Effects of ground-state correlations on collective excitations of ^{16}O

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The effects of the correlations in the ground state of ^{16}O on the octupole and dipole excitations are studied using the extended random phase approximation (ERPA) derived from the time-dependent density-matrix theory. It is found that the ground-state correlation effects are significant, especially in the octupole excitation. It is shown that the first 3^- state calculated in the random phase approximation (RPA) is shifted upward when the self-energy contributions are included in particle-hole pairs. The coupling to the two-particle–two-hole states plays a role in shifting the first 3^- state down to the right position. It is also found that the dipole strength is fragmented due to the partial occupation of the single-particle states and that the peak position of the giant dipole resonance calculated in ERPA is little changed from that in RPA due to the above-mentioned competing effects: the increase in particle-hole energy and the coupling to two-particle–two-hole configurations.

I. 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 double-closed-shell nuclei for which the HF theory would give a good description of the ground states. However, recent theoretical studies for ^{16}O indicate that the ground state of ^{16}O is a highly correlated state [1,2], which indicates the necessity of using beyond-RPA theories to study collective excitations of ^{16}O. In this paper we investigate how octupole and dipole excitations of ^{16}O are affected by ground-state correlations, using an extended RPA (ERPA) that has been derived from the time-dependent density-matrix theory (TDDM) [3,4]. We show that the octupole excitation of ^{16}O is quite sensitive to the ground-state correlation effects.

II. 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

$$n_{\alpha\alpha'}(t) = \langle\Phi(t)|a_{\alpha'}^{\dagger}a_{\alpha}|\Phi(t)\rangle, \tag{1}$$

$$C_{\alpha\beta\alpha'\beta'}(t) = \langle\Phi(t)|a_{\alpha'}^{\dagger}a_{\beta'}^{\dagger}a_{\beta}a_{\alpha}|\Phi(t)\rangle \\ - (n_{\alpha\alpha'}(t)n_{\beta\beta'}(t) - n_{\alpha\beta'}(t)n_{\alpha\beta'}(t)), \tag{2}$$

where $|\Phi(t)\rangle$ is the time-dependent total wave function $|\Phi(t)\rangle = \exp[-iHt]|\Phi(t=0)\rangle$. The equations of motion for reduced density matrices form a chain of coupled equations known as the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. In TDDM the BBGKY hierarchy is truncated by replacing a three-body density matrix with antisymmetrized products of the one-body and two-body density matrices. The TDDM equation for $C_{\alpha\beta\alpha'\beta'}$ contains all effects of two-body correlations: particle-particle, hole-hole, and particle-hole correlations. The ground state in TDDM is given as a stationary solution of the TDDM equations. The stationary solution can be obtained using the gradient method [1]. This method is also used in the present work. The

ERPA equations used here are derived as the small amplitude limit of TDDM and are written in matrix form for the one-body and two-body amplitudes $x_{\alpha\alpha'}^{\mu}$ and $X_{\alpha\beta\alpha'\beta'}^{\mu}$ [1]

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix}\begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix} = \omega_{\mu}\begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix}\begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix}. \tag{3}$$

The one-body sector of Eq. (3) $Ax^{\mu} = \omega_{\mu}S_1 x^{\mu}$ is formally the same as the equation in the self-consistent RPA (SCRPA) of Refs. [5–7], which includes the effects of ground-state correlations through $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$. We refer to the approximation $Ax^{\mu} = \omega_{\mu}S_1 x^{\mu}$ 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:

$$A(\alpha\alpha' : \lambda\lambda')$$
$$= (\epsilon_{\alpha} - \epsilon_{\alpha'})(n_{\alpha'\alpha'} - n_{\alpha\alpha})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'}$$
$$+ (n_{\alpha'\alpha'} - n_{\alpha\alpha})(n_{\lambda'\lambda'} - n_{\lambda\lambda})\langle\alpha\lambda'|v|\alpha'\lambda\rangle_A$$
$$- \delta_{\alpha'\lambda'}\sum_{\gamma\gamma'\gamma''}\langle\alpha\gamma|v|\gamma'\gamma''\rangle C_{\gamma'\gamma''\lambda\gamma}$$
$$- \delta_{\alpha\lambda}\sum_{\gamma\gamma'\gamma''}\langle\gamma\gamma'|v|\alpha'\gamma''\rangle C_{\lambda'\gamma''\gamma\gamma'}$$
$$+ \sum_{\gamma\gamma'}(\langle\alpha\gamma|v|\lambda\gamma'\rangle_A C_{\lambda'\gamma'\alpha'\gamma} + \langle\lambda'\gamma|v|\alpha'\gamma'\rangle_A C_{\alpha\gamma'\lambda\gamma})$$
$$- \sum_{\gamma\gamma'}(\langle\alpha\lambda'|v|\gamma\gamma'\rangle C_{\gamma\gamma'\alpha'\lambda} + \langle\gamma\gamma'|v|\alpha'\lambda\rangle C_{\alpha\lambda'\gamma\gamma'}), \tag{4}$$

$$S_1(\alpha\alpha' : \lambda\lambda')$$
$$= (n_{\alpha'\alpha'} - n_{\alpha\alpha})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'}, \tag{5}$$

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 $C_{\alpha\beta\alpha'\beta'}$ describe the self-energy of the particle-hole (p-h) state due to ground-state correlations [5], and the last four terms with $C_{\alpha\beta\alpha'\beta'}$ may be interpreted as the modification of the p-h interaction caused by ground-state correlations [5]. The difference between mRPA and SCRPA is in the method to determine $n_{\alpha\alpha}$ and $C_{\alpha\beta\alpha'\beta'}$: In SCRPA these matrices

are self-consistently determined using the amplitudes $x^{\mu}_{\alpha\alpha'}$ whereas here we calculate them in TDDM. Such a method of expressing $n_{\alpha\alpha}$ with the RPA amplitudes has been used in other beyond-RPA theories [8–12]. 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) [13], respectively. In SRPA calculations the so-called diagonal approximation where the correlations in matrix D are neglected has often been used [13]. In the ERPA calculations shown below all correlations in matrix D are included. It has been pointed out [14] 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 nonperturbatively in TDDM and the one-body amplitudes $x^{\mu}_{\alpha\alpha'}$ include the p-p and h-h components in addition to the p-h and h-p components. Therefore, ERPA and mRPA satisfy EWSR [15].

III. RESULTS

The occupation probability $n_{\alpha\alpha}$ and the correlation matrix $C_{\alpha\beta\alpha'\beta'}$ are calculated within TDDM using 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. 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 [16], 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: $t_3\rho_n\delta^3(r - r')$, $t_3\rho\delta^3(r - r')/2$, and $t_3\rho_p\delta^3(r - r')$ for the proton-proton, proton-neutron, and neutron-neutron interactions, respectively, where ρ_p, ρ_n, and ρ are the proton, neutron, and total densities, respectively. In the RPA, mRPA and ERPA calculations the one-body amplitudes $x^{\mu}_{\alpha\alpha'}$ are defined using a large number of single-particle states, including those in the continuum. We discretize the continuum states by confining the wave functions in a sphere with radius 15 fm and take all the single-particle states with $\epsilon_{\alpha} \leqslant 50$ MeV and $j_{\alpha} \leqslant 11/2\hbar$. 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 the 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 $X^{\mu}_{\alpha\beta\alpha'\beta'}$, we use the small

TABLE I. Single-particle energies ϵ_{α} and occupation probabilities $n_{\alpha\alpha}$ calculated in TDDM.

Orbit	ϵ_{α} [MeV]		$n_{\alpha\alpha}$	
	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

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 $X^{\mu}_{\alpha\beta\alpha'\beta'}$ with $|\epsilon_{\alpha} + \epsilon_{\beta} - \epsilon_{\alpha'} - \epsilon_{\beta'}| \leqslant E_{\max}$ MeV. By comparing the results with $E_{\max} = 40$, 50, and 60 MeV, we found that $E_{\max} = 60$ MeV is sufficient for the truncated single-particle space. For the matrix elements of the residual interaction which couple to $X^{\mu}_{\alpha\beta\alpha'\beta'}$, we use the same residual interaction (with $f = 1$) as that used for the ground-state calculation because the single-particle space for $X^{\mu}_{\alpha\beta\alpha'\beta'}$ is much smaller than that for $x^{\mu}_{\alpha\alpha'}$.

The occupation probabilities calculated in TDDM are shown in Table I. 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 a strongly correlated state. 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 ground-state correlations, which is given by the total energy difference between HF and TDDM, is 6.4 MeV, which is much smaller than $|E_c| = 23.7$ MeV.

The strength functions for the isoscalar octupole excitation calculated in RPA (blue [gray] dot-dashed line), SRPA (red [gray] dashed line), mRPA (dotted line), and ERPA (solid line) are shown in Fig. 1. The excitation operator used is
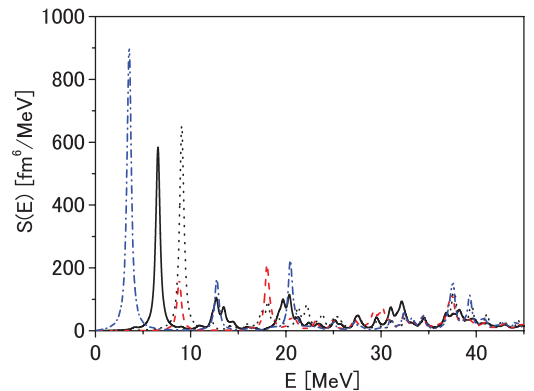

FIG. 1. (Color online) Strength functions calculated in RPA (blue [gray] dot-dashed line), SRPA (red [gray] dashed line), mRPA (dotted line), and ERPA (solid line) for the octupole excitation in ^{16}O. The distributions are smoothed with an artificial width $\Gamma = 0.5$ MeV.

$r^3 Y_{30}(\theta)$. In mRPA and ERPA the fractional occupation of the $2s_{1/2}$ states makes the transitions from these states to the continuum states possible, which gives some unphysical strength distributions in the very low-energy region. As is shown below, the unphysical contributions could in principle be eliminated by using the correlation matrix $C_{\alpha'\beta'\alpha\beta}$. However, it is difficult to completely eliminate the unphysical states. Therefore, we neglected the single-particle transitions from the $2s_{1/2}$ states. 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. 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 [17]. 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. We found that the last four terms in Eq. (4), which describe the modifications of the p-h interaction, play a role in slightly increasing the attractive p-h correlations. In ERPA the 3_1^- state is shifted downward to 6.56 MeV due to the coupling to the 2p-2h configurations. The $B(E3)$ value of the 3_1^- state calculated in ERPA is $130e^2$ fm^6, while the experimental value is $204 \pm 6e^2$ fm^6 [17]. The results in mRPA and ERPA demonstrate that both the ground-state correlations and the coupling to 2p-2h configurations play an important role in describing the properties of the 3_1^- state. Similar effects of ground-state correlations on collective excitations of metallic clusters have been reported by Gambacurta and Catara [12] using an extended SRPA approach.

We point out that the 3_1^- state in RPA somewhat depends on the parameters of the Skyrme interactions. For example, it has been reported that the SkM* parameter set [18] gives the 3_1^- state at 6.06 MeV with $B(E3) = 91.1e^2$ m^6 [19] and that a simple Skyrme type interaction with $t_0 = -1048$ MeV fm^3, $t_3 = 19150$ MeV fm^6, and $w_0 = 95$ MeV fm^5 gives the 3_1^- state at 6.05 MeV, which exhausts 10.5% of EWSR [20]. We also found that the parameter set of the Skyrme III force with $f = 0.62$, $x_0 = 0$, and $w_0 = 90$ MeV fm^5 gives the 3_1^- state at 6.12 MeV with $B(E3) = 211e^2$ fm^6 in RPA, which are close to the experimental data 6.13 MeV and $204 \pm 6e^2$ fm^6 [17]. However, this force also induces strong ground-state correlations and the 3_1^- state calculated in ERPA comes at 8.26 MeV, which is much higher than the data.

The strength functions for the isovector dipole excitation calculated in RPA (blue [gray] dot-dashed line) and SRPA (red [gray] dashed line) are shown in Fig. 2 and those in mRPA (dotted line) and ERPA (solid line) are shown in Fig. 3. The single-particle transitions from the partially occupied
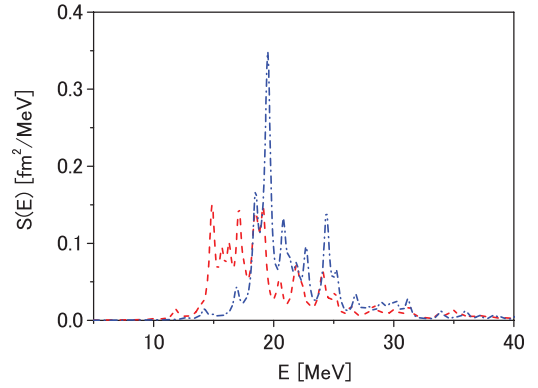

FIG. 2. (Color online) Strength functions calculated in RPA (blue [gray] dot-dashed line) and SRPA (red [gray] dashed line) for the isovector dipole excitation in ^{16}O. The distributions are smoothed with an artificial width $\Gamma = 0.5$ MeV.

$2s_{1/2}$ states are neglected in mRPA and ERPA. In RPA the summed energy-weighted strength exhausts 84% of the dipole sum rule including the enhancement term, which is given by the t_1 and t_2 parameters of the Skyrme III force and accounts for 26% of the sum rule value. To increase the sum of the energy-weighted strength, we need to include the momentum-dependent terms of the Skyme force in the residual interaction and also expand the single-particle space. The energy-weighted sums of the dipole strength in the other approximations give a value similar to that in RPA. Comparison of the result in SRPA with that in RPA shows that the main effect of the coupling to the 2p-2h configurations is to shift the RPA strength distribution downward. A similar downward shift of the dipole strength has been reported in large-scale SRPA calculations [21,22]. The centroid energies given by $\bar{E} = \int E S(E) dE / \int S(E) dE$ are 22.5, 21.9, 23.9, and 23.3 MeV in RPA, SRPA, mRPA, and ERPA, respectively. In mRPA the largest peak is upwardly shifted to 21.5 MeV from the position at 19.5 MeV in RPA. This upward shift is due to the self-energy contributions, mainly in the $(1p_{3/2})^{-1} - 1d_{5/2}$ pairs. In the case of the isovector dipole excitation, the last four terms in Eq. (4) play a role in slightly reducing the repulsive p-h correlations. The increase in the dipole strength below 15 MeV in mRPA and ERPA, which is consistent
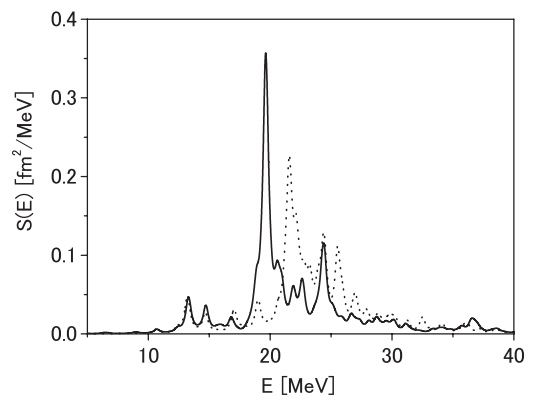

FIG. 3. Strength functions calculated in mRPA (dotted line) and ERPA (solid line) for the isovector dipole excitation in ^{16}O. The distributions are smoothed with an artificial width $\Gamma = 0.5$ MeV.
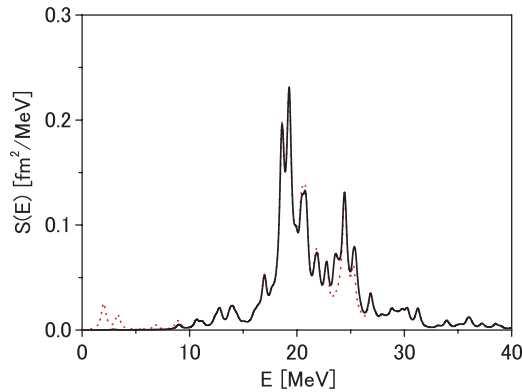
FIG. 4. (Color online) Strength functions calculated in mRPA (solid line) and RPA (red [gray] dotted line) for the isovector dipole excitation in ^{16}O. The partially occupied single-particle states obtained in TDDM are used in the RPA calculation. The correlation matrix $C_{\alpha'\beta'\alpha\beta}$ is inserted only to the $2s_{1/2}$-$2p_{3/2}$ and $2s_{1/2}$-$2p_{1/2}$ pairs in the mRPA calculation. The distributions are smoothed with an artificial width $\Gamma = 0.5$ MeV.

with the experiment [23], is due to the partial occupation of the $1d_{5/2}$ states allowing such low-energy p-h transitions as $1d_{5/2} \rightarrow 2p_{3/2}$. The strength distribution above 20 MeV in mRPA is about 2 MeV downwardly shifted in ERPA due to the coupling to the 2p-2h configurations. However, there is little difference between the mRPA and ERPA distributions in the energy region below 17 MeV. This indicates that the dipole states in the low-energy region weakly couple to the 2p-2h configurations. In the case of the isovector dipole excitation the effects of the ground-state correlations play a role in increasing the fragmentation of the dipole strength in the low-energy region. However, in the giant dipole resonance (GDR) region it seems that the increase in the energy of the p-h pairs is compensated by a downward shift of the dipole strength due to the coupling to the 2p-2h configurations. The experimental photoabsorption cross section [23] shows a broader GDR distribution than the result in ERPA. More two-body configurations should be included to improve the ERPA result. A similar downward shift of negative-parity states due to coupling to multiphonon states have been reported in a recent application of a multiphonon model to ^{16}O [24].

As mentioned above, partial occupation of the particle states could cause some unphysical low-lying transitions possible. To show this, we performed an RPA calculation for the isovector dipole excitation using the partially occupied single-particle states including the $2s_{1/2}$ states. The result is shown in Fig. 4 with the dotted line. The strength seen below 5 MeV comes from the transitions from the $2s_{1/2}$ states to the $2p_{3/2}$ and $2p_{1/2}$ states. The solid line in Fig. 4 shows the result in mRPA where the correlation matrix $C_{\alpha'\beta'\alpha\beta}$ is included only in the $2s_{1/2}$-$2p_{3/2}$ and $2s_{1/2}$-$2p_{1/2}$ p-h pairs. Since the norm matrix S_1 given by Eq. (5) for the $2s_{1/2}$-$2p_{3/2}$ and $2s_{1/2}$-$2p_{1/2}$ pairs is quite small (≈ 0.02, see Table I), the terms in Eq. (4) which contain $C_{\alpha\beta\alpha'\beta'}$ can drastically shift the energies of these pairs. In fact the inclusion of the correlation matrix eliminates the strength in the low-energy region and slightly increases the strength distribution around 25 MeV, as seen in Fig. 4. When the coupling of the p-h pairs to 2p-2h configurations is included in ERPA, it becomes difficult to completely eliminate the unphysical low-energy transitions from the partially occupied $2s_{1/2}$ states. This is the reason why we neglected such transitions in the mRPA and ERPA calculations shown above. The problems of unphysical components in beyond-RPA approaches have been discussed in Ref. [11], where a way to disentangle them is also suggested.

IV. CONCLUSION

In summary, the effects of the correlations in the ground state of ^{16}O on the octupole and dipole excitations were studied using the extended RPA. It was found that the ground-state correlation effects on the first 3^- state are significant: The first 3^- state is shifted upward due to the self-energy contributions. It was also found that the coupling to two-particle–two-hole states plays a role in producing the first 3^- at right excitation energy. In the case of the isovector dipole excitation, the effects of the ground-state correlations were found to increase the fragmentation of the dipole strength in low-energy region. However, the giant dipole resonance calculated in ERPA is little changed from that in RPA due to the competing effects: The increase in particle-hole energy and the coupling to two-particle–two-hole configurations. The mechanism to eliminate unphysical low-energy transitions originating from partial occupation of the particle states was also discussed. Our results demonstrate that the ground-state correlation effects in ^{16}O should be properly taken into account in the study of collective excitations. It is interesting to study these effects in other nuclei.

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