Dipole resonances in oxygen isotopes in time-dependent density-matrix theory

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The strength functions of isovector dipole resonances in the oxygen isotopes $^{18-24}\text{O}$ with even neutron numbers are calculated using an extended version of the time-dependent Hartree-Fock theory (TDDM). The results are compared with recent experimental data and also with a shell-model calculation. It is found that the observed isotope dependence of low-lying dipole strength is reproduced in TDDM when the strength of the residual interaction is appropriately chosen. It is also found that there is a difference between the TDDM prediction and the shell-model calculation for $^{24}\text{O}$. A tentative result for the strength function of an isoscalar quadrupole resonance in $^{24}\text{O}$ is presented.

1. Motivation

About seven years ago, one of the authors (M.T.) performed explorative calculations for isovector dipole ($E1$) and isoscalar quadrupole ($E2$) resonances in the unstable oxygen isotope $^{22}\text{O}$ based on the time-dependent density-matrix theory (TDDM). It was found that there are low-energy $E1$ and $E2$ modes associated with excess neutrons. At that time, there were no experimental data for comparison and the TDDM calculations were not highly quantitative: since spin-orbit force was neglected in the calculation of a mean-field potential, the neutron $2s$ and $1d$ states were assumed to be half occupied, apparently overestimating the effect of ground-state correlations. Recently, the isotope dependence of low-lying $E1$ strength has been measured at GSI for oxygen isotopes and compared with a shell-model calculation.

The main purpose of this report is to present more quantitative TDDM results than the previous ones for the isovector $E1$ resonances in oxygen isotopes. Two recent improvements make it possible to perform better TDDM calculations: one is the treatment of ground-state correlations. As will be described below, an adiabatic treatment of the residual interaction enables us to obtain a correlated ground state which is a stationary solution of TDDM. The other improvement is the extension of the TDDM program to include spin-orbit force, which has been done based on the TDHF code with spin-orbit extension of the TDDM program to include spin-orbit force.

This report is organized as follows: in Sec. 2 we briefly describe the equations of motion in TDDM and explain how the $E1$ strength function is calculated. The obtained results are presented and discussed in Sec. 3. A tentative result of the $E2$ strength function is also shown for $^{24}\text{O}$ in Sec. 3, and Sec. 4 is devoted to a summary.

2. TDDM and method for calculating the strength function

TDDM is an extended version of the time-dependent Hartree-Fock theory (TDHF) and is formulated in order to determine the time evolution of one-body and two-body density matrices $\rho$ and $\rho_2$ in a self-consistent manner. TDDM, therefore, includes the effects of both a mean-field potential and nucleon-nucleon correlations. The equations of motion for $\rho$ and $\rho_2$ can be derived by truncating the well-known BBGKY hierarchy for reduced density matrices; the equations of motion for $\rho$ and $\rho_2$ in the density-matrix formalism in general are

$$\frac{i\hbar}{\partial t} \rho(11') = (K(1) - K(1'))\rho + \int (v(12) - (21'))\rho_2(121'2)d2,$$

$$\frac{i\hbar}{\partial t} \rho_2(121'2) = (K(1) + K(2) - K(1') - K(2'))\rho_2 + (v(12) - v(1'2'))\rho,$$

$$+ \int (v(13) + v(23) - v(31') - v(32'))\rho_2(121'23)d3,$$

where the numbers indicate spatial, spin and isospin coordinates, $K$ is a kinetic-energy operator, and $v$ is a two-body interaction. The equation of motion for $\rho_2$ contains a three-body density matrix $\rho_3$. To close the hierarchy in the equations of motion, genuine three-body correlations are neglected and the three-body density matrix is assumed to be

$$\rho_3(1231'2'3') = AS(\rho(11')\rho(22')\rho(33')) + \rho(11')C_2(232'3'),$$

where $C_2$ is the correlated part of $\rho_2$, the operator $A$ anti-symmetrizes the operand under the exchange of coordinates $i$ and $j$, and $S$ symmetrizes it under the exchange of pairs of coordinates $(i'i)$ and $(jj')$. To solve the equations of motion for $\rho$ and $\rho_2$, we expand $\rho$ and $C_2$ using a finite number of single-particle states $\psi$, which satisfy a TDHF-like equation,

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

$$C_2(121'2', t) = \rho_2 - A(\rho) = \sum_{\alpha, \alpha', \gamma, \gamma'} C_{\alpha, \alpha', \gamma, \gamma'}(t) \times \psi_{\alpha}(1, t)\psi_{\gamma}(2, t)\psi_{\alpha'}^*(1', t)\psi_{\gamma'}^*(2', t).$$
Thus, the equations of motion of TDDM consist of the following three coupled equations:\(^1\)

\[
\frac{i\hbar}{\partial t} \psi_\alpha(t, \bar{\bar{r}}) = h(1, t) \psi_\alpha(t, \bar{\bar{r}}), \tag{6}
\]

\[
ih_n \dot{\alpha} = \sum_{\beta < \delta} [\langle \alpha | \beta \rangle \gamma_j \delta \rho_{\alpha, \beta, \alpha'} - \rho_{\alpha, \beta, \alpha'} (\gamma_j \delta | \alpha' \beta \rangle)], \tag{7}
\]

\[
ih_C_{\alpha, \beta, \alpha', \beta'} = B_{\alpha, \beta, \alpha', \beta'} + P_{\alpha, \beta, \alpha', \beta'} + H_{\alpha, \beta, \alpha', \beta'}, \tag{8}
\]

where \(h\) is the mean-field hamiltonian and \(v\) the residual interaction. The terms on the right-hand side of Eq.(8) are explicitly shown in the Appendix, where it may be easily understood that Eq.(8) contains all two-body correlations including those induced by the Pauli exclusion principle. The TDDM equations of motion satisfy conservation laws of the total number of particles and the total momentum and energy. The small amplitude limit of TDDM was investigated\(^8\) and it was found that if only the one particle - one hole and one particle - one hole - one particle elements of \(n_{\alpha, \alpha'}\) and \(C_{\alpha, \beta, \alpha', \beta'}\) are taken, the small amplitude limit of TDDM will be equivalent to the conventional second RPA (SRPA).\(^9\) Thus, TDDM is a more general framework than the conventional SRPA. It is also pointed out\(^10\) that keeping all the matrix elements of one-body and two-body amplitudes in SRPA as is always so in TDDM is essential to satisfy the property that a spurious state associated with the translational motion has zero excitation energy which RPA fulfills.

The E1 strength function is calculated in the following three steps:

1) A static Hartree-Fock (HF) calculation is performed to obtain the initial ground state. The Skyrme III with spin-orbit force is used as the effective interaction. Unoccupied single-particle states up to the 2s and 1d orbits are also calculated for both protons and neutrons to solve the TDDM equations for \(n_{\alpha, \alpha'}\) and \(C_{\alpha, \beta, \alpha', \beta'}\). The single-particle wavefunctions are confined to a cylinder with length 20 fm and radius 10 fm. (Axial symmetry is imposed to calculate the single-particle wavefunctions.)\(^5\) The mesh size used is 0.5 fm. The neutron 1d_{5/2} state is assumed to be partially occupied to obtain the HF ground states for \(^1\)H and \(^2\)O.

2) To obtain a correlated ground state, we evolve the HF ground state using the TDDM equations and the following time-dependent residual interaction of the \(\delta\)-function form

\[
v(t) = v_0 (1 - e^{-t/\tau}) \delta^3(\bar{\bar{r}} - \bar{\bar{r}}_0), \tag{9}
\]

The TDDM program is written for use with more complicated residual interactions such as the Skyrme force. To save computation time, however, we use the simple residual interaction in this report. The time constant \(\tau\) should be sufficiently large to obtain a nearly stationary solution of the TDDM equations.\(^5\) We choose \(\tau\) to be 150 fm/c. The strength of the residual interaction is determined to approximately reproduce the observed occupation probability of the proton 1d_{5/2} state in \(^5\)H. The obtained value of \(v_0\) is \(-230\) MeVfm\(^3\), which may be smaller than the value of approximately \(-300\) MeVfm\(^3\) found in the literature for pairing-gap calculations. The time step size used to solve the TDDM equations is 0.75 fm/c.

3) The E1 mode is excited by boosting the single-particle wavefunctions at \(t = 5\tau\) with the dipole velocity field:

\[
\psi_\alpha(t) \rightarrow e^{i k D(z)} \psi_\alpha, \tag{10}
\]

where

\[
D(z) = \begin{cases} 
\frac{\hbar z}{4} & \text{for protons,} \\
-\frac{\hbar z}{4} & \text{for neutrons.}
\end{cases} \tag{11}
\]

Here, \(Z\) and \(N\) are the numbers of protons and neutrons, respectively, and \(A = Z + N\). When the boosting parameter \(k\) is sufficiently small, the strength function defined by

\[
S(E) = \sum_{\alpha} |\langle \Phi_\alpha | \hat{D} | \Phi_0 \rangle|^2 \delta(E - E_\alpha) \tag{12}
\]

is obtained from the Fourier transformation of the time-dependent dipole moment \(D(t)\) as

\[
S(E) = \frac{1}{\pi \hbar k} \int_0^\infty D(t) \sin \frac{Et}{\hbar} dt, \tag{13}
\]

where

\[
D(t) = \int D(z) \rho(\bar{\bar{r}}, t) d^3 \bar{\bar{r}}. \tag{14}
\]

In Eq.(12) \(|\Phi_0\rangle\) is the total ground-state wavefunction and \(|\Phi_\alpha\rangle\) the wavefunction for an excited state with excitation energy \(E_\alpha\). It is very time consuming to solve the TDDM equations (especially Eq.(8)) for a long period. Thus, we stop TDDM calculations at \(t = 1200\) fm/c. The upper limit of the time integration in Eq.(13) is limited to 450 fm/c. To reduce fluctuations in \(S(E)\), the dipole moment is multiplied by a damping factor \(e^{-T \Gamma / 2 \hbar}\) with \(\Gamma = 1\) MeV before the time integration. Since the integration time is limited, the strength function in a very low energy region \((E \leq 2\hbar / 150 \approx 3\) MeV) is not well determined. The energy-weighted sum rule (EWSR) is expressed as

\[
\int S(E) EdE = \frac{1}{2} \langle \Phi_0 | [\hat{D}, [H, \hat{D}]] | \Phi_0 \rangle
\]

\[
= \frac{\hbar^2 Z N}{2m A} + \frac{t_1 + t_2}{4} \int \rho_n(\bar{\bar{r}}) \rho_n(\bar{\bar{r}}) d^3 \bar{\bar{r}}
\]

\[
+ \sum_{\alpha' \in \beta, \beta' \in \gamma} \int \psi^*_\alpha(\bar{\bar{r}}) \psi_{\alpha'}(\bar{\bar{r}}) d^3 \bar{\bar{r}} C_{\alpha', \beta', \alpha} \rangle, \tag{15}
\]

where \(m\) is the nucleon mass, and \(t_1\) and \(t_2\) are the parameters for the momentum-dependent parts of the Skyrme interaction. We assume that the hamiltonian \(H\) consists of a two-body interaction of the Skyrme type. The first term on the right-hand side of the above equation corresponds to the classical Thomas-Reiche-Kuhn (TRK) sum rule and the second term, the enhancement term, is due to the momentum dependence of the hamiltonian. The contribution of the momentum-dependent part is about 28% of the total EWSR value in the oxygen isotopes considered here and the term proportional to \(C_{\alpha, \beta, \alpha', \beta'}\) describing the effects of ground-state correlations is quite small (less than 1% of the total sum rule value).

3. Result and discussion

In order to demonstrate how the adiabatic method for obtaining a correlated ground state works, we show in Fig. 1...
the HF, correlation and total energies as functions of time for $^{22}$O. The correlation energy $E_{\text{corr}}$ is defined as

$$E_{\text{corr}} = \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} \langle \alpha\beta|v|\alpha'\beta' \rangle C_{\alpha'\beta'\alpha\beta}.$$  \hspace{1cm} (16)

Since all the two-body correlations are taken into account in the equation of motion for $C_{\alpha\beta\alpha'\beta'}$, the correlation energy includes both pairing-type and RPA-type correlation energies. The HF, correlation and total energies smoothly approach their final values without any visible fluctuations, and it has been checked\(^4\) that as long as $\tau$ is sufficiently large, the final values are independent of $\tau$. Fig. 1 also shows that the total energy is well conserved after $t = 750\text{fm/c}$. The energy conservation is subtle in TDDM. In the case that the excitation energy brought into the system is large as in heavy-ion collisions, the total energy is not well conserved.\(^7\) This originates in the truncation of the single-particle space. In the small amplitude limit of TDDM considered here, the energy conservation holds well. The calculated occupation probabilities of the neutron $2s_{1/2}$ and $1d_{3/2}$ states are 2-3% in the oxygen isotopes considered here. A small increase (of 1.3 MeV) in the HF energy and also in the total energy at $t = 750\text{fm/c}$ is due to the boosting of the single-particle wavefunctions to excite the $E_1$ mode. The value of the boosting parameter $k$ used in this calculation is 0.1 fm$^{-1}$. The time evolution of the dipole moment of $^{22}$O is shown in Fig. 2. The strength function is obtained from the Fourier transformation of this moment between $750\text{fm/c}$ and $1200\text{fm/c}$. Since the amplitude of the dipole moment linearly depends on $k$ as long as $k$ is small, the strength function is independent of $k$.

In Figs. 3-6, the $E1$ strength functions of $^{18-24}$O with even neutron numbers calculated in TDDM (solid line) are compared with those in TDHF (dotted line). The TDHF calculations presented here are equivalent to the RPA calculations without any truncation of unoccupied single-particle states because the TDHF equation for the boosted single-particle wavefunctions $\psi_{\alpha}$ is solved in coordinate space. The boundary condition for the continuum states, however, is not properly taken into account in our calculation because all the single-particle wave functions are confined to the cylinder. Therefore, the calculated strength functions slightly depend on the cylinder size. The difference between the TDDM and TDHF calculations is due to the effects of two-body correlations, which may have two aspects: one is to induce the ground-state correlations which increase the occupation probabilities of weakly bound neutron orbits. The increase in low-lying strength ($E < 15\text{MeV}$) seen in the TDDM results for all the isotopes is due to partial occupation of the neutron $2s_{1/2}$ and $1d_{3/2}$ states. The comparison between the TDDM result for $^{24}$O and those for other isotopes suggests

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**Fig. 1.** Time evolution of the HF (dotted line), correlation (dot-dashed line), and total energies (solid line) of $^{22}$O. The value of the boosting parameter $k$ is 0.1 fm$^{-1}$.

**Fig. 2.** Time evolution of the dipole moment of $^{22}$O. The value of the boosting parameter $k$ is 0.1 fm$^{-1}$.

**Fig. 3.** Strength functions of isovector dipole resonances in $^{18}$O calculated in TDDM (solid line) and in TDHF (dotted line).

**Fig. 4.** Strength functions of isovector dipole resonances in $^{20}$O calculated in TDDM (solid line) and in TDHF (dotted line).
that the occupation of the neutron $2s_{1/2}$ state is responsible for the increase in the $E1$ strength in the very low energy region (around $E = 5$ MeV). This is because the appearance of a prominent peak at 6 MeV in $^{20}$O is related to the nearly full occupation of the neutron $2s_{1/2}$ state. The other aspect of the two-body correlations is to increase the width of the giant dipole resonance (GDR) which is located around 25 MeV. There are background two particle - two hole states which consist of $1\hbar\omega$ excitations of protons and $0\hbar\omega$ excitations of neutrons. The coupling of the GDR to these states leads to the spreading of the GDR strength. The fractions of the EWSR values depleted over the energy range between 0 MeV to 40 MeV are about 85% in TDDM and about 90% in TDHF. The EWSR values depleted below 15 MeV are shown by circles in Fig. 7. The magnitude of the low-lying strength is increased and now becomes close to the experimental data except for $^{22}$O. The fact that the low-lying $E1$ strength in $^{20}$O is most increased with the use of the stronger residual interaction may be explained by the large fragmentation of the GDR strength as seen in Fig. 8.

The TDDM results for $^{24}$O shown in Fig. 7 significantly differ from the shell-model calculation. The difference originates in the fact that the shell-model calculation gives much smaller spreading width to the GDR in $^{24}$O than the TDDM calculations do. Since a large amount of the $E1$ strength is concentrated in the GDR, the low-lying $E1$ strength calculated in the shell model becomes small in $^{24}$O.

Finally, we show a tentative result for the isoscalar
quadrupole resonance in $^{24}$O. The quadrupole mode is excited by boosting the single-particle wavefunctions at $t = 5\pi$ with the quadrupole velocity field:

$$\psi_\alpha(5\pi) \rightarrow e^{iQ(z)}\psi_\alpha,$$

where we choose

$$Q(\vec{r}) = z^2 - \frac{1}{2}(x^2 + y^2).$$

The strength function for the quadrupole mode is expressed as

$$\int S(E) EdE = \frac{1}{2}\langle\Phi_0| [\hat{Q}, [\hat{H}, \hat{Q}]]|\Phi_0\rangle = \frac{\hbar^2 A}{2m}\langle\Phi_0| r^2 |\Phi_0\rangle.$$  \hspace{1cm} (19)

The strength function is calculated from the Fourier transform of the time-dependent quadrupole moment in a way similar to the dipole mode. In this calculation, the TDHF equations are solved until $t = 1500$ fm/c to better determine the strength function in the very low energy region. In Fig. 9, the strength function in TDHF is compared with that in TDDM. The peak at 2.6 MeV may be due to the one particle - one hole transition from the $2s_{1/2}$ state to the $1d_{5/2}$ state of neutrons. The fraction of the EWSR value depleted below 40 MeV is 95%. In the previous calculation $^{1)}$ for the quadrupole mode where the single-particle space was taken up to the $2p$ and $1f$ states, a downward shift of the giant quadrupole resonance (GQR) was obtained due to the coupling to two particle - two hole states. The low-lying states were not much affected by the coupling, however. Therefore, the small effect of the two-body correlations on the GQR in the present calculation may be due to the truncation of the single-particle space.

4. Summary

The strength functions of the isovector dipole resonances in the oxygen isotopes $^{18-24}$O with even neutron numbers were calculated using an extended version of TDHF known as TDDM. These calculations are much more improved and quantitative than the previous ones $^{1)}$ in two aspects: the inclusion of spin-orbit force in the mean-field potential and the use of the correlated ground state. The results were compared with recent experimental data and also with a shell-model calculation. It was found that if the strength of the residual interaction is appropriately chosen, TDDM approximately reproduces the observed isotope dependence of the low-lying $E1$ strength. It was also found that the TDDM prediction differs from the shell-model calculation for $^{24}$O. It was discussed that this originates in the spreading width of the GDR between the two models. The TDDM result for the isoscalar quadrupole resonance was also presented. It was found that the effects of two-body correlations are small for the quadrupole mode in the truncated single-particle space used here.

5. Appendix

The terms which consist of the equation of motion for the correlation matrix $C_{\alpha\alpha'\beta\beta'}$ Eq.(8) are explicitly shown below. The first term $B_{\alpha,\beta',\beta}^{\alpha'}$ describes the first-order terms of $v$ with the Pauli blocking factors and may be called the Born term:

$$B_{\alpha,\beta',\beta}^{\alpha'} = \sum_{\lambda_1,\lambda_2,\lambda_3,\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle \times \{ (\delta_{\lambda_2\lambda_1} - n_{\lambda_2\lambda_1})(\delta_{\beta\lambda_2} - n_{\beta\lambda_2}) n_{\lambda_3\alpha'} n_{\lambda_4\beta'} $$

$$- n_{\lambda_1\lambda_2}(\delta_{\lambda_2\lambda_1} - n_{\lambda_2\lambda_1})(\delta_{\lambda_3\alpha'} - n_{\lambda_3\alpha'})(\delta_{\lambda_4\beta'} - n_{\lambda_4\beta'}),$$

where subscript $A$ means that the two-body matrix is antisymmetrized. The first part of the right-hand side of the above equation may be regarded as a gain term and the second part, a loss term. The second term $P_{\alpha,\beta',\beta}^{\alpha'}$ on the right-hand side of Eq.(8) consists of terms with $C_{\alpha\alpha'\beta\beta'}$ and represents pairing-type higher order particle-particle (and hole-hole) correlations with the appropriate Pauli blocking factors:

$$P_{\alpha,\beta',\beta}^{\alpha'} = \sum_{\lambda_1,\lambda_2,\lambda_3,\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle \times \{ (\delta_{\lambda_1\lambda_2} - n_{\lambda_1\lambda_2})(\delta_{\lambda_1\alpha} - n_{\lambda_1\alpha})(\delta_{\lambda_2\beta'} - n_{\lambda_2\beta'}) $$

$$- (\delta_{\lambda_1\alpha}(\delta_{\lambda_1\alpha} - n_{\lambda_1\alpha})(\delta_{\lambda_2\beta'} - n_{\lambda_2\beta'})(\delta_{\lambda_1\alpha} - n_{\lambda_1\alpha})(\delta_{\lambda_2\beta'} - n_{\lambda_2\beta'}),$$

The last term $H_{\alpha,\beta',\beta}^{\alpha'}$ on the right-hand side of Eq.(8) also contains $C_{\alpha\alpha'\beta\beta'}$ and describes the contribution of RPA-type higher order correlations in the particle-hole channel:

$$H_{\alpha,\beta',\beta}^{\alpha'} = \sum_{\lambda_1,\lambda_2,\lambda_3,\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle \times \{ (\delta_{\lambda_1\lambda_2}(\delta_{\lambda_1\alpha} - n_{\lambda_1\alpha})(\delta_{\lambda_2\beta'} - n_{\lambda_2\beta'})(\delta_{\lambda_1\alpha} - n_{\lambda_1\alpha})(\delta_{\lambda_2\beta'} - n_{\lambda_2\beta'}) $$

Thus, the equation of motion for $C_{\alpha\alpha'\beta\beta'}$ includes all the two-body correlations (paring-type and RPA-type correlations, and the coupling between them) at infinite order.
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