Eigenstates of the time-dependent density-matrix theory

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Abstract. An extended time-dependent Hartree-Fock theory, known as the time-dependent density-matrix theory (TDDM), is solved as a time-independent eigenvalue problem for low-lying 2^+ states in ^{24}O to understand the foundation of the rather successful time-dependent approach. It is found that the calculated strength distribution of the 2^+ states has physically reasonable behavior and that the strength function is practically positive definite though the non-Hermitian Hamiltonian matrix obtained from TDDM does not guarantee it. A relation to an Extended RPA theory with hermiticity is also investigated. It is found that the density-matrix formalism is a good approximation to the Hermitian Extended RPA theory.

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1 Introduction

The time-dependent density-matrix theory (TDDM) [1] is a version of extended time-dependent Hartree-Fock theories which dynamically include two-body correlations. Although TDDM has been formulated to deal with large-amplitude collective motions [2,3], it has also been applied to small-amplitude oscillations: Dipole and quadrupole giant resonances in stable nuclei [4,5] and low-lying states in unstable oxygen isotopes [6,7]. Although the obtained results are quite reasonable, the foundation of TDDM for small-amplitude motions is not clear in its time-dependent form. In this paper an eigenvalue problem of the small-amplitude limit of TDDM (STDDM) is solved for low-lying 2^+ states in ^{24}O to better understand the time-dependent approach. ^{24}O is one of the neutron-rich nuclei which attract recent experimental and theoretical interests and is quite suitable for our present study: Although it is an open-shell nucleus, the Hartree-Fock (HF) assumption which we use to obtain a starting ground state is valid as first-order approximation, and the proton degrees of freedom which do not play a major role because of the proton shell closure can be neglected in a simple analysis condidered here. The Hamiltonian matrix of STDDM is not Hermitian as will be shown below. STDDM is compared with an Extended RPA (ERPA) theory which has hermiticity [8] and its relation to the ERPA theory is clarified. This paper is organized as follows: The formulation

of STDDM is presented in sect. 2. A numerical solution of STDDM for low-lying 2^+ states in ^{24}O is shown in sect. 3. A comparison of STDDM with a more elaborate ERPA with hermiticity is made in sect. 4 and sect. 5 is devoted to a summary.

2 Small-amplitude limit of TDDM

TDDM gives the time evolution of the one-body density-matrix $\rho(1,1')$ and the correlated part $C(12,1'2')$ of the two-body density-matrix, where numbers denote space, spin, and isospin coordinates. The equations of motion for ρ and C have been obtained by truncating the well-known Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy of reduced density matrices [9]. STDDM has been formulated according to the following steps [10]: 1) Linearizing the equations of motion for ρ and C with respect $\delta\rho$ 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. 2) Expanding $\delta\rho$ and δC with single-particle states ψ_α as

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

$$\delta C(121'2',t) = \sum_{\alpha_1\alpha_2\alpha_1'\alpha_2'} X_{\alpha_1\alpha_2\alpha_1'\alpha_2'}(t)\psi_{\alpha_1}(1,t)$$
$$\times\psi_{\alpha_2}(2,t)\psi_{\alpha_1'}^*(1',t)\psi_{\alpha_2'}^*(2',t), \tag{2}$$

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where ψ_α is chosen to be an eigenstate of the mean-field Hamiltonian $h_0(\rho_0)$:

$$h_0(\rho_0)\psi_\alpha(1) = -\frac{\hbar^2\nabla^2}{2m}\psi_\alpha(1) + \int d2v(1,2)[\rho_0(2,2)\psi_\alpha(1)$$
$$-\rho_0(1,2)\psi_\alpha(2)] = \epsilon_\alpha\psi_\alpha(1). \qquad (3)$$

Here, the one-body density matrix ρ_0 is given as

$$\rho_0(11') = \sum_{\alpha\alpha'} n^0_{\alpha\alpha'}\psi_\alpha(1)\psi^*_{\alpha'}(1'). \qquad (4)$$

After Fourier transforming the linearized equations, the equations for $x_{\alpha\alpha'}(\omega)$ and $X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(\omega)$ can be written in matrix form,

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix} = \omega \begin{pmatrix} x \\ X \end{pmatrix}, \qquad (5)$$

where ω is an eigenvalue. The matrices $a, b, c,$ and d are explicitly given in appendix A. Equation (5) can also be obtained from the following equations:

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

$$\langle\Phi_0|[a^+_{\alpha'_1}a^+_{\alpha'_2}a_{\alpha_2}a_{\alpha_1}, H]|\Phi\rangle = \omega\langle\Phi_0|a^+_{\alpha'_1}a^+_{\alpha'_2}a_{\alpha_2}a_{\alpha_1}|\Phi\rangle, \quad (7)$$

where [ ] stands for the commutation relation, H is the total Hamiltonian consisting of the kinetic energy term and a two-body interaction, $|\Phi_0\rangle$ is the ground-state wave function, and $|\Phi\rangle$ the wave function for the excited state with excitation energy ω. Linearizing eqs. (6) and (7) with respect to $x_{\alpha\alpha'} = \langle\Phi_0|a^+_{\alpha'}a_\alpha|\Phi\rangle$ and $X_{\alpha_1\alpha_2\alpha'_1\alpha'_2} = \langle\Phi_0|a^+_{\alpha'_1}a^+_{\alpha'_2}a_{\alpha_2}a_{\alpha_1}|\Phi\rangle$, and using the occupation matrix $n^0_{\alpha\alpha'} = \langle\Phi_0|a^+_{\alpha'}a_\alpha|\Phi_0\rangle$ and the two-body correlation matrix $C^0_{\alpha_1\alpha_2\alpha'_1\alpha'_2} = \langle\Phi_0|a^+_{\alpha'_1}a^+_{\alpha'_2}a_{\alpha_2}a_{\alpha_1}|\Phi_0\rangle - \mathcal{A}(n^0_{\alpha_1\alpha'_1}n^0_{\alpha_2\alpha'_2})$, where $\mathcal{A}$ is an antisymmetrization operator, we arrive at eq. (5). Equation (5) is reduced to the second RPA (SRPA) [11,12] under the following two assumptions: The first one is the HF approximation for the ground state, in which $n^0_{\alpha\alpha'} = \delta_{\alpha\alpha'}f_\alpha$ with $f_\alpha = 1$ (0) for occupied (unoccupied) states at zero temperature and $C^0_{\alpha_1\alpha_2\alpha'_1\alpha'_2} = 0$. The other is to restrict $X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}$ only to two-particle–two-hole components and their complex conjugates.

The Hamiltonian matrix of eq. (5) is not Hermitian, i.e. $b \neq c^+$, as is easily understood from its explicit form. For a non-Hermitian Hamiltonian matrix, the left-hand-side eigenvectors of the Hamiltonian matrix constitute a basis which is orthogonal to $(x_{\alpha\alpha'}, X_{\alpha_1\alpha_2\alpha'_1\alpha'_2})$, and the orthonormal condition is written as

$$\langle\tilde{\mu}|\mu'\rangle = \sum_{\alpha\alpha'}\tilde{x}^*_{\alpha\alpha'}(\mu)x_{\alpha\alpha'}(\mu')$$
$$+ \sum_{\alpha_1\alpha_2\alpha'_1\alpha'_2}\tilde{X}^*_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(\mu)X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(\mu') = \delta_{\mu\mu'}, \quad (8)$$

where $|\mu\rangle$ represents an eigenvector $(x_{\alpha\alpha'}, X_{\alpha_1\alpha_2\alpha'_1\alpha'_2})$ with the eigenvalue ω_μ, and $|\tilde{\mu}\rangle$ the left-hand-side eigenvector of the Hamiltonian matrix with the same eigenvalue:

$$(\tilde{x}^* \quad \tilde{X}^*) \begin{pmatrix} a & c \\ b & d \end{pmatrix} = \omega_\mu(\tilde{x}^* \quad \tilde{X}^*). \qquad (9)$$

The completeness relation is written as

$$\sum_\mu \begin{pmatrix} x_{\alpha\alpha'}(\mu) \\ X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(\mu) \end{pmatrix} \left(\tilde{x}^*_{\beta\beta'}(\mu) \ \tilde{X}^*_{\beta_1\beta_2\beta'_1\beta'_2}(\mu)\right) = I, \quad (10)$$

where I is the unit matrix. In general the strength function is defined as

$$S(E) = \sum_{E_\mu>0} |\langle\Psi_\mu|\hat{Q}|\Psi_0\rangle|^2\delta(E-E_\mu), \qquad (11)$$

where $|\Psi_0\rangle$ is the ground state, $|\Psi_\mu\rangle$ is an excited state with an excitation energy E_μ, and $\hat{Q}$ an excitation operator. The strength function in STDDM is calculated in a way similar to that used in TDDM. In TDDM, an initial excited wave function $|\Phi(t=0)\rangle$ is given by boosting the ground-state wave function $|\Phi_0\rangle$ as

$$|\Phi(t=0)\rangle = e^{ik\hat{Q}}|\Phi_0\rangle. \qquad (12)$$

Then the initial values of the time-dependent amplitudes $x_{\alpha\alpha'}$ and $X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}$ are given at first order of k as

$$x_{\alpha\alpha'}(0) = \langle\Phi(t=0)|a^+_{\alpha'}a_\alpha|\Phi(t=0)\rangle$$
$$\approx ik\langle\Phi_0|[a^+_{\alpha'}a_\alpha, \hat{Q}]|\Phi_0\rangle, \qquad (13)$$

$$X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(0) \approx ik\langle\Phi_0|[a^+_{\alpha'_1}a^+_{\alpha'_2}a_{\alpha_2}a_{\alpha_1}, \hat{Q}]|\Phi_0\rangle. \qquad (14)$$

In TDDM the time dependence of $x_{\alpha\alpha'}$ and $X_{\alpha_1\alpha_2\alpha'_1\alpha'_2}$ is determined by solving numerically the TDDM equations. It can also be expressed using the eigenstates of eq. (5) as

$$\begin{pmatrix} x(t) \\ X(t) \end{pmatrix} = \exp\left[-i\begin{pmatrix} a & c \\ b & d \end{pmatrix}t/\hbar\right]\begin{pmatrix} x(0) \\ X(0) \end{pmatrix} =$$
$$\sum_\mu \exp\left[-i\frac{\omega_\mu t}{\hbar}\right]\begin{pmatrix} x_\mu \\ X_\mu \end{pmatrix}(\tilde{x}^*_\mu \ \tilde{X}^*_\mu)\begin{pmatrix} x(0) \\ X(0) \end{pmatrix}, \quad (15)$$

where the completeness relation eq. (10) is inserted. The time-dependent moment $Q(t) = \langle\Phi(t)|\hat{Q}|\Phi(t)\rangle$ for a one-body operator becomes

$$Q(t) = \sum_{\text{Re}(\omega_\mu>0)} \left\{ \exp\left(-i\frac{\omega_\mu t}{\hbar}\right)\left(\sum_{\alpha\alpha'}\langle\alpha|Q|\alpha'\rangle x_{\alpha'\alpha}(\mu)\right) \right.$$
$$\left. \times(\tilde{x}^*_\mu x(0) + \tilde{X}^*_\mu X(0)) + \text{complex conjugate} \right\}, \quad (16)$$

where we use the fact that both states with ω_μ and $-\omega^*_\mu$ are eigenstates of eq. (5). The strength function in TDDM is obtained from the Fourier transformation of $Q(t)$ [1] as

$$S(E) = \frac{1}{\pi k\hbar}\int_0^\infty Q(t)e^{-\Gamma t/2\hbar}\sin\frac{Et}{\hbar}dt, \qquad (17)$$

where an artificial damping factor Γ is introduced to obtain a smooth distribution for $S(E)$. Equations (16) and

(17) suggest that the strength function in STDDM has the form

$$S(E) = -\frac{1}{\pi}\text{Im}\left\{\sum_{\text{Re}(\omega_\mu)>0}\left[\left(\sum_{\alpha\alpha'}\langle\alpha|Q|\alpha'\rangle x_{\alpha'\alpha}(\mu)\right)\right.\right.$$

$$\times\left(\sum_{\beta\beta'}\langle\beta|Q|\beta'\rangle\tilde{x}^t_{\beta'\beta}(\mu)\right)^*\frac{1}{E-\omega_\mu+i\Gamma/2}$$

$$-\left(\sum_{\alpha\alpha'}\langle\alpha|Q|\alpha'\rangle x_{\alpha'\alpha}(\mu)\right)^*$$

$$\left.\left.\times\left(\sum_{\beta\beta'}\langle\beta|Q|\beta'\rangle\tilde{x}^t_{\beta'\beta}(\mu)\right)\frac{1}{E+\omega_\mu^*+i\Gamma/2}\right]\right\}, (18)$$

where $\tilde{x}^t_{\alpha\alpha'}(\mu)$ is defined as

$$\tilde{x}^t_{\alpha\alpha'}(\mu) = \sum_{\lambda\lambda'}\langle\Phi_0|[a^+_{\alpha'}a_\alpha, a^+_\lambda a_{\lambda'}]|\Phi_0\rangle\tilde{x}_{\lambda\lambda'}(\mu)$$

$$+ \sum_{\lambda_1\lambda_2\lambda'_1\lambda'_2}\langle\Phi_0|[a^+_{\alpha'}a_\alpha, a^+_{\lambda_1}a^+_{\lambda_2}a_{\lambda'_2}a_{\lambda'_1}]|\Phi_0\rangle\tilde{X}_{\lambda_1\lambda_2\lambda'_1\lambda'_2}(\mu).$$

$$(19)$$

The strength function $S(E)$ in STDDM is not guaranteed to be positive definite, as is easily understood from its expression, eq. (18).

3 Numerical solution

In this section we present a numerical solution of eq. (5) calculated for low-lying 2^+ states in ^{24}O, where a time-dependent approach has previously been applied [7]. The $E2$ strength function is calculated according to the following steps:

1) A static HF calculation is performed to obtain the initial ground state. The neutron $2s_{1/2}$ state is assumed to be the last fully occupied neutron orbit of ^{24}O. The Skyrme III is used as the effective interaction. It has been used as one of the standard parameterizations of the Skyrme force in nuclear-structure calculations even for very neutron-rich nuclei [13,14]. The single-particle wave functions are confined to a sphere with radius of 12 fm. The mesh size used is 0.1 fm.

2) To obtain the correlated ground state $|\Phi_0\rangle$, we evolve the HF ground state using the TDDM equations for $\psi_\alpha(1,t)$, $n_{\alpha\alpha'}(t)$ and $C_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(t)$ [6,7] and the following time-dependent residual interaction:

$$v(t) = (1 - e^{-t/\tau})v(\boldsymbol{r} - \boldsymbol{r}'). \qquad (20)$$

The time constant τ should be sufficiently large to obtain a nearly stationary solution of the TDDM equations [15]. We choose τ to be 300 fm/c. In the calculation of $n_{\alpha\alpha'}(t)$ and $C_{\alpha_1\alpha_2\alpha'_1\alpha'_2}(t)$, the single-particle states are limited to the neutron orbits $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$. In a consistent calculation the residual interaction should be the same as
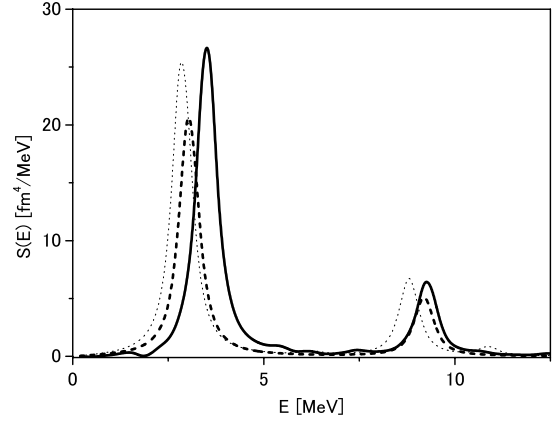
Fig. 1. Strength distributions of the neutron quadrupole modes in ^{24}O calculated in STDDM (solid line), RPA (dashed line) and SRPA (dotted line).

that used to generate the mean field. However, a Skyrme-type force contains momentum-dependent terms, which make the computation time of two-body matrix elements quite large. Therefore, we need to use a simple force of the δ-function form $v \propto \delta^3(\boldsymbol{r} - \boldsymbol{r}')$. We use the following pairing-type residual interaction of the density-dependent δ-function form [16]:

$$v(\boldsymbol{r} - \boldsymbol{r}') = v_0(1 - \rho(\boldsymbol{r})/\rho_0)\delta^3(\boldsymbol{r} - \boldsymbol{r}'), \qquad (21)$$

where $\rho(\boldsymbol{r})$ is the nuclear density. The parameters ρ_0 and v_0 are set to be 0.16 fm^{-3} and -1000 MeV fm^3, respectively. Similar values of ρ_0 and v_0 have been used in the Hartree-Fock-Bogoliubov calculations [17–19] in a truncated single-particle space. The time step used to solve the TDDM equations is 0.75 fm/c.

3) At $t = 5\tau$ we stop the TDDM calculation and solve eq. (5). Since we are interested in low-lying states which originate in inner-shell transitions, we use only the neutron $1d_{5/2}$, $2s_{1/2}$, and $1d_{3/2}$ states. The dimension of the Hamiltonian matrix is about 650×650 when these single-particle states are used. The strength function for 2^+ states is calculated using eq. (18) with $Q = r^2Y_{20}(\theta,\phi)$. We use $\Gamma = 0.5$ MeV.

The eigenvalues of some 2^+ states become imaginary because the Hamiltonian matrix of eq. (5) is not Hermitian. However, their imaginary components are quite small (less than 0.08 MeV). Some 2^+ states have also negative quadrupole strengths because the positivity of $S(E)$ is not guaranteed. However, the negative contributions are so small that $S(E)$ becomes almost positive in the entire energy region when it is smoothed with $\Gamma = 0.5$ MeV. The obtained result in STDDM (solid line) is shown in fig. 1, where the strength functions in RPA (dashed line) and SRPA (dotted line) are also presented for comparison. The first 2^+ state calculated in STDDM is energetically shifted upward and becomes significantly more collective as compared with that in RPA. The increase in the excitation energy is due to the lowering of the ground state, and the enhancement of the collectivity of the first 2^+ state

is due to the mixing of two-body configurations intensified by ground-state correlations. These properties of the first 2^+ state under the influence of ground-state correlations are similar to those obtained from quasi-particle RPA calculations [20,21] and also from the TDDM calculation [7]. Large single-particle space including continuum states has been used in these realistic calculations [20, 21,7] so as to deal with giant resonances as well as low-lying states. Therefore, only a semi-quantitative comparison between our previous TDDM result [7] and the present STDDM calculation, which can only be performed in very truncated single-particle space, should be made for lowest-lying states. In SRPA, where ground-state correlations are neglected, the 2^+ states become also collective due to the coupling to two-particle–two-hole configurations, as shown in fig. 1. However, their excitation energies are simply shifted downward. This might cause serious problems when unperturbed particle-hole energies are small and (or) when the coupling to two-body configurations is strong. The numerical solution of eq. (5) shown in this section is physically reasonable and also gives additional justification to its equivalent time-dependent approach.

4 Discussions

In this section we discuss a relation between STDDM and a more elaborate Extended RPA theory (ERPA) which has hermiticity [8]. First, we briefly present the ERPA theory. The ground state $|\Phi_0\rangle$ in ERPA is constructed so that

$$\langle \Phi_0|[H, a_\alpha^+ a_{\alpha'}]|\Phi_0\rangle = 0, \tag{22}$$

$$\langle \Phi_0|[H, a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'}]|\Phi_0\rangle = 0, \tag{23}$$

$$\langle \Phi_0|[H, a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_3}^+ a_{\alpha_3'} a_{\alpha_2'} a_{\alpha_1'}]|\Phi_0\rangle = 0 \tag{24}$$

are satisfied for any single-particle indices. In other words, $n_{\alpha\alpha'}^0$, $C_{\alpha_1\alpha_2\alpha_1'\alpha_2'}^0$, and the three-body correlation matrix $C_{\alpha_1\alpha_2\alpha_3\alpha_1'\alpha_2'\alpha_3'}^0$ are determined so that the above equations are satisfied. The explicit expressions for eqs. (22)-(24) are shown in ref. [8]. Although it is not evident to find an analytic solution of eqs. (22)-(24) [22], a method for obtaining $n_{\alpha\alpha'}^0$ and $C_{\alpha_1\alpha_2\alpha_1'\alpha_2'}^0$ numerically has been proposed in ref. [15] and already been tested for realistic nuclei [6,7,23] as was shown in sect. 3. The ERPA equations are formulated using the equation-of-motion approach [24,25] as

$$\langle \Psi_0|[[a_\alpha^+ a_{\alpha'}, H], Q^+]|\Psi_0\rangle = \omega\langle \Psi_0|[a_\alpha^+ a_{\alpha'}, Q^+]|\Psi_0\rangle \tag{25}$$

$$\langle \Psi_0|[[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H], Q^+]|\Psi_0\rangle = \\ \omega\langle \Psi_0|[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, Q^+]|\Psi_0\rangle, \tag{26}$$

where the operator Q^+ is defined as

$$Q^+ = \sum(x_{\lambda\lambda'} a_\lambda^+ a_{\lambda'} + X_{\lambda_1\lambda_2\lambda_1'\lambda_2'} : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :), \tag{27}$$

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

$$Q^+|\Psi_0\rangle = |\Psi\rangle, \tag{28}$$
$$Q|\Psi_0\rangle = 0. \tag{29}$$

In eqs. (26) and (27), : : stands for : $a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'}$:= $a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} - \mathcal{A}(a_{\alpha_1}^+ a_{\alpha_1'}\langle \Phi_0|a_{\alpha_2}^+ a_{\alpha_2'}|\Phi_0\rangle + a_{\alpha_2}^+ a_{\alpha_2'}\langle \Phi_0|a_{\alpha_1}^+ a_{\alpha_1'}|\Phi_0\rangle)$. Equations (25) and (26) can be written in matrix form

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix} = \omega \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix}, \tag{30}$$

where each matrix element is evaluated using the ground state $|\Phi_0\rangle$:

$$S_1(\alpha'\alpha : \lambda\lambda') = \langle \Phi_0|[a_\alpha^+ a_{\alpha'}, a_\lambda^+ a_{\lambda'}]|\Phi_0\rangle, \tag{31}$$

$$S_2(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda_1\lambda_2\lambda_1'\lambda_2') = \\ \langle \Phi_0|[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :]|\Phi_0\rangle, \tag{32}$$

$$T_1(\alpha'\alpha : \lambda_1\lambda_2\lambda_1'\lambda_2') = \\ \langle \Phi_0|[a_\alpha^+ a_{\alpha'}, : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :]|\Phi_0\rangle, \tag{33}$$

$$T_2(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda\lambda') = \\ \langle \Phi_0|[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, a_\lambda^+ a_{\lambda'}]|\Phi_0\rangle, \tag{34}$$

$$A(\alpha'\alpha : \lambda\lambda') = \langle \Phi_0|[[a_\alpha^+ a_{\alpha'}, H], a_\lambda^+ a_{\lambda'}]|\Phi_0\rangle, \tag{35}$$

$$B(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda\lambda') = \\ \langle \Phi_0|[[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H], a_\lambda^+ a_{\lambda'}]|\Phi_0\rangle, \tag{36}$$

$$C(\alpha'\alpha : \lambda_1\lambda_2\lambda_1'\lambda_2') = \\ \langle \Phi_0|[[a_\alpha^+ a_{\alpha'}, H], : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :]|\Phi_0\rangle, \tag{37}$$

$$D(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda_1\lambda_2\lambda_1'\lambda_2') = \\ \langle \Phi_0|[[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H], : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :]|\Phi_0\rangle. \tag{38}$$

All matrices in the above are written in terms of $n_{\alpha\alpha'}^0$, $C_{\alpha_1\alpha_2\alpha_1'\alpha_2'}^0$, and $C_{\alpha_1\alpha_2\alpha_3\alpha_1'\alpha_2'\alpha_3'}^0$, which are shown in ref. [8]. Due to eqs. (22)-(24), the above matrices have the following symmetries:

$$A(\alpha'\alpha : \lambda\lambda') = A(\lambda'\lambda : \alpha\alpha') = A(\lambda\lambda' : \alpha'\alpha)^*, \tag{39}$$

$$B(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda\lambda') = C(\lambda'\lambda : \alpha_1\alpha_2\alpha_1'\alpha_2') = \\ C(\lambda\lambda' : \alpha_1'\alpha_2'\alpha_1\alpha_2)^*, \tag{40}$$

$$D(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda_1\lambda_2\lambda_1'\lambda_2') = D(\lambda_1'\lambda_2'\lambda_1\lambda_2 : \alpha_1\alpha_2\alpha_1'\alpha_2') = \\ D(\lambda_1\lambda_2\lambda_1'\lambda_2' : \alpha_1'\alpha_2'\alpha_1\alpha_2)^*. \tag{41}$$

We explain in more detail the last relation as an example. The following relation always holds due to the operator identity

$$D(\alpha_1'\alpha_2'\alpha_1\alpha_2 : \lambda_1\lambda_2\lambda_1'\lambda_2') - D(\lambda_1'\lambda_2'\lambda_1\lambda_2 : \alpha_1\alpha_2\alpha_1'\alpha_2') = \\ \langle \Phi_0|[[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H], : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :]|\Phi_0\rangle \\ -\langle \Phi_0|[[: a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :, H], : a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :]|\Phi_0\rangle = \\ -\langle \Phi_0|[H, [: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :]]|\Phi_0\rangle. \tag{42}$$

The commutation relation between the two-body operators in the last line of the above equation is reduced to three-body operators at most. Since eqs. (22)-(24) are valid, the last line of eq. (42) is identical to zero. Thus, the symmetry of the matrix D is proven.

The orthonormality condition in ERPA is given by [26]

$$(x_{\mu'}^* \ X_{\mu'}^*) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x_\mu \\ X_\mu \end{pmatrix} = \delta_{\mu\mu'}, \qquad (43)$$

where x_μ and X_μ constitute an eigenstate of eq. (30) with $\omega = \omega_\mu$. The completeness relation becomes

$$\sum_\mu \begin{pmatrix} x_\mu \\ X_\mu \end{pmatrix} (x_\mu^* X_\mu^*) \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} = I. \qquad (44)$$

The transition amplitudes for one-body and two-body operators, $z_{\alpha\alpha'} = \langle \Psi_0 | a_{\alpha'}^+ a_\alpha | \Psi \rangle$ and $Z_{\alpha_1\alpha_2\alpha_1'\alpha_2'} = \langle \Psi_0 | : a_{\alpha_1'}^+ a_{\alpha_2'}^+ a_{\alpha_1} a_{\alpha_2} : | \Psi \rangle$, are calculated as follows:

$$\begin{pmatrix} z \\ Z \end{pmatrix} = \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix}. \qquad (45)$$

Now we show a relation between STDDM and ERPA. When the eigenvector (x, X) in STDDM is transformed to (y, Y) as

$$\begin{pmatrix} x \\ X \end{pmatrix} = \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2' \end{pmatrix} \begin{pmatrix} y \\ Y \end{pmatrix}, \qquad (46)$$

where S_2' has no terms with the three-body correlation matrices, the equation in STDDM becomes

$$\begin{pmatrix} aS_1 + cT_2 & aT_1 + cS_2' \\ bS_1 + dT_2 & bT_1 + dS_2' \end{pmatrix} \begin{pmatrix} y \\ Y \end{pmatrix} = \omega \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2' \end{pmatrix} \begin{pmatrix} y \\ Y \end{pmatrix}. \qquad (47)$$

It is straightforward to prove that when the three-body correlation matrices $C_{\alpha_1\alpha_2\alpha_3\alpha_1'\alpha_2'\alpha_3'}$ are neglected, three blocks of the above Hamiltonian matrix satisfy the identities $A = aS_1 + cT_2$, $B = bS_1 + dT_2$, and $C = aT_1 + cS_2'$. We explain the relation $B = bS_1 + dT_2$ in detail. When two-body and three-body operators are decomposed using $a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} =: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} : + \mathcal{A}(a_{\alpha_1}^+ a_{\alpha_1'} \langle \Phi_0 | a_{\alpha_2}^+ a_{\alpha_2'} | \Phi_0 \rangle + a_{\alpha_2}^+ a_{\alpha_2'} \langle \Phi_0 | a_{\alpha_1}^+ a_{\alpha_1'} | \Phi_0 \rangle)$ for a two-body operator and a similar relation for a three-body operator, the commutation relation $[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H]$ becomes

$$[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H] = \sum_{\lambda\lambda'} b(\alpha_1\alpha_2\alpha_1'\alpha_2' : \lambda\lambda') a_{\lambda'}^+ a_\lambda$$

$$+ \sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'} d(\alpha_1\alpha_2\alpha_1'\alpha_2' : \lambda_1\lambda_2\lambda_1'\lambda_2') : a_{\lambda_1'}^+ a_{\lambda_2'}^+ a_{\lambda_2} a_{\lambda_1} :$$

$$+ \sum_{\lambda_1\lambda_2\lambda_3\lambda_1'\lambda_2'\lambda_3'} e(\alpha_1\alpha_2\alpha_1'\alpha_2' : \lambda_1\lambda_2\lambda_3\lambda_1'\lambda_2'\lambda_3')$$

$$: a_{\lambda_1'}^+ a_{\lambda_2'}^+ a_{\lambda_3'}^+ a_{\lambda_3} a_{\lambda_2} a_{\lambda_1} :, \qquad (48)$$

where the matrix e consists of matrix elements of the two-body interaction. In STDDM, the last term on the right-hand side of the above equation is neglected. It is clear from eq. (48) that $B = \langle \Phi_0 | [[: a_{\alpha_1}^+ a_{\alpha_2}^+ a_{\alpha_2'} a_{\alpha_1'} :, H], a_\lambda^+ a_{\lambda'}] | \Phi_0 \rangle = bS_1 + dT_2$. The matrix D

has some terms which cannot be written by using $bT_1 + dS_2'$ even if the three-body correlation matrices are neglected: For example, all terms with the square of the two-body correlation matrix cannot be expressed with bT_1. Thus, it is found that STDDM is identical to ERPA under the following two assumptions: The first is that the three-body correlation matrices can be neglected and the second is that $D \approx bT_1 + dS_2'$. Our numerical calculations so far performed suggest that these assumptions are quite reasonable. However, whether the non-hermiticity problem is always contained within reasonable limits or not is a subject to be investigated in further applications.

5 Summary

The eigenstates of the small amplitude limit of the time-dependent density-matrix theory (STDDM) were calculated for the low-lying 2^+ states in ^{24}O to better understand the foundation of its corresponding time-dependent approach. It is found that STDDM properly deals with the effects of ground-state correlations on the low-lying 2^+ states and that the non-hermiticity of STDDM is quite moderate: The eigenvalues have quite small imaginary parts and the strength function is practically positive definite although it is not guaranteed because of its non-Hermitian form. A comparison of STDDM and an Extended RPA (ERPA) theory with hermiticity was also made, and it is found that STDDM is a reasonable approximation to the ERPA theory. STDDM involves diagonalization of a Hamiltonian matrix whose dimension rapidly increases with increasing number of single-particle orbits. In realistic calculations, therefore, the time-dependent approach (TDDM) which simply follows the time evolution of the one-body and two-body amplitudes seems more practical than STDDM: In fact, all the single-particle states up to the $2p_{3/2}$ and $1f_{7/2}$ were taken for both protons and neutrons in the TDDM calculation for ^{24}O [7].

Appendix A.

The matrices in eq. (5) are given as

$$a(\alpha\alpha' : \lambda\lambda') = (\epsilon_\alpha - \epsilon_{\alpha'})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'}$$
$$- \sum_\beta (\langle \beta\lambda' | v | \alpha'\lambda \rangle_A n_{\alpha\beta}^0 - \langle \alpha\lambda' | v | \beta\lambda \rangle_A n_{\beta\alpha'}^0), \quad (A.1)$$

$$b(\alpha_1\alpha_2\alpha_1'\alpha_2' : \lambda\lambda') = -\delta_{\alpha_1\lambda}\left\{ \sum_{\beta\gamma\delta} [(\delta_{\alpha_2\beta} - n_{\alpha_2\beta}^0)n_{\gamma\alpha_1'}^0 n_{\delta\alpha_2'}^0 \right.$$
$$+ n_{\alpha_2\beta}^0(\delta_{\gamma\alpha_1'} - n_{\gamma\alpha_1'}^0)(\delta_{\delta\alpha_2'} - n_{\delta\alpha_2'}^0)]\langle \lambda'\beta | v | \gamma\delta \rangle_A$$
$$+ \sum_{\beta\gamma} (\langle \lambda'\alpha_2 | v | \beta\gamma \rangle C_{\beta\gamma\alpha_1'\alpha_2'}^0 + \langle \lambda'\beta | v | \alpha_1'\gamma \rangle_A C_{\alpha_2\gamma\alpha_2'\beta}^0$$
$$\left. - \langle \lambda'\beta | v | \alpha_2'\gamma \rangle_A C_{\alpha_2\gamma\alpha_1'\beta}^0 \right\}$$

$$+\delta_{\alpha_2\lambda}\Bigg\{\sum_{\beta\gamma\delta}[(\delta_{\alpha_1\beta}-n^0_{\alpha_1\beta})n^0_{\gamma\alpha'_1}n^0_{\delta\alpha'_2}$$

$$+n^0_{\alpha_1\beta}(\delta_{\gamma\alpha'_1}-n^0_{\gamma\alpha'_1})(\delta_{\delta\alpha'_2}-n^0_{\delta\alpha'_2})]\langle\lambda'\beta|v|\gamma\delta\rangle_A$$

$$+\sum_{\beta\gamma}[\langle\lambda'\alpha_1|v|\beta\gamma\rangle C^0_{\beta\gamma\alpha'_1\alpha'_2}$$

$$+\langle\lambda'\beta|v|\alpha'_1\gamma\rangle_A C^0_{\alpha_1\gamma\alpha'_2\beta}-\langle\lambda'\beta|v|\alpha'_2\gamma\rangle_A C^0_{\alpha_1\gamma\alpha'_1\beta}]\Bigg\}$$

$$+\delta_{\alpha'_1\lambda'}\Bigg\{\sum_{\beta\gamma\delta}[(\delta_{\delta\alpha'_2}-n^0_{\delta\alpha'_2})n^0_{\alpha_1\beta}n^0_{\alpha_2\gamma}$$

$$+n^0_{\delta\alpha'_2}(\delta_{\alpha_1\beta}-n^0_{\alpha_1\beta})(\delta_{\alpha_2\gamma}-n^0_{\alpha_2\gamma})]\langle\beta\gamma|v|\lambda\delta\rangle_A$$

$$+\sum_{\beta\gamma}[\langle\beta\gamma|v|\lambda\alpha'_2\rangle C^0_{\alpha_1\alpha_2\beta\gamma}$$

$$+\langle\alpha_1\beta|v|\lambda\gamma\rangle_A C^0_{\alpha_2\gamma\alpha'_2\beta}-\langle\alpha_2\beta|v|\lambda\gamma\rangle_A C^0_{\alpha_1\gamma\alpha'_2\beta}]\Bigg\}$$

$$-\delta_{\alpha'_2\lambda'}\Bigg\{\sum_{\beta\gamma\delta}[(\delta_{\delta\alpha'_1}-n^0_{\delta\alpha'_1})n^0_{\alpha_1\beta}n^0_{\alpha_2\gamma}$$

$$+n^0_{\delta\alpha'_1}(\delta_{\alpha_1\beta}-n^0_{\alpha_1\beta})(\delta_{\alpha_2\gamma}-n^0_{\alpha_2\gamma})]\langle\beta\gamma|v|\lambda\delta\rangle_A$$

$$+\sum_{\beta\gamma}[\langle\beta\gamma|v|\lambda\alpha'_1\rangle C^0_{\alpha_1\alpha_2\beta\gamma}$$

$$+\langle\alpha_1\beta|v|\lambda\gamma\rangle_A C^0_{\alpha_2\gamma\alpha'_1\beta}-\langle\alpha_2\beta|v|\lambda\gamma\rangle_A C^0_{\alpha_1\gamma\alpha'_1\beta}]\Bigg\}$$

$$+\sum_{\beta}[\langle\alpha_1\lambda'|v|\beta\lambda\rangle_A C^0_{\beta\alpha_2\alpha'_1\alpha'_2}-\langle\alpha_2\lambda'|v|\beta\lambda\rangle_A C^0_{\beta\alpha_1\alpha'_1\alpha'_2}$$

$$-\langle\beta\lambda'|v|\alpha'_2\lambda\rangle_A C^0_{\alpha_1\alpha_2\alpha'_1\beta}+\langle\beta\lambda'|v|\alpha'_1\lambda\rangle_A C^0_{\alpha_1\alpha_2\alpha'_2\beta}],\tag{A.2}$$

$$c(\alpha\alpha':\lambda_1\lambda_2\lambda'_1\lambda'_2)=\langle\alpha\lambda'_2|v|\lambda_1\lambda_2\rangle\delta_{\alpha'\lambda'_1}$$
$$-\langle\lambda'_1\lambda'_2|v|\alpha'\lambda_2\rangle\delta_{\alpha\lambda_1},\tag{A.3}$$

$$d(\alpha_1\alpha_2\alpha'_1\alpha'_2:\lambda_1\lambda_2\lambda'_1\lambda'_2)=$$
$$(\epsilon_{\alpha_1}+\epsilon_{\alpha_2}-\epsilon_{\alpha'_1}-\epsilon_{\alpha'_2})\delta_{\alpha_1\lambda_1}\delta_{\alpha_2\lambda_2}\delta_{\alpha'_1\lambda'_1}\delta_{\alpha'_2\lambda'_2}$$

$$+\delta_{\alpha'_1\lambda'_1}\delta_{\alpha'_2\lambda'_2}\sum_{\beta\gamma}(\delta_{\alpha_1\beta}\delta_{\alpha_2\gamma}-\delta_{\alpha_2\gamma}n^0_{\alpha_1\beta}$$

$$-\delta_{\alpha_1\beta}n^0_{\alpha_2\gamma})\langle\beta\gamma|v|\lambda_1\lambda_2\rangle$$

$$-\delta_{\alpha_1\lambda_1}\delta_{\alpha_2\lambda_2}\sum_{\beta\gamma}(\delta_{\alpha'_1\beta}\delta_{\alpha'_2\gamma}-\delta_{\alpha'_2\gamma}n^0_{\beta\alpha'_1}$$

$$-\delta_{\alpha'_1\beta}n^0_{\gamma\alpha'_2})\langle\lambda'_1\lambda'_2|v|\beta\gamma\rangle$$

$$+\delta_{\alpha_2\lambda_2}\delta_{\alpha'_2\lambda'_2}\sum_{\beta}(\langle\alpha_1\lambda'_1|v|\beta\lambda_1\rangle_A n^0_{\beta\alpha'_1}$$

$$-\langle\beta\lambda'_1|v|\alpha'_1\lambda_1\rangle_A n^0_{\alpha_1\beta})$$

$$+\delta_{\alpha_2\lambda_2}\delta_{\alpha'_1\lambda'_1}\sum_{\beta}(\langle\alpha_1\lambda'_2|v|\beta\lambda_1\rangle_A n^0_{\beta\alpha'_2}$$

$$-\langle\beta\lambda'_2|v|\alpha'_2\lambda_1\rangle_A n^0_{\alpha_1\beta})$$

$$+\delta_{\alpha_1\lambda_1}\delta_{\alpha'_1\lambda'_1}\sum_{\beta}(\langle\alpha_2\lambda'_2|v|\beta\lambda_2\rangle_A n^0_{\beta\alpha'_2}$$

$$-\langle\beta\lambda'_2|v|\alpha'_2\lambda_2\rangle_A n^0_{\alpha_2\beta})$$

$$+\delta_{\alpha_1\lambda_1}\delta_{\alpha'_2\lambda'_2}\sum_{\beta}(\langle\alpha_2\lambda'_1|v|\beta\lambda_2\rangle_A n^0_{\beta\alpha'_1}$$

$$-\langle\beta\lambda'_1|v|\alpha'_1\lambda_2\rangle_A n^0_{\alpha_2\beta}),\tag{A.4}$$

where $n^0_{\alpha\alpha'}=\langle\Phi_0|a^+_{\alpha'}a_\alpha|\Phi_0\rangle$ and $C^0_{\alpha_1\alpha_2\alpha'_1\alpha'_2}=\langle\Phi_0|a^+_{\alpha'_1}a^+_{\alpha'_2}a_{\alpha_2}a_{\alpha_1}|\Phi_0\rangle-\mathcal{A}(n^0_{\alpha_1\alpha'_1}n^0_{\alpha_2\alpha'_2})$, and the subscript A indicates that the corresponding matrix element is antisymmetrized.

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