamma_1\gamma_2\rangle+\sum_{\alpha\lambda}\langle\alpha|\nabla|\gamma_1\rangle\cdot\langle\gamma_1'\gamma_2'|v\nabla_2|\lambda\gamma_2\rangle n_{\lambda\alpha}$$
$$+\sum_{\alpha\lambda}\langle\alpha|\nabla|\gamma_2\rangle\cdot\langle\gamma_1'\gamma_2'|v\nabla_1|\gamma_1\lambda\rangle n_{\lambda\alpha}$$
$$+\ \langle\gamma_2'|\nabla|\gamma_2\rangle\cdot\sum_{\alpha\lambda}(\langle\alpha\gamma_1'|\nabla_1 v|\lambda\gamma_1\rangle_A-\langle\alpha\gamma_1'|v\nabla_1|\lambda\gamma_1\rangle_A)n_{\lambda\alpha}$$
$$+\sum_{\alpha\lambda}((\langle\alpha|\nabla|\gamma_2\rangle\cdot\langle\gamma_1'\gamma_2'|\nabla_1 v|\lambda\gamma_1\rangle_A$$
$$-\ \langle\gamma_1'|\nabla|\lambda\rangle\cdot\langle\alpha\gamma_2'|v\nabla_1|\gamma_2\gamma_1\rangle_A)n_{\lambda\alpha}$$
$$+\ \langle\gamma_1'|\nabla|\gamma_1\rangle\cdot\sum_{\alpha\lambda}(\langle\alpha\gamma_2'|\nabla_1 v|\lambda\gamma_2\rangle_A-\langle\alpha\gamma_2'|v\nabla_1|\lambda\gamma_2\rangle_A)n_{\lambda\alpha}$$
$$+\sum_{\alpha\lambda}((\langle\alpha|\nabla|\gamma_1\rangle\cdot\langle\gamma_2'\gamma_1'|\nabla_1 v|\lambda\gamma_2\rangle_A$$
$$-\ \langle\gamma_2'|\nabla|\lambda\rangle\cdot\langle\alpha\gamma_1'|v\nabla_1|\gamma_1\gamma_2\rangle_A)n_{\lambda\alpha}. \tag{73}$$

First we consider the following sum of the terms in Eqs.(72) and (73) which do not have the summation over α and λ:

$$\begin{aligned}
&\langle\gamma_1'\gamma_2'|\nabla_1^2 v|\gamma_1\gamma_2\rangle-\langle\gamma_1'\gamma_2'|v\nabla_1^2|\gamma_1\gamma_2\rangle\\
&+\langle\gamma_1'\gamma_2'|\nabla_1\cdot\nabla_2 v|\gamma_1\gamma_2\rangle-\langle\gamma_1'\gamma_2'|v\nabla_1\cdot\nabla_2|\gamma_1\gamma_2\rangle\\
&=\langle\gamma_1'\gamma_2'|(\nabla_1^2 v)+2(\nabla_1 v)\cdot\nabla_1|\gamma_1\gamma_2\rangle\\
&+\langle\gamma_1'\gamma_2'|(\nabla_1\cdot\nabla_2 v)+(\nabla_1 v)\cdot\nabla_2+(\nabla_2 v)\cdot\nabla_1|\gamma_1\gamma_2\rangle\\
&=\langle\gamma_1'\gamma_2'|(\nabla_1^2 v)+(\nabla_1\cdot\nabla_2 v)|\gamma_1\gamma_2\rangle\\
&+\langle\gamma_1'\gamma_2'|[(\nabla_1 v)+(\nabla_2 v)]\cdot\nabla_1|\gamma_1\gamma_2\rangle\\
&+\langle\gamma_1'\gamma_2'|(\nabla_1 v)\cdot(\nabla_1+\nabla_2)|\gamma_1\gamma_2\rangle,
\end{aligned}\tag{74}$$

where $(\nabla_1\cdot\nabla_2 v)$ means that both ∇_1 and ∇_2 act only on v. The first two terms in the last line of the above equation vanish because $(\nabla_1^2 v)+(\nabla_1\nabla_2 v)=0$ and $(\nabla_1 v)+(\nabla_2 v)=0$ for translationally invariant v. The last term also vanishes because the symmetric term under exchange of indices such as $(\gamma_1,\gamma_2,\gamma_1',\gamma_2')\Longleftrightarrow(\gamma_2,\gamma_1,\gamma_2',\gamma_1')$ contributes in Eq.(54).

Next we consider the sum of the terms with $\langle\gamma_1'|\nabla|\gamma_1\rangle$ in Eq.(73):

$$\langle\gamma_1'|\nabla|\gamma_1\rangle\cdot(\langle\gamma_2'|[\nabla,h]|\gamma_2\rangle+\sum_{\alpha\lambda}(\langle\alpha\gamma_2'|\nabla_1 v|\lambda\gamma_2\rangle_A-\langle\alpha\gamma_2'|v\nabla_1|\lambda\gamma_2\rangle_A)n_{\lambda\alpha}). \tag{75}$$

The above sum is zero because the expression in the parentheses is the same as Eq.(63). Similarly, the sum of the terms with $\langle\gamma_2'|\nabla|\gamma_2\rangle$ vanishes. Finally we consider the terms with $\langle\alpha|\nabla|\gamma_1\rangle$ and the summation over two single-particle indices:

$$\sum_{\alpha\lambda}\langle\alpha|\nabla|\gamma_1\rangle\cdot(2\langle\gamma_1'\gamma_2'|v\nabla_1|\lambda\gamma_2\rangle + \langle\gamma_1'\gamma_2'|v\nabla_2|\lambda\gamma_2\rangle + \langle\gamma_2'\gamma_1'|\nabla_1 v|\lambda\gamma_2\rangle_A)n_{\lambda\alpha}, \tag{76}$$

where the first term in the sum comes from Eq.(72). After the addition of terms obtained from the exchange of single-particle indices such as $(\gamma_1,\gamma_2,\gamma_1',\gamma_2')\Longleftrightarrow(\gamma_2,\gamma_1,\gamma_2',\gamma_1')$ and $(\gamma_1',\gamma_2')\Longleftrightarrow(\gamma_2',\gamma_1')$ according to Eq.(56), the above sum becomes

$$\sum_{\alpha\lambda}2\langle\alpha|\nabla|\gamma_1\rangle\cdot(\langle\gamma_1'\gamma_2'|v\nabla_1|\lambda\gamma_2\rangle + \langle\gamma_1'\gamma_2'|v\nabla_2|\lambda\gamma_2\rangle + \langle\gamma_2'\gamma_1'|\nabla_1 v|\lambda\gamma_2\rangle_A - \langle\gamma_2'\gamma_1'|v\nabla_1|\lambda\gamma_2\rangle - \langle\gamma_2'\gamma_1'|v\nabla_2|\lambda\gamma_2\rangle - \langle\gamma_1'\gamma_2'|\nabla_1 v|\lambda\gamma_2\rangle_A)n_{\lambda\alpha}. \tag{77}$$

Using

$$\langle\gamma_1'\gamma_2'|\nabla_1 v|\lambda\gamma_2\rangle_A = \langle\gamma_1'\gamma_2'|(\nabla_1 v)|\lambda\gamma_2\rangle_A + \langle\gamma_1'\gamma_2'|v\nabla_1|\lambda\gamma_2\rangle - \langle\gamma_1'\gamma_2'|v\nabla_1|\gamma_2\lambda\rangle, \tag{78}$$

we can reduce Eq.(77) to

$$-\sum_{\alpha\lambda}2\langle\alpha|\nabla|\gamma_1\rangle\cdot(\langle\gamma_1'\gamma_2'|(\nabla_1 v)|\lambda\gamma_2\rangle_A + \langle\gamma_1'\gamma_2'|(\nabla_2 v)|\lambda\gamma_2\rangle_A). \tag{79}$$

This vanishes because $\nabla_1 v + \nabla_2 v = 0$ for translationally invariant v. Similarly, the sum of the terms with $\langle\alpha|\nabla|\gamma_2\rangle$, $\langle\gamma_1'|\nabla|\lambda\rangle$ and $\langle\gamma_2'|\nabla|\lambda\rangle$ vanish. Thus, it is shown that Eq.(54) is fulfilled for the double excitation of translational motion. As discussed above, the unrestricted summation over α and α' in Eq.(72) and over α, β, α' and β' in Eq.(73) is necessary to satisfy Eq.(54). This means that extended RPA theories should contain all components of one-body and two-body amplitudes to have a zero energy solution for the double excitation of translational motion: any truncation of α and α' in c and α, β, α' and β' in d destroys the structure of $[\hat{H}, i\boldsymbol{P}\cdot i\boldsymbol{P}]$. Eq.(53) can be proved in a similar way, though the ground state condition Eq.(5) is required. The proof of Eq. (55) is straightforward.

5 Summary

We presented an extended theory of RPA (ERPA) which enables us to calculate both one-body and two-body transition amplitudes. Our ERPA is of quite general form in the sense that the effects of ground-state correlations are consistently taken in to account. Some symmetry properties of ERPA were discussed and it was pointed out that ERPA preserves the energy-weighted sum rule. Using ERPA we discussed the conditions that ERPA has zero-energy solutions for spurious modes in the case of spontaneously broken symmetries. It was found that the conservation of the structure of the commutation relation between the hamiltonian and the operators associated with spurious modes is essential for ERPA to have such symmetry properties. It was shown that the small amplitude limit of the time-dependent density-matrix theory (STDDM), an approximate form of ERPA used for realistic applications, also has zero-energy solutions for spurious modes. The single and double excitations of translational motion were considered as illustrative examples of spurious modes and it was shown that all components of one-body and two-body amplitudes are necessary to have a zero energy solution for the double excitation of translational motion. We are investigating the feasibility of our ERPA using solvable models. The obtained results will be published elsewhere.

A

We here give the explicit expressions for the matrices a, b, c, d and e.

The single-particle states are given by Eq.(8).

$$a(\alpha\alpha':\lambda\lambda') = (\epsilon_\alpha - \epsilon_{\alpha'})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'} - \sum_\beta(\langle\beta\lambda'|v|\alpha'\lambda\rangle_A n_{\alpha\beta} - \langle\alpha\lambda'|v|\beta\lambda\rangle_A n_{\beta\alpha'}), \tag{80}$$

$$
\begin{aligned}
& b\ (\alpha_1\alpha_2\alpha_1'\alpha_2' : \lambda\lambda') \\
& = -\delta_{\alpha_1\lambda}\{\sum_{\beta\gamma\delta}[(\delta_{\alpha_2\beta} - n_{\alpha_2\beta})n_{\gamma\alpha_1'}n_{\delta\alpha_2'} + n_{\alpha_2\beta}(\delta_{\gamma\alpha_1'} - n_{\gamma\alpha_1'})(\delta_{\delta\alpha_2'} - n_{\delta\alpha_2'})]\langle\lambda'\beta|v|\gamma\delta\rangle_A \\
& + \sum_{\beta\gamma}[\langle\lambda'\alpha_2|v|\beta\gamma\rangle C_{\beta\gamma\alpha_1'\alpha_2'} + \langle\lambda'\beta|v|\alpha_1'\gamma\rangle_A C_{\alpha_2\gamma\alpha_2'\beta} - \langle\lambda'\beta|v|\alpha_2'\gamma\rangle_A C_{\alpha_2\gamma\alpha_1'\beta}]\} \\
& + \delta_{\alpha_2\lambda}\{\sum_{\beta\gamma\delta}[(\delta_{\alpha_1\beta} - n_{\alpha_1\beta})n_{\gamma\alpha_1'}n_{\delta\alpha_2'} + n_{\alpha_1\beta}(\delta_{\gamma\alpha_1'} - n_{\gamma\alpha_1'})(\delta_{\delta\alpha_2'} - n_{\delta\alpha_2'})]\langle\lambda'\beta|v|\gamma\delta\rangle_A \\
& + \sum_{\beta\gamma}[\langle\lambda'\alpha_1|v|\beta\gamma\rangle C_{\beta\gamma\alpha_1'\alpha_2'} + \langle\lambda'\beta|v|\alpha_1'\gamma\rangle_A C_{\alpha_1\gamma\alpha_2'\beta} - \langle\lambda'\beta|v|\alpha_2'\gamma\rangle_A C_{\alpha_1\gamma\alpha_1'\beta}]\} \\
& + \delta_{\alpha_1'\lambda'}\{\sum_{\beta\gamma\delta}[(\delta_{\delta\alpha_2'} - n_{\delta\alpha_2'})n_{\alpha_1\beta}n_{\alpha_2\gamma} + n_{\delta\alpha_2'}(\delta_{\alpha_1\beta} - n_{\alpha_1\beta})(\delta_{\alpha_2\gamma} - n_{\alpha_2\gamma})]\langle\beta\gamma|v|\lambda\delta\rangle_A \\
& + \sum_{\beta\gamma}[\langle\beta\gamma|v|\lambda\alpha_2'\rangle C_{\alpha_1\alpha_2\beta\gamma} + \langle\alpha_1\beta|v|\lambda\gamma\rangle_A C_{\alpha_2\gamma\alpha_2'\beta} - \langle\alpha_2\beta|v|\lambda\gamma\rangle_A C_{\alpha_1\gamma\alpha_2'\beta}]\} \\
& - \delta_{\alpha_2'\lambda'}\{\sum_{\beta\gamma\delta}[(\delta_{\delta\alpha_1'} - n_{\delta\alpha_1'})n_{\alpha_1\beta}n_{\alpha_2\gamma} + n_{\delta\alpha_1'}(\delta_{\alpha_1\beta} - n_{\alpha_1\beta})(\delta_{\alpha_2\gamma} - n_{\alpha_2\gamma})]\langle\beta\gamma|v|\lambda\delta\rangle_A \\
& + \sum_{\beta\gamma}[\langle\beta\gamma|v|\lambda\alpha_1'\rangle C_{\alpha_1\alpha_2\beta\gamma} + \langle\alpha_1\beta|v|\lambda\gamma\rangle_A C_{\alpha_2\gamma\alpha_1'\beta} - \langle\alpha_2\beta|v|\lambda\gamma\rangle_A C_{\alpha_1\gamma\alpha_1'\beta}]\} \\
& + \sum_{\beta}[\langle\alpha_1\lambda'|v|\beta\lambda\rangle_A C_{\beta\alpha_2\alpha_1'\alpha_2'} - \langle\alpha_2\lambda'|v|\beta\lambda\rangle_A C_{\beta\alpha_1\alpha_1'\alpha_2'} \\
& - \langle\beta\lambda'|v|\alpha_2'\lambda\rangle_A C_{\alpha_1\alpha_2\alpha_1'\beta} + \langle\beta\lambda'|v|\alpha_1'\lambda\rangle_A C_{\alpha_1\alpha_2\alpha_2'\beta}],
\end{aligned}
\tag{81}
$$

$$
c(\alpha\alpha' : \lambda_1\lambda_2\lambda_1'\lambda_2') = \langle\alpha\lambda_2'|v|\lambda_1\lambda_2\rangle\delta_{\alpha'\lambda_1'} - \langle\lambda_1'\lambda_2'|v|\alpha'\lambda_2\rangle\delta_{\alpha\lambda_1},
\tag{82}
$$

$$
\begin{aligned}
d(\alpha_1\alpha_2\alpha_1'\alpha_2' \ :\ \lambda_1\lambda_2\lambda_1'\lambda_2') &= (\epsilon_{\alpha_1} + \epsilon_{\alpha_2} - \epsilon_{\alpha_1'} - \epsilon_{\alpha_2'})\delta_{\alpha_1\lambda_1}\delta_{\alpha_2\lambda_2}\delta_{\alpha_1'\lambda_1'}\delta_{\alpha_2'\lambda_2'} \\
& + \delta_{\alpha_1'\lambda_1'}\delta_{\alpha_2'\lambda_2'}\sum_{\beta\gamma}(\delta_{\alpha_1\beta}\delta_{\alpha_2\gamma} - \delta_{\alpha_2\gamma}n_{\alpha_1\beta} - \delta_{\alpha_1\beta}n_{\alpha_2\gamma})\langle\beta\gamma|v|\lambda_1\lambda_2\rangle \\
& - \delta_{\alpha_1\lambda_1}\delta_{\alpha_2\lambda_2}\sum_{\beta\gamma}(\delta_{\alpha_1'\beta}\delta_{\alpha_2'\gamma} - \delta_{\alpha_2'\gamma}n_{\beta\alpha_1'} - \delta_{\alpha_1'\beta}n_{\gamma\alpha_2'})\langle\lambda_1'\lambda_2'|v|\beta\gamma\rangle \\
& + \delta_{\alpha_2\lambda_2}\delta_{\alpha_2'\lambda_2'}\sum_{\beta}(\langle\alpha_1\lambda_1'|v|\beta\lambda_1\rangle_A n_{\beta\alpha_1'} - \langle\beta\lambda_1'|v|\alpha_1'\lambda_1\rangle_A n_{\alpha_1\beta}) \\
& + \delta_{\alpha_2\lambda_2}\delta_{\alpha_1'\lambda_1'}\sum_{\beta}(\langle\alpha_1\lambda_2'|v|\beta\lambda_1\rangle_A n_{\beta\alpha_2'} - \langle\beta\lambda_2'|v|\alpha_2'\lambda_1\rangle_A n_{\alpha_1\beta}) \\
& + \delta_{\alpha_1\lambda_1}\delta_{\alpha_1'\lambda_1'}\sum_{\beta}(\langle\alpha_2\lambda_2'|v|\beta\lambda_2\rangle_A n_{\beta\alpha_2'} - \langle\beta\lambda_2'|v|\alpha_2'\lambda_2\rangle_A n_{\alpha_2\beta}) \\
& + \delta_{\alpha_1\lambda_1}\delta_{\alpha_2'\lambda_2'}\sum_{\beta}(\langle\alpha_2\lambda_1'|v|\beta\lambda_2\rangle_A n_{\beta\alpha_1'} - \langle\beta\lambda_1'|v|\alpha_1'\lambda_2\rangle_A n_{\alpha_2\beta}).
\end{aligned}
\tag{83}
$$

$$
\begin{aligned}
e(\alpha_1\alpha_2\alpha_1'\alpha_2' : \gamma_1\gamma_2\gamma_3\gamma_1'\gamma_2'\gamma_3') &= -\langle\alpha_1\gamma_3'|v|\gamma_1\gamma_2\rangle\delta_{\alpha_2\gamma_3}\delta_{\alpha_1'\gamma_1'}\delta_{\alpha_2'\gamma_2'} \\
& + \langle\alpha_2\gamma_3'|v|\gamma_1\gamma_2\rangle\delta_{\alpha_1\gamma_3}\delta_{\alpha_1'\gamma_1'}\delta_{\alpha_2'\gamma_2'} \\
& + \langle\gamma_1'\gamma_2'|v|\alpha_1'\gamma_3\rangle\delta_{\alpha_1\gamma_1}\delta_{\alpha_2\gamma_2}\delta_{\alpha_2'\gamma_3'} \\
& - \langle\gamma_1'\gamma_2'|v|\alpha_2'\gamma_3\rangle\delta_{\alpha_1\gamma_1}\delta_{\alpha_2\gamma_2}\delta_{\alpha_1'\gamma_3'}.
\end{aligned}
\tag{84}
$$

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