Variation after $K$-projection in antisymmetrized molecular dynamics for low-energy dipole excitations in $^{10}$Be and $^{16}$O

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A novel method of variation after $K$-projection is proposed to study dipole excitations in the framework of antisymmetrized molecular dynamics with the $\beta$-constraint. The method is applied to $^{10}$Be and $^{16}$O to describe low-energy dipole excitations. In the application to $^{10}$Be, two dipole states in the low-energy region are obtained. For $^{16}$O, the $1^{-}_1$ and $1^{-}_2$ states are obtained with remarkable dipole strength. The $1^{-}_1$ state is characterized by significant toroidal dipole (TD) strength and compressional dipole strength, whereas the $1^{-}_2$ state has significant TD strength and shows a developed $\alpha + ^{12}$C cluster structure. Dipole properties in $^{16}$O are discussed by analyzing the current densities of the dipole transitions.

1. Introduction

In recent nuclear excitation studies in stable and unstable nuclei, low-energy dipole (LED) strength, which is found in low-energy regions rather than in giant dipole resonances, has attracted experimental [1–3] and theoretical [4] attention. LED strength has been observed in some $N = Z$ nuclei [5–8], as well as in various neutron-rich nuclei, such as $^{18}$O [9,10], $^{20}$O [11], and $^{26}$Ne [12,13]. The properties and origins of LED excitations are often discussed in relation to the symmetry energy of nuclear matter [14–16], the neutron skin thickness in neutron-rich nuclei [17–21], and the neutron capture rate from astrophysical considerations [22–24]; however, they are yet to be clarified.

In theoretical studies of LED excitations, several different LED modes have been proposed. For example, the Pigmy mode in $N > Z$ nuclei, in which excess neutrons oscillate in an opposite direction to the core [25], contributes to the isovector dipole strengths [26–28]. Another mode type is the toroidal dipole (TD) mode, which is characterized by a vortical nature, as suggested by Ref. [29]. The TD mode can produce isoscalar dipole (ISD) strength and is expected to appear in neutron-rich and $N = Z$ nuclei. In recent years, the TD mode has been intensively studied by microscopic models [30–33]. Kvasil et al. introduced the TD operator to measure the toroidal feature, demonstrating that it is a sensitive probe for the TD mode [32]. However, experimental observation of the TD strength is yet to be confirmed. The third mode type is the cluster excitation mode. As pointed out by Chiba et al. [34], the ISD strength can be enhanced in the cluster excitation mode. In the low-energy spectra, these dipole modes do not necessarily appear as identical states but, instead, may mix with each other in the low-energy $1^{-}$ spectra.
In deformed nuclei, due to the coupling of the dipole modes with nuclear deformation, many interesting features of the LED excitations can be found. In a strong coupling regime, the dipole excitations can be classified by $K$ quantum number, indicating the $z$-component of the total angular momentum in a body-fixed frame. Nesterenko et al. investigated the LED excitations in deformed nuclei with a mean field approach [35–37], and showed that compressional dipole (CD) and TD modes appear as $K = 0$ and $K = 1$ states, respectively. The LED excitations in a deformed system of $^{10}$Be have also been discussed in our previous work [38], in which LED properties are discussed in terms of $K$ quantum number in the prolately deformed system.

Our future goal is to investigate LED excitations in various nuclei, including stable and unstable nuclei, with a microscopic framework to reveal their fundamental features and origins. Accordingly, it is essential to describe various LED modes, such as the Pigmy, TD, and cluster excitation modes, in general nuclei both with and without deformations.

In this paper, we propose a novel method of variation after $K$-projection to study LED excitations in the framework of antisymmetrized molecular dynamics (AMD) with the $\beta$-constraint. Using the AMD wave function, energy variation is performed after the parity- and $K$-projections under the quadrupole deformation constraint. AMD is a useful microscopic approach for the structural study of light nuclei, and can describe developed cluster structures, shell-model-like states, and their intermediate states [39–41]. To study deformed nuclei, AMD has been developed for the $\beta$-constraint and $\beta\gamma$-constraint versions, in which the quadrupole deformation parameters $\beta$ and $(\beta, \gamma)$ are constrained in the energy variation [42–44]. The latter approach is better than the former for the detailed description of deformations, specifically for axial-asymmetric structures; however, it is limited insofar as it requires an enormous number of basis wave functions in the two-dimensional space of the constraint parameters and is difficult to apply to heavy-mass nuclei. In the present study, we improve the $\beta$-constraint by performing the $K$-projection in the energy variation to efficiently obtain basis wave functions essential to LED excitations.

As a test case of light deformed nuclei, we apply the present method to $^{10}$Be, the structure of which has been investigated by many different models, such as the cluster model [45,46], molecular orbital model [47,48], and AMD [49,50], which show the $2\alpha + nn$ cluster structures of low-energy states. To show the applicability of the $K$-projection method, we compare the results of the $\beta$-constraint and $\beta\gamma$-constraint AMD methods both with and without $K$-projection, after which we apply the present method to study dipole excitations of $^{16}$O.

The article is organized as follows: Section 2 explains $K$-projection after variation in the AMD framework and also describes the generator coordinate method (GCM) and the expression of dipole operators. The interactions used in the present calculation are expressed in Sect. 3. Section 4 applies the present method to $^{10}$Be, while Section 5 investigates the LED excitations in $^{16}$O. Finally, the article is summarized in Sect. 6.

2. Formalism

To investigate the dipole excitations, we propose constrained AMD with variation after $K$-projection as well as with parity projection; i.e. energy variation is performed for the AMD wave function projected onto the parity and $z$-component of the angular momentum eigenstate under the quadrupole constraint ($\beta$ or $\beta\gamma$). After energy variation, AMD wave functions are superposed with GCM. The AMD framework has been described in detail in Refs. [39,43,51].
2.1. AMD

An AMD wave function is given by a Slater determinant as

\[ \Phi = \mathcal{A} [\psi_1 \psi_2 \cdots \psi_A], \]  

where \( \psi_i \) \((i = 1, 2, \ldots, A)\) denotes the \(i\)th single-particle wave function given by a localized Gaussian wave packet as

\[ \psi_i = \phi(Z_i) \chi(\xi_i) \tau_i, \]

\[ \phi(Z_i) = \left( \frac{2\nu}{\pi} \right)^{\frac{3}{4}} \exp \left[ -\nu \left( r - \frac{Z_i}{\sqrt{\nu}} \right)^2 \right], \]

\[ \chi(\xi_i) = \xi_i \uparrow | \uparrow \rangle + \xi_i \downarrow | \downarrow \rangle, \]

\[ \tau_i = p \text{ or } n, \]

where \( Z_i \) and \( \xi_i \) denote the Gaussian centroids and nucleon spin orientations, respectively, which are treated independently as variational parameters determined by the energy optimization. \( \nu \) denotes the width parameter, which is taken to be common for all nucleons.

In a simple version of AMD, the energy variation

\[ \delta \left( \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right) = 0 \]

is performed for the parity-projected AMD wave function \( | \Psi \rangle = \hat{P}_\pi | \Phi \rangle \) with the parity projection operator \( \hat{P}_\pi \).

2.2. Quadrupole constraint AMD

To perform \( K \)-projection, energy variation is performed under the constraint of the quadrupole deformation parameter \( \beta \) or \( \beta \gamma \). The deformation parameters \( \beta \) and \( \gamma \) can be defined as

\[ \beta \cos \gamma = \frac{\sqrt{5}}{3} \frac{2 \langle z^2 \rangle - \langle x^2 \rangle - \langle y^2 \rangle}{R^2}, \]

\[ \beta \sin \gamma = \frac{\sqrt{5}}{3} \frac{\langle x^2 \rangle - \langle y^2 \rangle}{R^2}, \]

\[ R^2 = \frac{5}{3} \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle, \]

where \( \langle r \rangle \) denotes the expectation value of the operator \( \hat{r} \) by the AMD wave function without projection.

In this paper we use two types of constraint AMD: \( \beta \gamma \)-constraint AMD (\( \beta \gamma \)-AMD) [44] and \( \beta \)-constraint AMD (\( \beta \)-AMD) [43]. For a given constraint value \( \beta_0 \) (or values \( \beta_0, \gamma_0 \)), the energy variation is conducted by imposing the constraint \( \beta = \beta_0 \) (\( \beta = \beta_0, \gamma = \gamma_0 \)). Here we keep the condition for the off-diagonal components of the moment of inertia, i.e. \( \langle xy \rangle = \langle yz \rangle = \langle zx \rangle = 0 \). After the energy variation for each parity \((\pi = \pm)\) state, the optimized AMD wave function with the given quadrupole deformation \( | \Phi^\pi (\beta_0) \rangle \) (\( | \Phi^\pi (\beta_0, \gamma_0) \rangle \)) is obtained.
Table 1. Summary list for the constraints and projections used in the present calculations with K-VAP and P-VAP: their acronyms of the methods, the constraints and projection operators imposed on the wave function $\Phi$ in the energy variation given in Eq. 6, the parity ($\pi$) and $K$ quantum number, and the AMD wave functions ($\phi$) obtained after the energy variation.

| Method                | Constraints | $|\psi\rangle$ | $\pi, K$ | $\Phi$ |
|-----------------------|-------------|----------------|-----------|--------|
| $\beta$-AMD with P-VAP | $\beta$     | $\hat{P}_\beta |\phi\rangle$ | $\pi = \pm$ | $\Phi^\pi (\beta)$ |
| $\beta$-AMD with K-VAP | $\beta$     | $\hat{P}_K \hat{P}_\beta |\phi\rangle$ | $K^\pi = 0^+, 0^-, 1^-$ | $\Phi^\pi_K (\beta)$ |
| $\beta \gamma$-AMD with P-VAP | $\beta, \gamma$ | $\hat{P}_\beta |\phi\rangle$ | $\pi = \pm$ | $\Phi^\pi (\beta, \gamma)$ |
| $\beta \gamma$-AMD with K-VAP | $\beta, \gamma$ | $\hat{P}_K \hat{P}_\beta |\phi\rangle$ | $K^\pi = 0^+, 0^-, 1^-$ | $\Phi^\pi_K (\beta, \gamma)$ |

2.3. K-projection variation after projection (VAP)

In the present method, the energy variation in Eq. (6) is performed for the $K$- and parity-projected AMD wave function $|\psi\rangle = \hat{P}_K \hat{P}_\beta |\phi\rangle$ instead of $|\psi\rangle = \hat{P}_\beta |\phi\rangle$ without the $K$ projection. Here, $\hat{P}_K$ denotes the $K$-projection operator, which can be given as

$$\hat{P}_K = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-iK\theta} \hat{R}(\theta),$$

(10)

where $\hat{R}(\theta)$ is the rotation operator around the principal axis in a body-fixed frame. We call the present method K-VAP and the conventional method P-VAP. As a result of K-VAP, the AMD wave function can be optimized for the given parity and $K$ quantum number. To describe the ground state wave functions of $^{10}$Be and $^{16}$O, the $K^\pi = 0^+$ projection is performed in K-VAP, and the resultant AMD wave function is called the $K^\pi = 0^+$ basis. For the dipole excitations (i.e. the $1^-$ excitation states), $K^\pi = 0^-$ and $K^\pi = 1^-$ projections are performed, and the obtained AMD wave functions are called $K^\pi = 0^-$ and $K^\pi = 1^-$ bases, respectively. The obtained AMD wave function of $\beta$-AMD ($\beta \gamma$-AMD) with K-VAP is denoted as $|\Phi^\pi_K (\beta)\rangle$ ($|\Phi^\pi_K (\beta, \gamma)\rangle$). In Table 1 we provide a summary list of the constraints and projections adopted in the present calculations with K-VAP and P-VAP.

2.4. GCM

To construct wave functions for the ground and $1^-$ states, GCM is applied for $\beta$-AMD with K-VAP with respect to the generator coordinate $\beta$, which is to say the basis wave functions are superposed as

$$\Psi^\pi (J_m) = \sum_{K, K'} \sum_{\beta} c_{KK'}(\beta) \hat{P}^J_{MK} \hat{P}^\pi_K |\Phi^\pi_K (\beta)\rangle,$$

(11)

where parity projection and total angular momentum projection $\hat{P}^J_{MK}$ are performed. It should be noted that, for the $1^-$ states, the $K = 0$ and $K = 1$ bases are adopted and the mixing of $K'$ components is taken into account. The coefficients $c_{KK'}(\beta)$ are determined by solving the Hill–Wheeler equation [52,53]. In a similar way, for comparison, the GCM calculation with the wave functions of P-VAP bases, $|\Phi^\pi (\beta_0)\rangle$, is performed. For the width parameter, we set $\nu = 0.235 \text{ fm}^{-2}$ for $^{10}$Be and $\nu = 0.19 \text{ fm}^{-2}$ for $^{16}$O, which are the same as in Refs. [38,54].
2.5. Dipole operator

To analyze the LED excitations, we use three dipole operators: $E_1$, CD, and TD [32], which can be defined as

$$\hat{M}_{E_1}(\mu) = \frac{N}{A} \sum_{i \in p} r_i Y_1(\hat{r}_i) - \frac{Z}{A} \sum_{i \in n} r_i Y_1(\hat{r}_i),$$  \hspace{1cm} (12)

$$\hat{M}_{CD}(\mu) = -\frac{1}{10\sqrt{2c}} \int dr \nabla \cdot j_{\text{nucl}}(r) r^3 Y_1(\hat{r}),$$  \hspace{1cm} (13)

$$\hat{M}_{TD}(\mu) = -\frac{1}{10\sqrt{2c}} \int dr (\hat{\nabla} \times j_{\text{nucl}}(r)) \cdot r^3 Y_{11}(\hat{r}),$$  \hspace{1cm} (14)

where $j_{\text{nucl}}$ denotes the convection nuclear current and $Y_{jL}(\hat{r})$ the vector spherical:

$$j_{\text{nucl}}(r) = -\frac{i}{\hbar} \frac{2m}{A} \sum_{k=1}^{A} \{\nabla_k \delta(r - r_k) + \delta(r - r_k) \nabla_k\},$$  \hspace{1cm} (15)

$$Y_{jL}(\hat{r}) = \sum_{\alpha, \beta} \langle L\alpha, 1\beta | j_{\mu} \rangle Y_L(\hat{r}) e_\beta.$$  \hspace{1cm} (16)

The transition strength of the dipole operator $\hat{M}_D$ for the $0^+_1 \rightarrow 1^-_k$ transition is given as

$$B(D; 0^+_1 \rightarrow 1^-_k) = |\langle 1^-_k | \hat{M}_D | 0^+_1 \rangle|^2.$$  \hspace{1cm} (17)

The TD and CD operators are isoscalar-type rank-one operators. The former probes the nuclear vorticity, as discussed in Ref. [36], whereas the latter probes the compressional mode and corresponds to the ordinary ISD operator

$$\hat{M}_{ISD}(\mu) = \int dr \rho(r) r^3 Y_1(\hat{r})$$  \hspace{1cm} (18)

with the relation

$$B(CD; 0^+_1 \rightarrow 1^-_k) = \left(\frac{1}{10 \hbar c} \frac{E_k}{E_1} \right)^2 B(ISD; 0^+_1 \rightarrow 1^-_k),$$  \hspace{1cm} (19)

where $E_k$ is the excitation energy of the $1^-_k$ state.

3. Effective interaction

The Hamiltonian of the total system is given as

$$H = \sum_i t_i - T_G + \sum_{i<j} v^{\text{Coulomb}}_{ij} + V_{\text{eff}},$$  \hspace{1cm} (20)

where $t_i$ and $T_G$ denote the kinetic energy of the $i$th nucleon and the center of mass motion, respectively; $v^{\text{Coulomb}}_{ij}$ denotes the two-body Coulomb potential, which is approximated by a seven-range Gaussian form; and $V_{\text{eff}}$ denotes the effective nuclear interaction of the central and spin–orbit forces. We use the same effective interactions as Refs. [38,55] for $^{10}$Be, and those from Refs. [54,56] for $^{16}$O. That is, for $^{10}$Be, we use the Volkov No.2 force [57] with $W = 1 - M = 0.4$ and $B = H = 0.125$ for the central force and G3RS spin–orbit force [58,59] with $u_1 = -u_2 = -1600$ MeV. This parameter set describes well the energy spectra of $^{10}$Be. For $^{16}$O, we use the MV1 central force with the case-1
parametrization of $W = 1 - M = 0.38$ and $B = H = 0$, and the G3RS spin–orbit force with $u_1 = -u_2 = -3000$ MeV, which describes the energy spectra of $^{12}\text{C}$ with AMD [60]. The Volkov central force is a finite-range two-body interaction, which describes the $\alpha-\alpha$ scattering phase shifts; it is often used for light nuclei and has an over-binding problem when applied to heavy-mass nuclei. The MV1 central force consists of finite-range two-body and zero-range three-body terms and can systematically reproduce the binding energies of $\alpha$, $^{12}\text{C}$, and $^{16}\text{O}$ [56] without the over-binding problem.

4. Application to $^{10}\text{Be}$

In this section we apply the present method (i.e. $\beta$-AMD with K-VAP) to $^{10}\text{Be}$. We also apply $\beta\gamma$-AMD with P-VAP and K-VAP for comparison, and discuss how the new method works for dipole excitations.

4.1. Energy surfaces and spectra

For detailed analysis, we discuss the energy surfaces on the $\beta-\gamma$ plane obtained by $\beta\gamma$-AMD with K-VAP and P-VAP. In Fig. 1, the calculated energy surfaces are shown. In particular, Figs. 1(a) and (b) show the P-VAP results for the positive- and negative-parity projections, respectively, and Figs. 1(c), (d), and (e) show the K-VAP result with $K_\pi = 0^+$, $K_\pi = 0^-$, and $K_\pi = 1^-$, respectively. The K-VAP energy surfaces show a broad flat region around the energy minimum area. It should be noted that an energy minimum area is located at $\gamma \sim 0$ in the P-VAP energy surfaces, corresponding to a prolate minimum, but extends (or shifts) towards a triaxial deformation area ($\gamma \sim 30^\circ$) in the $K_\pi = 0^+$ and $K_\pi = 0^-$ energy surfaces (Figs. 1(c) and (d)). This indicates that the axial symmetric deformation is favored before $K$-projection, whereas triaxial deformation is favored after $K$-projection.

The solid lines with filled circles represent the $\gamma$-optimized paths for bases of $\beta$-AMD, where $\gamma$ is optimized for each $\beta$ value. In the case of P-VAP, the path moves along the $\gamma = 0$ line, meaning that $\beta$-AMD with P-VAP gives approximately axial-symmetric states. Alternatively, in the K-VAP result, the path goes through a $\gamma \neq 0$ area in the energy valley, meaning that triaxially deformed
configurations can be obtained by K-VAP with \( \beta \)-AMD. As shown later, these triaxial configurations are essential to describe the \( K^\pi = 0^- \) dipole mode.

We perform the GCM calculation for \( \beta^\gamma \)-AMD (\( \beta \)-AMD) with P-VAP and K-VAP by superposing the obtained basis wave functions to obtain the energy spectra as well as the final wave functions of \(^{10}\)Be. The calculated energy spectra are compared with the experimental spectra for corresponding states in Fig. 2. In the K-VAP result, energies are globally lower by a few MeV compared with the P-VAP result for all states, meaning that further energy optimization is achieved by \( K \)-projection. For dipole states, two \( 1^- \) states (\( 1^-_1, 2 \)) are obtained in both the \( \beta^\gamma \)-AMD and \( \beta \)-AMD calculations with K-VAP. However, for P-VAP, the \( 1^-_2 \) state is obtained by \( \beta^\gamma \)-AMD and not by \( \beta \)-AMD, because the latter calculation (\( \beta \)-AMD with P-VAP) does not contain triaxially deformed bases, as shown in the \( \gamma \)-optimized path in Fig. 1(b).

### 4.2. Properties of dipole excitations

In this subsection we discuss the properties of dipole excitations based on the results of \( \beta \)-AMD with K-VAP. The excitation energies and dipole transition strengths for the \( E1, CD, \) and \( TD \) operators are shown in Table 2. The intrinsic densities of the basis wave functions obtained by \( \beta \)-AMD with K-VAP and P-VAP are shown in Figs. 3 and 4, respectively. In the K-VAP result, the \( 0^+_1 \) state has the largest overlap with the configuration at \( (\beta, \gamma) = (0.60, 4.6^\circ) \) in Fig. 3(a), whereas the \( 1^-_1 \) state dominantly contains the \( K = 1 \) component of the intrinsic state at \( (\beta, \gamma) = (0.72, 1.7^\circ) \) in Fig. 3(f). In addition, they show approximately axial-symmetric shapes \( (\gamma \sim 0) \) with an \( \alpha + ^6\)He-like structure. In these states, two clusters are close to each other and not well developed. The \( 1^-_1 \) state has a strong TD transition and can be regarded as the \( K = 1 \) excitation built on the compact \( \alpha + ^6\)He state. This remarkable TD strength is caused by vortical current in the transition current density and it is considered that the excitation mode to the \( 1^-_1 \) state is the vortical mode consistent with that discussed in Refs. [38,61]. For the \( 0^+_1 \) and \( 1^-_1 \) states, the P-VAP result has similar features to the K-VAP result in the TD transition but differs from the K-VAP result with respect to CD strength. In other words, the K-VAP calculation has a CD strength for the \( 1^-_1 \) state that is three times larger than that of the P-VAP calculation because of the significant mixing of the \( K = 0 \) component of the triaxially
Table 2. The excitation energies and transition strengths in $^{10}$Be obtained by $\beta$-AMD with P-V AP and K-V AP, as well as experimental data [62].

|        | $E_x$ [MeV] | $B$(TD) [fm$^4$] | $B$(CD) [fm$^4$] | $B$(E1) [fm$^4$] |
|--------|-------------|------------------|------------------|------------------|
| P-V AP |             |                  |                  |                  |
| $I_1^+$| 9.05        | $2.66 \times 10^{-3}$ | $6.79 \times 10^{-5}$ | $6.42 \times 10^{-3}$ |
| $I_2^+$| —           | —                | —                | —                |
| K-V AP |             |                  |                  |                  |
| $I_1^+$| 7.96        | $2.39 \times 10^{-3}$ | $2.39 \times 10^{-4}$ | $6.92 \times 10^{-3}$ |
| $I_2^+$| 14.9        | $2.59 \times 10^{-4}$ | $2.89 \times 10^{-4}$ | $2.47 \times 10^{-1}$ |
| Exp.   |             |                  |                  |                  |
| $I_1^+$| 5.96        | —                | —                | $2.72 \times 10^{-6}$ |
| $I_2^+$| —           | —                | —                | —                |

Fig. 3. Intrinsic densities of $^{10}$Be at given $\beta$ values obtained by $\beta$-AMD with K-V AP. The top, middle, and bottom panels show the densities of the $K^\pi = 0^+, 0^-, 1^-$ bases, respectively.

deformed configurations (see Fig. 3(c)). For the $E1$ transition, the calculated $0_1^+ \rightarrow 1_1^-$ transition is weak and qualitatively consistent with the experimental data, but quantitatively overestimates the observed value of $B(E1 : 0_1^+ \rightarrow 1_1^-)$ by a few orders of magnitude.
Fig. 4. Intrinsic densities of $^{10}\text{Be}$ at given $\beta$ values obtained by $\beta$-AMD with P-V AP. The optimized values of $\gamma$ for each $\beta$ are written in the panels. Panels (a) and (b) show the densities of the positive-parity bases, and panels (c) and (d) show those of the negative-parity bases.

The $1^-_2$ state is dominantly formed by the $K = 0$ component of the triaxially deformed configurations obtained by $\beta$-AMD with K-V AP for $K^\pi = 0^-$. It has dominant overlap ($\sim 70\%$) with the basis wave function at $(\beta, \gamma) = (0.84, 5.5^\circ)$ with a remarkably developed $\alpha + ^6\text{He}$ cluster structure, as shown in Fig. 3(d). In addition, it has significant overlap ($\sim 52\%$) with the base at $(\beta, \gamma) = (0.48, 29^\circ)$ in Fig. 3(c). In these configurations, the $^6\text{He}$ cluster is deformed in a tilted or perpendicular orientation from the $Z$-axis, thereby contributing the triaxiality of the whole system. The $K = 0$ component projected from these triaxial configurations plays a crucial role in generating the $1^-_2$ state.

In the transition properties, remarkable $E1$ strength is obtained for the $1^-_2$ state: the energy-weighted strength ($EB(E1 : 0^+_1 \rightarrow 1^-_2)$) accounts for about 10% of the TRK sum rule. Moreover, it also has significant CD transition strength due to the $K = 0$ component of the developed $\alpha + ^6\text{He}$ cluster structure. Furthermore, due to the mixing of the large triaxial configuration in Fig. 3(c), the CD strength and $E1$ strength are enhanced because the excitation from the ground state to the aforementioned triaxial configurations involves the spatial expansion of excess neutron distribution in $^6\text{He}$, which induces the $E1$ and CD strengths as described in Ref. [38].

For $^{10}\text{Be}$, $\beta$-AMD with K-V AP can efficiently generate important bases for the LED excitations ($1^-_1$ and $1^-_2$ states) and, moreover, obtains equivalent results to $\beta\gamma$-AMD. In particular, the K-VAP treatment can obtain triaxial configurations within $\beta$-AMD, which are essential for the $1^-_2$ state ($K = 0$ mode). This is an advantage over $\beta\gamma$-AMD since it reduces computational costs, and it is also superior to the standard $\beta$-AMD with the P-VAP framework, which favors axial-symmetric configurations rather than axial-asymmetric ones.
5. Results for $^{16}\text{O}$

In this section we apply $\beta$-AMD with K-V AP to $^{16}\text{O}$ and present the results obtained for LED excitations.

5.1. Energy surfaces and intrinsic structures

$K$-projected energy curves obtained by $\beta$-AMD with K-V AP are shown in Fig. 5 compared with the P-V AP result. Figures 5(a), (b), and (c) show the $K^\pi = 0^+, 0^-$, and $1^-$ projected energy surfaces, respectively. In all cases, the energy minimum corresponds to the normal deformation (ND) around $\beta = 0.2–0.4$, indicating a relatively smaller deformation in $^{16}\text{O}$ than in $^{10}\text{Be}$. In the negative-parity results, the energy difference between the $K^\pi = 0$ and $K^\pi = 1$ bases is a few MeV at the energy minimum but gets larger as $\beta$ increases: the energy curve for the $K^\pi = 0^-(K^\pi = 1^-)$ bases is soft (steep) against $\beta$.

Figure 6 shows the intrinsic densities of the K-V AP bases. For all cases of $K^\pi = 0^+, 0^-$, and $1^-$, an $\alpha$ cluster is formed at the surface of a $^{12}\text{C}$ core in the ND region, which develops as $\beta$ increases. The $K^\pi = 0^+$ bases around the energy minimum at $\beta \sim 0.4$ have a tetrahedral-like structure, as shown in Fig. 6(a), which contributes to the ground state obtained by the GCM calculation. In the large-$\beta$ region, the $K^\pi = 0^+$ bases show a developed $^{12}\text{C} + \alpha$ cluster structure (see Fig. 6(b)), which dominantly contributes to the $0^+_2$ state. In the $K^\pi = 0^-$ and $K^\pi = 1^-$ bases, the intrinsic configurations at $\beta \sim 0.4$ (ND region) are similar to each other, as shown in Figs. 6(c) and (e). These two bases have large overlaps with the $1^-_1$ state obtained by the GCM calculation. At large $\beta$ values, the $K^\pi = 0^-$ and $K^\pi = 1^-$ bases have developed $^{12}\text{C} + \alpha$ cluster configurations, where the $^{12}\text{C}$ cluster is deformed with tilted orientation against the $Z$-axis, as shown in Figs. 6(d) and (f). Consequently, the total system is axial asymmetric. The $K^\pi = 0^-$ bases with this axial-asymmetric cluster structure play an important role in constructing the $1^-_2$ state, which will be discussed later.

5.2. GCM results and LED strengths

The energy spectra obtained by the GCM calculation with K-V AP bases are shown in Fig. 7 compared with the experimental data. In Fig. 8, the GCM amplitudes, which are given by the squared overlaps of the GCM states with K-V AP bases, are shown as functions of $\beta$. In Fig. 8(a), the GCM amplitudes...
Fig. 6. Intrinsic densities of $^{16}$O at given $\beta$ values obtained by $\beta$-AMD with K-VAP. The top, middle, and bottom panels show the densities of the $K^\pi=0^+$, $0^-$, and $1^-$ bases, respectively.

Fig. 7. Energy spectra of $^{16}$O obtained by the GCM calculation of $\beta$-AMD with P-VAP and K-VAP bases. The experimental energy spectra of the corresponding states are shown for comparison.

for the $0^+_1$ and $0^+_2$ states are shown by square and circle points, respectively. In Figs. 8(b) and (c), the GCM amplitudes for the $1^-_1$ and $1^-_2$ states are shown, respectively, with square (circle) points for $K^\pi=0^-$ ($1^-$) bases.

The calculated binding energy of the ground state is 120.3 MeV, which slightly underestimates the experimental value of 127.6 MeV. The ground state has the largest GCM amplitude as $\sim$90% with the base at $\beta=0.4$, as shown in Fig. 6(a). The lowest $1^-$ state at the excitation energy 9.8 MeV largely contains the $K^\pi=0^-$ and $K^\pi=1^-$ components in the $\beta\sim0.4$ (ND) region (see Fig. 8(b)). The $0^+_2$ state at 10.55 MeV and the $1^-_2$ state at 12.47 MeV are constructed from the $K^\pi=0^+$ and $K^\pi=0^-$ bases with the developed $\alpha+^{12}$C cluster structure, respectively, as can be seen in their
Fig. 8. GCM amplitudes as functions of β for the K-V AP results of 16O. In panel (a), the GCM amplitudes for the 0⁺ and 0⁺ states are plotted with square and circle points, respectively. Panels (b) and (c) show the amplitude for the 1−1 and 1−2 states, respectively. The K = 0 component of the GCM amplitude for the Kπ = 0− basis and the K = 1 component of the GCM amplitude for the Kπ = 1− basis are denoted by square and circle points, respectively.

Table 3. The excitation energies and the TD and CD transition strengths in 16O. The EWS ratio fISD for the ISD transition is also shown. The EWS for the ISD operator is calculated as EWS(ISD) = \( \frac{3}{8} \pi^2 m A \left( \frac{1}{11} \langle r^4 \rangle - \frac{25}{3} \langle r^2 \rangle^2 - 10 \epsilon \langle r^2 \rangle \right) \), where \( \epsilon = \frac{\hbar^2}{3mA} \left( \frac{4}{E_{ISGQR}} + \frac{5}{E_{ISGMR}} \right) \) with \( E_{ISGQR} = 65.4^{-1/3} \text{MeV} \) and \( E_{ISGMR} = 80.4^{-1/3} \text{MeV} \), as given in Ref. [5]. Experimental data are taken from Refs. [5,63].

|       | E [MeV] | B(TD) [fm^4] | B(CD) [fm^4] | fISD [%] |
|-------|---------|--------------|--------------|---------|
| P-VAP | 1⁻      | 9.88         | 2.93 × 10⁻³  | 3.49 × 10⁻³ | 5.30    |
|       | 1₂      | 13.20        | 3.98 × 10⁻³  | 1.65 × 10⁻⁵ | 0.108   |
| K-VAP | 1⁻      | 9.78         | 3.62 × 10⁻³  | 2.87 × 10⁻³ | 3.96    |
|       | 1₂      | 12.47        | 3.80 × 10⁻³  | 9.35 × 10⁻⁵ | 0.0713  |
| Exp.  | 1⁻      | 7.12         | —            | —        | 4.2     |
|       | 1₂      | 9.59         | —            | —        | —       |

large GCM amplitudes in the 0.6 ≲ β ≲ 0.8 region (see Figs. 8(a) and (c)). This result is consistent with the cluster model assignment of the 0⁺ and 1− states as the band-head states of the parity doublet (Kπ = 0⁺ and Kπ = 0−) \( \alpha + \text{^{12}C} \) cluster bands.

The calculated dipole transition strengths and the ratio of the energy-weighted sum (EWS) for the ISD transition as well as experimental data [5,63] are shown in Table 3. The present calculation obtains significant TD and CD strengths for the 1⁻ state, which is qualitatively consistent with the previous AMD result obtained by variation after spin-parity projections [56]. The TD strength is also shared by the 1− state due to the mixing of the TD mode and the \( \alpha + \text{^{12}C} \) cluster mode. More details of the two dipole modes are discussed later. The calculated EWS ratio fISD = 3.96% for the ISD transition to the 1⁻ state reproduces the observed value fISD = 4.2%. The E1 transitions for the low-lying 1⁻ states are essentially unobtainable for \( N = Z \) nuclei due to the charge symmetry. Although nonzero contributions come from slight symmetry breaking, the precise evaluation of such tiny components is beyond the present model, in which the isospin projection and T-mixing are not taken into account.

5.3. Comparison between K-VAP and P-VAP methods

For comparison, we perform β-AMD with P-VAP for 16O and compare the results with the present K-VAP method. The K-projected energy curves obtained from the P-VAP bases are shown in Fig. 5 by the square points, and the intrinsic densities of the P-VAP bases are shown in Fig. 9. Generally,
We analyze the dipole modes and discuss the origins of significant dipole strength for the present K-VAP method for $^{16}$O. We define the “intrinsic state” of each GCM state as the specific base state with the largest GCM amplitude. Since the energy optimization does not work for such minor components, the P-V AP method for the negative-parity projection fails to obtain a smooth curve with respect to the $K^\pi = 1^-$ projected energy, as shown in Fig. 5(c). This is a general trend of the P-V AP method, which favors an axial-symmetric configuration (i.e. the $K = 0$ dominant bases), as seen in the intrinsic densities of Fig. 9.

In the GCM energies of the $^{16}$O states obtained by superposing K-VAP or P-V AP bases, the GCM states obtained by the K-VAP bases gain 1–2 MeV of energy compared with the P-V AP result. In particular, the binding energy of the K-VAP result is 1.4 MeV larger than the P-V AP result. Further energy gains are obtained for the $^{12}$C $+ \alpha$ ($K^\pi = 0^-$) cluster band due to the rotational degree of freedom of the deformed $^{12}$C cluster in the K-VAP bases. The properties of dipole excitations are compared with the P-V AP and K-V AP results in Table 3, from which it is evident that the two methods provide qualitatively similar results for the excitation energies as well as the TD and CD transition strengths of the $1^+_{11}$ and $1^+_{12}$ states, meaning that, for $^{16}$O, the essential bases for LED states can be obtained by the P-V AP method, even though the K-VAP method results in extra energy gains due to the higher-order effects.

### 5.4. Excitation modes and origin of strengths

We analyze the dipole modes and discuss the origins of significant dipole strength for the present K-VAP method for $^{16}$O. We define the “intrinsic state” of each GCM state as the specific base state with the largest GCM amplitude. For the $0^+_1$ state, the intrinsic state is defined as the $K^\pi = 0^+$ base at $\beta = 0.4$, as shown in Fig. 6(a). In the $1^-_1$ state, the $K^\pi = 0^-$ and $K^\pi = 1^-$ bases at the $\beta \sim 0.4$ (ND) region are strongly mixed, and both have large GCM amplitudes, and therefore two choices of the intrinsic states are possible: $K^\pi = 0^-$ base at $\beta = 0.40$, as shown in Fig. 6(c), and $K^\pi = 1^-$ base at $\beta = 0.32$, as shown in Fig. 6(e). We call these intrinsic states $0^+_1$ $^{12}$C $\alpha$ ($K = 0$), and $1^-_{ND}$ ($K = 1$). The $1^-_2$ state mainly contains $K^\pi = 0^-$ components with the developed $\alpha + ^{12}$C structure. Therefore, as the intrinsic state of the $1^-_2$ state, we choose the $K^\pi = 0^-$ base at $\beta = 0.92$ (Fig. 6(f)), which we label as $1^-_{cl}$.

To clarify the dipole excitation modes, we calculate the transition current densities $\mathbf{j}^{K}(\mathbf{r})$ and local matrix elements of the CD and TD operators $M^D(r)$ ($D = CD$ or TD) for the transitions between $K$-projected states in the intrinsic frame. These are defined as

$$
\mathbf{j}^K(\mathbf{r}) \equiv \langle \mathbf{j}^K \mathbf{j}_{\text{nucl}}(\mathbf{r}) | i \rangle, 
$$

(21)
\[ \mathcal{M}_{\text{TD}}^{K=0}(r) = \frac{1}{c} \left[ (2X^2 + 2Y^2 + Z^2)J_Z^{K=0} - ZY_J^{K=0} - YZ_J^{K=0} \right], \]  
(22)

\[ \mathcal{M}_{\text{TD}}^{K=1}(r) = \frac{1}{c} \left[ (X^2 + 2Y^2 + 2Z^2)J_Z^{K=1} - XY_J^{K=1} - ZY_J^{K=1} \right], \]  
(23)

\[ \mathcal{M}_{\text{CD}}^{K=0}(r) = \frac{1}{c} \left[ -(X^2 + Y^2 + 2Z^2)J_Z^{K=0} - 2ZY_J^{K=0} - YZ_J^{K=0} \right], \]  
(24)

\[ \mathcal{M}_{\text{CD}}^{K=1}(r) = \frac{1}{c} \left[ -(3X^2 + Y^2 + 2Z^2)J_Z^{K=1} - 2XY_J^{K=1} - 2XZ_J^{K=1} \right], \]  
(25)

where the initial state \( |i\rangle \) is taken as \( \hat{P}_{K=0}|0^+_{gs}\rangle \), and the final state \( |f^K\rangle \) is \( \hat{P}_K |f\rangle \) with \( |f\rangle = |1_{\text{ND}}(K = 0)\rangle \), \( |1_{\text{ND}}(K = 1)\rangle \), or \( |1_{\text{cl}}\rangle \), and \( \mathcal{M}_{\text{TD(CD)}}^{K} \) is the local matrix element at \( r \) corresponding to the integrand of the TD (CD) strength, which is called the “TD (CD) strength density” in the present paper. Here, we specify the \( \mu \) component of the dipole operator in the TD strength \( Y_{1\mu=0} \) with the label \( K = 0 \) and \(- (Y_{1\mu=1} - Y_{1\mu=-1})/\sqrt{2} \) with \( K = 1 \), and, moreover, specify the \( \mu \) component of the dipole operator in the CD strength \( Y_{1\mu=0} \) with the label \( K = 0 \) and \(- (Y_{1\mu=1} - Y_{1\mu=-1})/\sqrt{2} \) with \( K = 1 \).

The calculated transition current densities for the \( 0^+_{gs} \rightarrow 1_{\text{ND}}(K = 0) \) and \( 0^+_{gs} \rightarrow 1_{\text{ND}}(K = 1) \) transitions are shown in Fig. 10, from which it is evident that, in the vector plot of \( r \), two dipole modes are present, characterized by the \( K \) quantum number: the \( K = 0 \) oscillation mode and the \( K = 1 \) vortical mode. The former shows the translational current along the \( Z \)-direction (see Fig. 10(a)) caused by the \( \alpha \) cluster oscillation relative to the \( ^{12}\text{C}(3\alpha) \) core, which is a \( K^\pi = 0^- \) excitation of the relative motion between two asymmetric clusters. The latter shows the remarkable vortical current (see Fig. 10(b)) arising from the tilted \( ^{12}\text{C} \) configuration in Fig. 6(c). It should be noted that, in the \( J^\pi = 1^- \) projected states, the two dipole modes of the \( K = 0 \) and \( K = 1 \) components overlap each other and are significantly contained in the \( 1_{\text{ND}}^- \) state, meaning that the \( 1_{\text{ND}}^- \) state has the dual nature of dipole excitations characterized by the \( K \) quantum number.

To discuss the contributions of these two dipole modes to the TD and CD transition strengths, we show in Fig. 11 the strength densities in the \( Z-X \) plane at \( Y = 0 \), \( \mathcal{M}_{\text{TD}}^{K}(X, 0, Z) \) and \( \mathcal{M}_{\text{CD}}^{K}(X, 0, Z) \), defined by Eqs. (22)–(25). The upper and lower panels of Fig. 11 show the calculated results of the TD and CD strengths, respectively, for the transitions from the \( 0^+_{gs} \) to the three \( 1^- \) states: \( 1_{\text{ND}}(K = 0) \), \( 1_{\text{ND}}^- (K = 1) \), and \( 1_{\text{cl}}^- \). The \( K = 0 \) oscillation (i.e. the \( \alpha \) cluster oscillation) generates strong

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**Fig. 10.** The transition current densities for the \( K \)-projected intrinsic states of \(^{16}\text{O} \). Panels (a) and (b) show the transition currents to \( 1_{\text{ND}}(K = 0) \) and \( 1_{\text{ND}}(K = 1) \), respectively. The densities are plotted on the \( Z-X \) plane.
CD strength density, as seen in Fig. 11(b), whereas the $K = 1$ vortical current contributes to the TD strength density, as can be seen in Fig. 11(c). Compared with the $0^+_\text{gs} \rightarrow 1^-_{\text{ND}}(K = 0)$ and $0^+_\text{gs} \rightarrow 1^-_{\text{ND}}(K = 1)$ transitions, the strength densities $M^K_D(r)$ are very weak in the $1^-_{\text{cl}}$ excitation (see Figs. 11(e) and (f)) because of the small overlap between the initial and final states, i.e. the compact ground state and the developed cluster state.

In the present analysis of the dominant intrinsic configurations, the pure $K^\pi = 0^-$ cluster excitation does not generate strong TD and CD strengths. The $K^\pi = 0^-$ cluster component is the main component of the $1^-_1$ state. Nevertheless, the $1^-_1$ state has significant TD strength in the GCM result, because it is not a pure $K^\pi = 0^-$ cluster state but, rather, contains significant mixing ($\sim 30\%$) of the $K = 1$ component at the $\beta \sim 0.4$ (ND) region. In other words, the TD strength of the $1^-_1$ state can be attributed to the mixing of the $K^\pi = 1^-$ vortical mode in the dominant $K^\pi = 0^-$ cluster mode.

The TD strength of the $1^-_2$ state is sensitive to the mixing ratio of the $K = 1$ configuration. To examine this sensitivity, we artificially vary the mixing ratio by changing the strength $V_{LS}$ of the spin–orbit force to $V_{LS}' = \lambda V_{LS}$. We perform the GCM calculation with $\lambda = 0.8$ and 0.9 for 80% and 90% weaker spin–orbit strengths. As $\lambda$ decreases, the energy interval between the $1^-_1$ and $1^-_2$ states increases and mixing reduces. As a result, the TD strength is concentrated on the $1^-_1$ state. For instance, for $\lambda = 0.8$, the TD strengths are $B(\text{TD}; 0^+_1 \rightarrow 1^-_1) = 8.30 \times 10^{-3}$ fm$^4$ and $B(\text{TD}; 0^+_1 \rightarrow 1^-_2) = 1.41 \times 10^{-3}$ fm$^4$. For the original strength ($\lambda = 1.0$), the result of $B(\text{TD}; 0^+_1 \rightarrow 1^-_1) = 3.62 \times 10^{-3}$ fm$^4$ and $B(\text{TD}; 0^+_1 \rightarrow 1^-_2) = 3.80 \times 10^{-3}$ fm$^4$ is a transient situation of the level crossing between the lower $K^\pi = 1^-$ vortical mode and the higher $K^\pi = 0^-$ cluster mode, where the TD strength from the $K^\pi = 1^-$ vortical mode is fragmented into the $1^-_1$ and $1^-_2$ states. Since model ambiguity remains in the effective interaction between parameters, we cannot obtain a conclusion for the mixing ratio. Accordingly, to understand the detailed properties of LED excitations in $^{16}\text{O}$, further experimental information is required.
6. Summary

We proposed a new method, $\beta$-AMD with K-VAP, in which variation is performed after $K$- and parity-projection under the $\beta$-constraint, which was applied to the LED excitations of $^{10}$Be and $^{16}$O.

For $^{10}$Be, the present method obtained essential configurations for LED excitations, which are more accurate than those obtained by the standard $\beta$-AMD with P-VAP (without $K$-projection). In particular, $\beta$-AMD with K-VAP can describe triaxially deformed configurations, whereas $\beta$-AMD with P-VAP only favors axial-symmetric ($\gamma \sim 0$) configurations. In the GCM calculation, $\beta$-AMD with K-VAP obtained results that are equivalent to the GCM results with respect to full $\beta\gamma$-AMD configurations for the 1$^-_1$ and 1$^-_2$ states. This suggests that $\beta$-AMD with K-VAP is a useful and numerically cost-effective approach for describing LED excitations.

For $^{16}$O, the present method obtained two LED states: 1$^-_1$ and 1$^-_2$. The ground and the 1$^-_1$ states are dominated by small deformation bases, whereas the 1$^-_1$ state has significant TD and CD transition strengths. Alternatively, the 1$^-_2$ state is mainly composed of bases with developed $\alpha + ^{12}$C cluster structures and is regarded as the band-head state of the $K^\pi = 0^-$ cluster band. In addition, by analyzing the strengths and current densities of the TD and CD dipole transitions, we discussed the dipole excitation properties and showed that the $K = 0$ and $K = 1$ natures play an important role. In particular, the 1$^-_1$ state has the duality of the $K = 0$ and $K = 1$ modes: the $K = 0$ oscillation mode is described by the relative motion between asymmetric clusters, whereas the $K = 1$ vortical mode is generated by the tilted configuration of the deformed $^{12}$C cluster. The 1$^-_2$ state is dominantly described by the $K = 0$ dipole motion of the $\alpha$ cluster relative to the $^{12}$C cluster.

Overall, the results suggest that the present method is a useful tool in studying LED in light nuclei.

In future studies, we will apply this method to the $Z \neq N$ nuclei in the sd-shell region, such as $^{18}$O and $^{20}$O. In addition, the experimental signal of the TD mode requires further study. For instance, the transverse-charge form factors would provide useful experimental information as a sensitive probe for the TD transition strengths, as pointed out by Nesterenko et al. [64].

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