Application of extended random-phase approximation with ground-state correlations to collective excitations of $^{16}\text{O}$

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Abstract. The ground-state correlation effects on the octupole excitation of $^{16}\text{O}$ are studied using the extended random phase approximation (ERPA) derived from the time-dependent density-matrix theory. ERPA includes the effects of ground-state correlations through the fractional occupation of single-particle states and a correlated two-body density matrix. The coupling to two particle - two hole configurations is also included in ERPA. It is found that the first $3^{-}$ state calculated in the random phase approximation (RPA) is shifted upward when the self-energy contributions due to ground-state correlations are included in particle - hole pairs and that the coupling to two particle - two hole states plays a role in shifting the first $3^{-}$ state down to the right position.

1. Introduction
The random phase approximation (RPA) based on the Hartree-Fock (HF) ground state has extensively been used to study nuclear collective excitations. It is generally considered that the HF + RPA approach is the most appropriate for doubly closed-shell nuclei such as $^{16}\text{O}$, $^{40}\text{Ca}$, $^{48}\text{Ca}$ and $^{208}\text{Pb}$ for which the HF theory would give a good description of the ground states. However, it has also been known that the ground state of $^{16}\text{O}$ actually is a highly correlated state (see Refs.[1, 2] for recent theoretical studies.) This indicates the necessity of using beyond RPA theories to study collective excitations of $^{16}\text{O}$, though the HF + RPA approach has commonly been used for $^{16}\text{O}$. In this report we investigate how the octupole excitation of $^{16}\text{O}$, which has a collective low-lying state, is affected by ground-state correlations, using an extended RPA (ERPA) that has been derived from the time-dependent density-matrix theory (TDDM) [3, 4]. The advantage of ERPA is that it not only includes the effects of ground-state correlations but also describes the coupling to two particle - two hole configurations. We show that the first octupole state in $^{16}\text{O}$ is quite sensitive to the ground-state correlation effects and the coupling to the higher amplitudes.

2. Formulation
The TDDM consists of the coupled equations of motion for the one-body density matrix $n_{\alpha\alpha'}$ (the occupation matrix) and the correlated part of the two-body density matrix $C_{\alpha\beta\alpha'\beta'}$ (the correlation matrix). These matrices are defined as

$$n_{\alpha\alpha'}(t) = \langle \Phi(t)|a_{\alpha'}^\dagger a_{\alpha}|\Phi(t)\rangle,$$

(1)
dependent HF theory (TDHF). The TDDM equation for \( C_{\alpha\beta'\gamma'}(t) \) is truncated by replacing a three-body density matrix with anti-symmetrized products of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. In TDDM the BBGKY hierarchy equations of motion for reduced density matrices form a chain of coupled equations known as the RPA corresponds to the small amplitude limit of TDHF and are written in matrix form for the one-body and two-body amplitudes \( x_{\alpha\alpha'} \) and \( X_{\alpha\beta'\alpha'} \) [1]

\[
\begin{pmatrix}
A & C \\
B & D
\end{pmatrix}
\begin{pmatrix}
x^\mu \\
X^\mu
\end{pmatrix} = \omega \begin{pmatrix}
S_1 & T_1 \\
T_2 & S_2
\end{pmatrix}
\begin{pmatrix}
x^\mu \\
X^\mu
\end{pmatrix},
\]

where the matrix on the left-hand side is the Hamiltonian matrix and that on the right-hand side the norm matrix. The one-body sector of Eq. (3) \( Ax^\mu = \omega S_1 x^\mu \) is formally the same as the equation in the self-consistent RPA (SCRPA) of Refs. [5, 6, 7], which also includes the effects of ground-state correlations through \( n_{\alpha\alpha'} \) and \( C_{\alpha\beta'\alpha} \). We refer to the approximation \( Ax^\mu = \omega S_1 x^\mu \) as the modified RPA (mRPA). To explain the role of the correlation matrix in the mRPA equation, we explicitly show the matrices \( A \) and \( S_1 \):

\[
A(\alpha\alpha' : \lambda\lambda') = (\epsilon_\alpha - \epsilon_\alpha') (n_{\alpha'\alpha'} - n_{\alpha\alpha}) \delta_{\alpha\lambda} \delta_{\alpha'\lambda'} + (n_{\alpha'\alpha'} - n_{\alpha\alpha})(n_{\lambda'\lambda'} - n_{\lambda\lambda}) (\alpha\lambda | v | \alpha'\lambda')_A \\
- \delta_{\alpha\lambda} \sum_{\gamma\gamma'} (\alpha\gamma | v | \gamma'\gamma')_{C_{\gamma\gamma'}} \lambda_{\gamma'} \\
- \delta_{\lambda\lambda'} \sum_{\gamma\gamma'} (\gamma\gamma' | v | \alpha'\gamma')_{C_{\lambda\gamma'}} \lambda_{\gamma'} \\
+ \sum_{\gamma\gamma'} ((\alpha\gamma | v | \lambda\gamma')_{A} C_{\lambda'\gamma'\alpha'\gamma} + (\gamma'\gamma | v | \alpha'\gamma')_{A} C_{\alpha\gamma'\lambda}) \\
- \sum_{\gamma\gamma'} ((\alpha\lambda' | v | \gamma\gamma')_{A} C_{\gamma'\gamma'\alpha'\lambda} + (\gamma\gamma' | v | \alpha'\lambda)_{C_{\lambda'\gamma'}}),
\]

where the subscript \( A \) means that the corresponding matrix is antisymmetrized and \( n_{\alpha\alpha'} \) is assumed to be diagonal. The first two terms on the right-hand side of Eq. (4) are the same as those in the RPA equation, the next two terms with \( C_{\alpha\beta'\alpha} \) describe the self-energy of the particle - hole (p-h) state due to ground-state correlations [5], and the last four terms with \( C_{\alpha\beta'\alpha} \) may be interpreted as the modification of the p-h interaction caused by ground-state correlations [5]. If the correlated ground state is replaced by the HF ground state, mRPA and ERPA become the same as RPA and the second RPA (SRPA) [8], respectively. In SRPA calculations the so-called diagonal approximation where the correlations in matrix \( D \) are neglected has often been used [8]. In the ERPA calculations shown below all correlations in matrix \( D \) are included. It has
been pointed out [9] that if the effects of ground-state correlations are included perturbatively in extended RPA theories, the energy-weighted sum rule (EWSR) is not satisfied. In our ERPA and mRPA the ground state is calculated non-perturbatively in TDDM and the one-body amplitudes $x_{\mu \alpha'}$ include the p-p and h-h components in addition to the p-h and h-p components. Therefore, ERPA and mRPA satisfy EWSR [10].

3. Results
3.1. Calculational details
The occupation probability $n_{\alpha \alpha}$ and the correlation matrix $C_{\alpha \beta \alpha' \beta'}$ are calculated within TDDM using the gradient method [1] and the single-particle states, the $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$ and $2s_{1/2}$ states for both protons and neutrons. For the calculations of the single-particle states we use the Skyrme III force, which has often been used for nuclear structure calculations. To reduce the dimension size, we only consider the two particle - two hole (2p-2h) and 2h-2p elements of $C_{\alpha \beta \alpha' \beta'}$. A simplified interaction which contains only the $t_0$ and $t_3$ terms of the Skyrme III force is used as the residual interaction. The spin-orbit force and Coulomb interaction are also omitted from the residual interaction. To avoid a cumbersome treatment of the rearrangement effects of a density-dependent force in extended RPA theories [11], we use the three-body version of the Skyrme interaction, $v_3 = t_3 \delta^3(r_1 - r_2) \delta^3(r_1 - r_3)$, which gives the following density-dependent two-body residual interaction: $t_3 \rho_p \delta^3(r - r')$, $t_3 \rho_n \delta^3(r - r')$ for the proton-proton, proton-neutron and neutron-neutron interactions, respectively, where $\rho_p, \rho_n$ and $\rho$ are the proton, neutron and total densities, respectively. In the RPA, mRPA and ERPA calculations the one-body amplitudes $x_{\mu \alpha'}$ are defined using a large number of single-particle states including those in the continuum. We discretize the continuum states by confining the wavefunctions in a sphere with radius 15 fm and take all the single-particle states with $\varepsilon_\alpha \leq 50$ MeV and $j_\alpha \leq 11/2h$. As the residual interaction, we use the same simple force as that used in the ground-state calculation. Since the residual interaction is not consistent with the effective interaction used in the calculation of the single-particle states, it is necessary to adjust its strength so that the collective states calculated in RPA come at right positions. We use the reduction factor $f = 0.62$ so that the spurious mode corresponding to the center-of-mass motion comes at zero excitation energy in RPA. The p-h interaction in the second term on the right-hand side of Eq. (4) is multiplied with this $f$. This rather large reduction of the strength is a direct consequence of inconsistency of the residual interaction but the reduction procedure has been found [1] to give an excitation energy of the giant quadrupole resonance of $^{16}$O that is comparable to the result of a self-consistent RPA calculation. To define the two-body amplitudes $X_{\alpha \beta \alpha' \beta'}$, we use the small single-particle space consisting of the $1s_{1/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}, 2s_{1/2}, 1d_{3/2}, 2p_{3/2}, 2p_{1/2}$ and $1f_{7/2}$ for both protons and neutrons. To reduce the number of the two-body amplitudes, we consider only the 2p-2h and 2h-2p components of $X_{\alpha \beta \alpha' \beta'}$ with $|\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_\alpha' - \varepsilon_\beta'| \leq 60$ MeV. For the matrix elements of the residual interaction which couple to $X_{\alpha \beta \alpha' \beta'}^\mu$, we use the same residual interaction (with $f = 1$) as that used for the ground-state calculation because the single-particle space for $X_{\alpha \beta \alpha' \beta'}^\mu$ is much smaller than that for $x_{\mu \alpha'}$.

3.2. Ground state of $^{16}$O
The occupation probabilities in the ground state of $^{16}$O calculated in TDDM are shown in Table 1. The deviation from the HF values ($n_{\alpha \alpha}$=1 or 0) is more than 10%, which means that the ground state of $^{16}$O is strongly correlated. A recent shell-model calculation by Utsuno and Chiba [2] also gives a similar result for the ground state of $^{16}$O. The correlation energy $E_c$ in the ground state, which is defined by $E_c = \sum_{\alpha \beta' \alpha' \beta'} \langle \alpha \beta' | v | \alpha' \beta' \rangle C_{\alpha \beta' \alpha' \beta}/2$, is $-23.7$ MeV. A large portion of the correlation energy is compensated by the increase in the mean-field energy due to the fractional occupation of the single-particle states. The resulting energy gain due to the
Table 1. Single-particle energies $\epsilon_\alpha$ and occupation probabilities $n_{\alpha\alpha}$ in the ground state of $^{16}\text{O}$ calculated in TDDM.

| orbit, proton | neutron | proton | neutron |
|---------------|---------|--------|---------|
| 1p$_{3/2}$    | -18.3   | -21.9  | 0.894   | 0.893   |
| 1p$_{1/2}$    | -12.3   | -15.7  | 0.868   | 0.865   |
| 1d$_{5/2}$    | -3.8    | -7.1   | 0.108   | 0.109   |
| 2s$_{1/2}$    | 1.1     | -1.6   | 0.019   | 0.021   |

Figure 1. Strength functions calculated in RPA (chain line), SRPA (dashed line), mRPA (dotted line) and ERPA (full line) for the octupole excitation in $^{16}\text{O}$. The distributions are smoothed with an artificial width $\Gamma = 0.5$ MeV.

3.3. Octupole excitation

The strength functions for the isoscalar octupole excitation calculated in RPA (chain line), SRPA (dashed line), mRPA (dotted line) and ERPA (full line) are shown in Figure 1. We used the excitation operator $r^3Y_{30}(\theta)$ to calculate the transition strength. In RPA the summed energy-weighted strength exhausts 97% of the EWSR value. The energy-weighted sum of the octupole strength in ERPA and mRPA is about 10% larger than that in RPA. However, $\langle r^{2L-2}\rangle$ (with $L = 3$) for the TDDM ground state is also larger than that for the HF ground state because the radius of the correlated ground state is slightly larger than that of the HF ground state. Consequently, 96% of the EWSR value is exhausted in ERPA and mRPA. The excitation energy of the first 3$^{-}$ (3$^{-}_{1}$) state in RPA is 3.54 MeV, which is much smaller than the experimental data 6.13 MeV [12]. In SRPA the state corresponding to the 3$^{-}_{1}$ state becomes an imaginary solution due to the coupling to the 2p-2h configurations. The results in RPA and SRPA suggest that the approaches based on the HF ground state cannot give a correct excitation energy of the 3$^{-}_{1}$ state. The excitation energy of the 3$^{-}_{1}$ state in mRPA is 9.1 MeV, which is much larger than that
in RPA. This is explained by the self-energy contributions (see Eq. (4)) in the p-h pairs such as $(1p_{1/2})^{-1} \times 2d_{5/2}$ and $(1p_{3/2})^{-1} \times 2d_{5/2}$. The self-energy contributions increase the energy of the p-h pairs, reflecting the fact that the ground-state energy is lowered by the ground-state correlations. In ERPA the $3^-_1$ state is shifted downward to 6.56 MeV due to the coupling to the 2p-2h configurations. The results in mRPA and ERPA demonstrate that both the ground-state correlations and the coupling to the 2p-2h configurations play an important role in describing the properties of the $3^-_1$ state. The importance of the ground-state correlations and the coupling to 2p -2h configurations has also been found in other excitation modes [1, 13].

4. Summary

The effects of the correlations in the ground state of $^{16}$O on the octupole excitation were studied using the extended RPA (ERPA). ERPA contains the ground-state correlation effects through the fractional occupation of single-particle states and the correlated part of the two-body density matrix. It also includes the coupling of the one particle - one hole amplitudes to two particle - two hole ones. It was found that the ground-state correlation effects on the first $3^-_1$ state are significant: the first $3^-_1$ state is shifted upward due to the self-energy contributions induced by the ground-state correlations. It was also found that the coupling to two particle - two hole states plays a role in producing the first $3^-_1$ at the right position. Our results demonstrate that the ground-state correlation effects should be properly taken into account in the study of nuclear collective excitations.

[1] Tohyama M 2007 Phys. Rev. C 75 044310
[2] Utsuno Y and Chiba S 2011 Phys. Rev. C 83 021301(R)
[3] Wang S J and Cassing W 1985 Ann. Phys. 159 328
[4] Gong M and Tohyama M 1990 Z. Phys. A335 153
[5] Janssen D and Schuck P 1991 Z. Phys. A339 43
[6] Dukelsky J and Schuck P 1990 Nucl. Phys. A 512 466
[7] Dukelsky J and Schuck P 1996 Phys. Lett. B 387 233
[8] Drozd S, Nishizaki S, Speth J and Wambach J 1990 Phys. Rep. 197 1
[9] Adachi S and Lipparini E 1988 Nucl. Phys. A 489 445
[10] Tohyama M and Schuck P 2007 Eur. Phys. J. A 32 139
[11] Gambacurta D, Grasso M and Catara 2011 J. Phys. G 38 035103
[12] Firestone R B 1996 Table of Isotopes (New York: John Wiley & Sons)
[13] Tohyama M 2013 Phys. Rev. C 87 054330