Structure of Excited States of $^{10}$Be studied with Antisymmetrized Molecular Dynamics

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We study structure of excited states of $^{10}$Be with the method of variation after spin parity projection in the frame work of antisymmetrized molecular dynamics. Present calculations describe many excited states and reproduce the experimental data of $E2$ and $E1$ transitions and the new data of the $\beta$ transition strength successfully. We make systematic discussions on the molecule-like structures of light unstable nuclei and the important role of the valence neutrons based on the results obtained with the framework which is free from such model assumptions as the existence of inert cores and clusters.

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I. INTRODUCTION

Owing to the radioactive nuclear beams, the data of unstable nuclei are increasing rapidly. Recently the structure of excited states as well as the ground states are very attractive in the study of unstable nuclei. In the light nuclear region, one of the hot and important subjects has been the clustering features. The clustering structures of the ground states are already well known to be developed in some light ordinary nuclei such as $^7$Li, $^8$Be and $^{20}$Ne. In the studies of the light unstable nuclei $^{11}$Be and $^{12}$C the clustering structures were predicted also in the very neutron-rich nuclei. It is natural that various molecule-like states may appear in the excited states of light unstable nuclei because the excitation due to relative motion between clusters is important in the light nuclear region. The clustering structure must be one of the important aspects to understand the exotic features of the unstable nuclei. However there remain many mysterious problems of clustering development and the role of valence nucleons in the unstable nuclei. Our aim is to make systematic study of structure change with the increase of the excitation energy. We are to find new features of unstable nuclei such as exotic shapes and molecule-like structures in the excited states and to understand the mechanism of the various structures.

$^{10}$Be, one of the challenges in the study of light unstable nuclei, were and are studied hard theoretically. Recent experiments of the charge exchange reactions $^{10}$B(3He,t)$^{10}$Be let us know the strength of the Gamow-Teller transitions to the excited states of $^{10}$Be. These new data of $\beta$ transition strength which are deduced from the cross sections at the forward angle are very helpful to study the structure of the excited states.

In the theoretical researches on the structure of the ground states of Be isotopes such as the reference [2], it was found that the developed $2\pi$ clustering structure in $^{8}$Be weakens in the $^{10}$Be because of the excess two neutrons. As for the excited states of $^{10}$Be, the previous calculations [13] with a simplest version (variation after parity projection) of antisymmetrized molecular dynamics (AMD) predicted that the largely deformed states with the $2\alpha+2n$ clustering structure construct a rotational band $K=1^+$ in low energy region which is supported by the experimental energy levels.

The problem of the abnormal spin parity $1/2^+$ in the ground state of $^{11}$Be is considered to have a close relation with the deformed non-normal parity states of $^{10}$Be. In the simple shell model consideration the normal parity of $^{11}$Be is negative because of the valence neutron in the $p_{1/2}$ shell, however, the ground states is known to be $J^\pi = 1/2^+$. It is suggested that one of the reasons for the parity inversion in $^{11}$Be is the energy gain of the $sd_{1/2}$ mixing orbit in the prolate deformed system due to the developed clustering. The $sd_{1/2}$ orbit of neutrons in neutron-rich Be isotopes is interesting and essential to understand the structure of light neutron-rich nuclei and is easily connected with the deformed structure of the non-normal parity states of $^{10}$Be. Furthermore it is natural that the negative parity band due to the deformed states of $^{10}$Be makes us imagine a corresponding positive parity band constructed by the analogous deformed intrinsic state where the neutrons in the $sd_{1/2}$ orbit play important roles.

Recently W. Von Oertzen proposed a dimer model [8] to describe the excited states of Be and B isotopes systematically. In his idea he supposed $2\alpha$ clusters and surrounding nucleons in molecular orbits like $\sigma$ and $\pi$ bonds as the orbits of electrons in the molecule. The neutron-rich Be nuclei can be written by $2\alpha$ and neutrons which occupy the
molecule-like $\sigma$ and $\pi$ orbits. This idea is helpful to understand the level structure of many excited states of $^9$Be and $^{10}$Be and to study the mechanism of the deformation of Be isotopes.

A. Doté et al. studied Be isotopes by microscopic calculations with the simplest version of AMD under a constraint on the deformation parameter $c$. They analyzed the single-particle orbits of the valence neutrons and found the importance of molecular orbits. It was found that in the negative parity state of $^{10}$Be the main component of the valence neutrons is the positive parity orbit which seems to be the $\sigma$ orbit in terms of the dimer model. They tried to represent the excited $0^+_2$ state of $^{10}$Be by constructing 2p-2h states using the wave function of the negative parity state which is considered to be 1p-1h state. Comparing the optimum deformation parameters for three states $0^+_1$, $1^-$ and $0^+_2$, they found that the intrinsic deformation is larger in $1^-$ than $0^+_1$ and largest in $0^+_2$. The results are consistent with the ones predicted by W. Von Oertzen. They calculated excited states $0^+_2$ of $^{10}$Be without assuming any cluster cores for the first time and confirmed that the $2\alpha$ cluster cores may exist in the excited states. However since the total-angular-momentum projection was not done microscopically, the discussion didn’t go beyond the intrinsic system and it is not easy to study other excited states. They have not mentioned the data such as $E1$, $E2$ and $\beta$ transitions which are important in the study of excited states.

$^{10}$Be has been studied with other microscopic models such as multi cluster models [7], AMD+GCM(Generator Coordinate Method) [8] and the parity-projected Hartree-Fock(HF) calculations [9]. In the former two method the existence of $\alpha$ clusters was assumed. In the last work with parity-projected HF calculations they assumed the excited $0^+_2$ state as a 2p-2h state by choosing the positive parity eigen state for the valence two neutrons. In the work with HF calculations, the analysis was limited in the intrinsic system and it is not easy to study the higher excited states.

Our aim is to make systematic studies on the structure of many excited states of the light unstable nuclei with a microscopic model which is free from such assumptions as the inert cores, the existence of clusters, and the particle-hole configurations. For this aim we adopt a method of antisymmetrized molecular dynamics(AMD). AMD has been already proved to be a very useful theoretical approach for the structure of the light nuclei [10,11,12,13]. In the AMD framework basis wave functions of the system are written by Slater determinants where the spatial part of each single-particle wave function is a Gaussian wave packet. In the previous works on the structure of Li, Be and B isotopes [2,3,4], we applied the simplest version of AMD in which the energy variation is done after the parity projection but before the total-angular momentum projection. It was found that the structure of the ground state changes rapidly between the shell-model-like structure and the clustering structure as the neutron number increases up to the neutron-drip line. The AMD calculations succeeded to reproduce well the experimental data for electro-magnetic properties such as the magnetic dipole moments and the electric quadrupole moments. It owes to the flexibility of the AMD wave function which can represent the clustering structures of light unstable nuclei without assuming any inert cores and clusters.

In the present paper, we study the structure of the excited states of $^{10}$Be by performing variational calculations after the spin parity projection with finite-range interactions in the framework of AMD. For higher states, AMD wave functions are superposed so as to be orthogonal to the lower states. The AMD approach of the variation after spin parity projection(VAP) has been already found to be advantageous for the study of excited states of the light nuclei and be very useful to describe various molecule-like structures [13-14]. We do not rely on any assumptions such as the inert cores, the single-particle orbits in the mean field, and the existence of clusters. By microscopic calculations of the expectation values of the corresponding operators, we can acquire the theoretical values of $E2$, $E1$ and $\beta$ transitions which are the valuable informations of the excited states to be compared directly with the experimental data.

In Sec. II, we explain the formulation of AMD for the study of the nuclear structure of excited states. The effective interactions are described in Sec. III, and the results are presented in Sec. IV comparing with the experimental data. In Sec. V, the detailed discussions on the structures and on the mechanism of the development of the molecule-like structures are made. Finally summary is given in Sec. VI.

II. FORMULATION

In this section we explain the formulation of AMD for the study of nuclear structure of the excited states [13-14].

A. Wave function

The wave function of a system is written by AMD wavefunctions,

$$\Phi = c\Phi_{AMD} + c'\Phi'_{AMD} + \cdots$$  \hspace{1cm} (1)$$

An AMD wavefunction of a nucleus with mass number $A$ is a Slater determinant of Gaussian wave packets;
\[ \Phi_{AMD}(Z) = \frac{1}{\sqrt{A!}} A\{\varphi_1, \varphi_2, \cdots, \varphi_A\}, \]  
(2)

\[ \varphi_i = \phi_{X_i} \chi_{\xi_i} \tau_i : \left\{ \begin{array}{l} \phi_{X_i}(r_j) \propto \exp \left[ -\nu \left( r_j - \frac{X_{ni}}{\sqrt{\nu}} \right)^2 \right], \\ \chi_{\xi_i} = \left( \frac{1}{2} + \xi_i \right), \\ \tau_i \end{array} \right. \]  
(3)

where the \( i \)-th single-particle wave function \( \varphi_i \) is a product of the spatial wave function, the intrinsic spin function and the isospin function. The spatial part \( \phi_{X_i} \) is presented by complex parameters \( X_{ni} \), \( X_{ni} \), \( X_{ni} \), \( X_{ni} \), \( X_{ni} \), \( X_{ni} \) is the intrinsic spin function parameterized by \( \xi_i \), and \( \tau_i \) is the isospin function which is fixed to be up(proton) or down(neutron) in the present calculations. Thus an AMD wave function is parameterized by a set of complex parameters \( Z \equiv \{ X_{ni}, \xi_i \} (n = 1, 3 \text{ and } i = 1, A) \), where \( X_{ni} \)'s indicate the centers of Gaussians of the spatial part and \( \xi_i \)'s are the parameters for the directions of the intrinsic spins.

If we consider a parity eigen state projected from an AMD wave function the total wave function consists of two Slater determinants,

\[ \Phi(Z) = (1 \pm P) \Phi_{AMD}(Z), \]  
(4)

where \( P \) is a parity projection operator. In case of a total-angular momentum eigen state the wave function of a system is represented by integral of the rotated states,

\[ \Phi(Z) = P_{MK}^{J} \Phi_{AMD}(Z) = \int d\Omega D_{MK}^{J*}(\Omega) R(\Omega) \Phi_{AMD}(Z), \]  
(5)

for which the expectation values of operators are numerically calculated by a summation of mesh points on the Euler angles \( \Omega \).

In principal the total wave function can be superposition of independent AMD wave functions. In order to construct higher excited states we consider superposition of the spin parity projected AMD wave functions \( P_{MK}^{J\pm} \Phi_{AMD} \),

\[ \Phi = c P_{MK}^{J+} \Phi_{AMD}(Z) + c' P_{MK}^{J-} \Phi_{AMD}(Z') + \cdots. \]  
(6)

The detail is mentioned later in subsection II D.

**B. Energy variation**

We make variational calculations to find the state which minimizes the energy of the system:

\[ \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} \]  
(7)

by the method of frictional cooling. Regarding the frictional cooling method in AMD, the reader is referred to papers [2,11]. For the wave function \( \Phi(Z) \) parameterized by \( Z \), the time development of the parameters are given by the frictional cooling equations,

\[ \frac{dX_{nk}}{dt} = (\lambda + i \mu) \frac{1}{i \hbar} \frac{\partial}{\partial X_{nk}^*} \langle \Phi(Z) | H | \Phi(Z) \rangle, \quad (n = 1, 3 \text{ and } k = 1, A) \]  
(8)

\[ \frac{d\xi_k}{dt} = (\lambda + i \mu) \frac{1}{i \hbar} \frac{\partial}{\partial \xi_k^*} \langle \Phi(Z) | H | \Phi(Z) \rangle, \quad (k = 1, A) \]  
(9)

with arbitrary real numbers \( \lambda \) and \( \mu < 0 \). It is easily proved that the energy of the system decreases with time. After sufficient time steps of cooling, the parameters for the wave function of minimum-energy state are obtained.
C. Lowest $J^\pm$ states

In order to obtain the wave function for the lowest $J^\pm$ state, we perform the energy variation for the spin parity eigenstates projected from an AMD wave function. In this case the trial function is $\Phi = P^{J^\pm}_{MK',\text{AMD}}(Z)$. In the previous works with the simplest version of AMD for the study of nuclear structure, the approach was variation after only the parity projection but variation before the total spin projection(VBP). In the present paper, the approach is variation after the spin parity projection(VAP). First we make VBP calculations to prepare an initial wave function after only the parity projection but variation before the total spin projection(VBP). In the present paper, the approach previous works [2,3] with the simplest version of AMD for the study of nuclear structure, the approach was variation deformation where the $K$ with the adopted $J'$ quantum of the lower $J^\pm$ state, we perform the energy variation for the spin parity $J^\pm$ states as follows. The parameters $J^\pm_{n,K}$, $\Phi_{AMD}$ under the constraint on the principal axis $z$ as equal to the 3-axis.

D. Higher excited states

As mentioned above, with the VAP calculation for $\Phi(Z) = P^{J^\pm}_{MK',\text{AMD}}(Z)$ of the $J^\pm$ eigen state with $K'$, we obtain the set of parameters $Z = Z^\pm_{1}$ which present the wave function for the first $J^\pm$ state. To search the parameters $Z$ for the higher excited $J^\pm$ states in the $n$-th $K^\pm = K'^\pm$ band, the wave functions are superposed to be orthogonal to the lower states as follows. The parameters $Z^\pm_{n,K}$ for the $n$-th $J^\pm$ state are reached by varying the energy of the orthogonal component to the lower states:

$$
\Phi(Z) = P^{J^\pm}_{MK',\text{AMD}}(Z) - \sum_{k=1}^{n-1} \langle P^{J^\pm}_{MK',\text{AMD}}(Z_{k}^\pm)|P^{J^\pm}_{MK',\text{AMD}}(Z) \rangle P^{J^\pm}_{MK',\text{AMD}}(Z_{k}^\pm).
$$

E. Expectation values

After VAP calculations for various $J^\pm_{n,K}$ states, the intrinsic states $\Phi^{1}_{AMD}, \Phi^{2}_{AMD}, \ldots, \Phi^{n}_{AMD}$, which approximately correspond to the $J^\pm_{n,K}$ states, are obtained as much of the number of the calculated levels. Finally we determine the wave functions for the $J^\pm_{n,K}$ states by diagonalizing the Hamiltonian matrix $(P^{J^\pm}_{MK',\text{AMD}}|H|P^{J^\pm}_{MK'',\text{AMD}})$ and the norm matrix $(P^{J^\pm}_{MK',\text{AMD}}|P^{J^\pm}_{MK'',\text{AMD}})$ simultaneously with regard to $(i,j)$ for all the intrinsic states and $(K',K'')$. In comparison with the experimental data such as energy levels and $E2$ transitions, the theoretical values are calculated with the final states after diagonalization.

III. INTERACTIONS

The adopted interaction for the central force is the case 3 of MV1 force [17], which contains a zero-range three-body force $V^{(3)}$ as a density dependent term in addition to the two-body interaction $V^{(2)}$ of the modified Volkov No.1 force,

$$
V_{DD} = V^{(2)} + V^{(3)}
$$

$$
V^{(2)} = (1 - m + bP_{s} - \hbar P_{r} - mP_{s}P_{r}) \left\{ V_{A} \exp \left[ - \left( \frac{r_{1}}{r_{A}} \right)^{2} \right] + V_{R} \exp \left[ - \left( \frac{r_{r}}{r_{R}} \right)^{2} \right] \right\},
$$

$$
V_{A} = -83.34 \text{MeV}, \ r_{A} = 1.60 \text{fm}, \ V_{R} = 99.86 \text{MeV}, \ r_{R} = 0.82 \text{fm},
$$

$$
V^{(3)} = \nu^{(3)}(r_{1} - r_{2})\delta(r_{1} - r_{3}), \ \nu^{(3)} = 5000 \text{MeV fm}^{6},
$$
where $P_s$ and $P_t$ stand for the spin and isospin exchange operators, respectively. As for the two-body spin-orbit force $V_{LS}$, we adopted the G3RS force \cite{18} as follows,

$$V_{LS} = \left\{ u_I \exp (-\kappa_I r^2) + u_{II} \exp (-\kappa_{II} r^2) \right\} \frac{(1 + P_s)}{2} \frac{(1 + P_t)}{2} \mathbf{L} \cdot (\mathbf{S}_1 + \mathbf{S}_2),$$

(15)

$$\kappa_I = 5.0 \, \text{fm}^{-2}, \kappa_{II} = 2.778 \, \text{fm}^{-2}.$$  

(16)

The Coulomb interaction $V_C$ is approximated by a sum of seven Gaussians.

We treat the resonance states within a bound state approximation by situating an artificial barrier $\mathcal{E}_{\text{barr}}$. In the variational calculation we variate the modified energy $\mathcal{E}' = \mathcal{E} + \mathcal{E}_{\text{barr}}$ with the additional artificial energy $\mathcal{E}_{\text{barr}}$ instead of $\mathcal{E} = \langle \Phi | H | \Phi \rangle / \langle \Phi | \Phi \rangle$, where $H$ is the Hamiltonian operator; $H = T + V_{DD} + V_{LS} + V_C$. For the barrier in the present calculations we adopt a function of the real part of the centers $X_i$ of the single-particle wave functions as follows,

$$\mathcal{E}_{\text{barr}} = V_W \sum_{i=1}^A \exp \left[ -2 \nu \left( r_a - \frac{|\text{Re}[X_i]|}{\sqrt{\nu}} \right)^2 \right]$$

(17)

where $Z$ and $N$ are proton and neutron numbers, respectively. We put the artificial barrier only in the variational calculation we variate the modified energy $\mathcal{E}'$ instead of $\mathcal{E}$ of the single-particle wave functions as follows,

$$r_a = r_0 \left( 2 \text{Max}[Z, N]^{1/3} + b \right)$$

(18)

$$V_W = 2.5 \, \text{MeV}, \ r_0 = 1.2 \, \text{fm}, \ b = 2.5 \, \text{fm},$$

(19)

where $Z$ and $N$ are proton and neutron numbers, respectively. We put the artificial barrier only in the variational calculation, but do not put the barrier in the diagonalization of the Hamiltonian matrix after VAP calculations. In the present calculations of $^{10}\text{Be}$, the artificial energies due to the barrier are found to be a few hundreds keV at most and make no significant effect on the results in most levels.

IV. RESULTS

The structure of the excited states of $^{10}\text{Be}$ is studied with the VAP calculations in the framework of AMD. In this section we display the theoretical results of the excitation energies, $E2$, $E1$, and $\beta$ transitions which can be directly compared with the experimental data. The detail of the structures are discussed in the next section. The adopted parameters of the interactions are $m = 0.62$, $b = h = 0$ for the Majorana, Bertlett and Heisenberg terms of the central force and the strength of the spin-orbit force $u_I = -u_{II} = 3000 \, \text{MeV}$ (case(1)). Trying another set of parameters case(2) with $m = 0.65$, $b = h = 0$ and $u_I = -u_{II} = 3700 \, \text{MeV}$, we did not find significant differences in the results. The set of parameters case(1) is the one adopted in the work on $^{12}\text{C}$ \cite{13}. On the other hands, the VAP calculations with the set of interactions case(2) reproduce the parity inversion of the ground state of $^{11}\text{Be}$. The optimum width parameters $\nu$ of wave packets are chosen to be 0.17 fm$^{-2}$ for case(1) and 0.19 fm$^{-2}$ for case(2) which give the minimum energies in VBP calculations of $^{10}\text{Be}$. The resonance states are treated within a bound state approximation by situating an artificial barrier out the surface as mentioned in section II.

The lowest $J^\pm$ states are obtained by VAP calculations for $P_{MK}^{J^\pm} \Phi_{\text{AMD}}$ with ($J^\pm, K^\pm$) = (0$^+$, 0), (2$^+$, 0), (3$^+$, +2), (4$^+$, 0), (1$^-$, 0), (2$^-$, 0), (3$^-$, 0), (4$^-$, 0). Considering 0$^+_2$ state to be 0$^+$ state in the second $K^\pi = 0^+$ band, the 0$^+_2$ state is calculated by VAP as the higher excited state orthogonal to the lowest 0$^+_1$ state as explained in the subsection II. That is to say that the 0$^+_2$ state is obtained by VAP for $\Phi(Z)$ in Eq. (10) with ($J^\pm, K', n) = (0^+, 0, 2)$. In the case of higher 2$^+$ states, we put the constraint that the approximately principal z-axis of the intrinsic deformation equals to the 3-axis of the Euler angle in the total-spin projection. According to VBP calculations the second 2$^+$ state is described as the band head of the lowest $K^\pi = 2^+$ band. Therefore we construct the state 2$^+_2$ by choosing ($J^\pm, K'$) of $P_{MK}^{J^\pm} \Phi_{\text{AMD}}$ as ($J^\pm, K' = (2^+, +2)$ under the constraint on the principal z-axis which keeps the approximately orthogonality to the lowest 2$^+$ state with ($J^\pm, K' = (2^+, 0)$). The third 2$^+_3$ state is easily conjectured to be 2$^+$ state in the second $K^\pi = 0^+_2$ band like 0$^+_2$ state. We obtain the 2$^+_3$ state by VAP for $\Phi(Z)$ in Eq. (10) with ($J^\pm, K', n) = (2^+, 0, 2)$ in the same way as the 0$^+_2$ state, under the constraint on the principal z-axis mentioned above. It means that the orthogonal condition to 2$^+_1$ is kept by superposing two wave functions as described in the subsection II, while the orthogonality to 2$^+_2$ ($K^\pi = 2^+$) is taken into account by choosing the different $K$ quantum $K' = 0^+$.

The binding energy obtained with the case(1) interactions is 61.1 MeV, and the one with case(2) is 61.3 MeV. The excitation energies of the results are displayed in Fig. 1. By diagonalization of the Hamiltonian matrix the excited states 4$^+_2$, 6$^+$ are found in the rotational band $K^\pi = 0^+_2$ and 5$^-$ is seen in the $K^\pi = 1^-$ band. Comparing with the experimental data, the level structure is well reproduced by theory. Although it is difficult to estimate the width of resonance within the present framework, the theoretical results suggest the existence of 3$^+$, 4$^+$, 6$^+$ and 5$^-$ states...
FIG. 1. Excitation energies of the levels in $^{10}$Be. Theoretical results are calculated by the diagonalization of the states obtained with VAP by using the interactions case(1).
TABLE I. E2 and E1 transition strength. The theoretical results with the interactions case(1) are compared with the experimental data [9].

| transitions         | Mult. | exp.         | theory (e fm²) |
|---------------------|-------|--------------|----------------|
| 2\(^+_1\) → 0\(^+_1\) | E2    | 10.5±1.1 (e fm²) | 11 (e fm²)     |
| 0\(^+_1\) → 2\(^+_1\) | E2    | 3.3±2.0 (e fm²) | 0.6 (e fm²)    |
| 0\(^-_1\) → 1\(^-_1\) | E1    | 1.3±0.6×10⁻² (e fm) | 0.6×10⁻² (e fm) |

which are not experimentally identified yet. The excited levels can be classified as the rotational bands \(K^\pi = 0^+, 2^+, 0^+\) and 1\(^-\). The intrinsic structures of these bands are discussed in detail in the next section.

The data of transition strength are of great help to investigate the structures of the excited states. The theoretical results with the interaction case (1) and the experimental data of E2 and E1 transition strength are presented in Table I. The theoretical values well agree with the experimental data.

The strength of the \(\beta\) decays of Gamow-Teller(GT) type transitions can be deduced from the cross sections at the 0° forward angle of the charge exchange reactions which have been measured recently [9]. These new data for the Gamow-Teller type \(\beta\) transitions are very useful probes to discuss the structures of the excited states of unstable nuclei. Table I shows the values of \(B(GT)\). The experimental values for the \(\beta\) transitions from \(^{10}\text{Be}(3+)\) to \(^{10}\text{Be}^*\) are deduced from the data of the reaction \(^{10}\text{B}(^3\text{He})^{10}\text{Be}\). As for the theoretical values, the wave functions for the neighbor nucleus \(^{10}\text{B}\) are calculated with VAP where \((J^\pi, K^\pi)\) are chosen to be \((3^+, -3)\) for the ground \(3^+_1\) state and \((1^+, -1)\) for the \(1^+_1\) state. \(^{10}\text{Be}\) and \(^{10}\text{B}\) are calculated with the case (1) and (2) interactions. The theoretical values reasonably match to the experimental data. The strength is not so sensitive to the interactions except for the decay \(^{10}\text{B}(3^+)\rightarrow^{10}\text{Be}(2^+_1)\). The results of the GT transition \(^{10}\text{B}(3^+)\rightarrow^{10}\text{Be}(2^+_1)\) with case(1) and case(2) interactions underestimate the experimental data, while with another set of interactions; Volokov No.2 is calculated to be 0.41 (\(\frac{g_2}{4\pi}\)) which is larger than the experimental data. Since the data for \(^{10}\text{B}(3^+)\rightarrow^{10}\text{Be}(9.4\text{MeV})\) correspond to the theoretical value of \(^{10}\text{B}(3^+)\rightarrow^{10}\text{Be}(3^+_1)\), it is natural to consider the excited level of \(^{10}\text{Be}\) at 9.4MeV as the \(3^+_1\) state. The result of \(B(GT)\) for \(^{10}\text{Be}(0^+_1)\rightarrow^{10}\text{B}(1^+)\) is consistent with the experimental data of the \(\beta\) decay from the mirror nucleus \(^{10}\text{C}(0^+_1)\rightarrow^{10}\text{B}(1^+)\). It is suggested that the \(B(GT)\) for \(^{10}\text{B}(3^+)\rightarrow^{10}\text{Be}(2^+_1)\) is not large because of the well developed clustering structure of \(^{10}\text{Be}(2^+_1)\). We will discuss again the \(\beta\) decays combining with the structures of excited states in the next section. In the reference [9] of the measurements of the strength \(B(GT)\), they mentioned about the isospin symmetry violation of \(\beta\) decay strength comparing \(B(GT_+)\) for \(^{10}\text{B}(3^+)\rightarrow^{10}\text{Be}(2^+_1)\) with \(B(GT_-)\) for the mirror reaction to \(^{10}\text{C}\). In the present calculations, we could not find the difference between \(B(GT_-)\) and \(B(GT_+)\) because there is little violation of isospin symmetry between the structures of \(^{10}\text{Be}(2^+_1)\) and the mirror state of \(^{10}\text{C}\). Taking into account of the experimental information that there exists a significant difference between the excitation energies of the daughter states of \(^{10}\text{Be}\) and \(^{10}\text{C}\), the isospin violation of the structures of these mirror states may be possible. We need more detailed investigations to discuss the problem of the isospin symmetry violation of \(B(GT)\).

V. DISCUSSION

In this section we discuss the structure of the excited states by analyzing the wave functions. Even though the states obtained by VAP mix after the diagonalization of the Hamiltonian matrix, the state \(P_{MK}\Phi_{AMD}(Z_{\pm}^n)\) projected from a Slater determinant obtained in VAP with \((J^\pm, K', n)\) is dominant in the final result of the \(J^\pm_n\) state. In this section we consider the Slater determinant \(\Phi_{AMD}(Z_{\pm}^n)\) as the intrinsic state for the \(J^\pm_n\) state.

A. intrinsic structure

In the excited states, various kinds of structures are found. Here we analyze the structures of the intrinsic states \(\Phi_{AMD}(Z_{\pm}^n)\). It is found that the excited levels are classified into rotational bands as \(0^+_1, 2^+_1, 4^+_1\) states in \(K^\pi = 0^+_1\) band, \(2^+_2, 3^+_2, 4^+_2\) in \(K^\pi = 2^+_1\) band, \(0^+_2, 2^+_3, 4^+_3, 6^+_3\) in the second \(K^\pi = 0^+_2\) band and \(1^-, 2^-, 3^-, 4^-, 5^-\) in \(K^\pi = 1^-\) band. Particularly the molecule-like states with the well-developed \(2\alpha\) cores construct the rotational bands \(K^\pm = 0^+_2\) and \(1^-\) in which the level spacing is small because of the large moments of inertia. The density distributions of matter, protons and neutrons in the intrinsic states \(\Phi_{AMD}(Z_{\pm}^n)\) are presented in Fig. 2. We found the \(2\alpha + 2n\) structures in

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the orthonormal base as follows \([5,12]\); \(\varphi\) of an AMD wavefunction into an orthonormal base \(\tilde{\text{H}}\) Hamiltonian by the analogy with Hartree-Fock theory. First we transform the set of single-particle wave functions and the single-particle energies of an intrinsic state are determined by diagonalizing the single-particle Hamiltonian by the analogy with Hartree-Fock theory. We study the behavior of the valence neutrons surrounding \(2\) nuclei. Considering that an intrinsic state is written by a Slater determinant \(\Phi\) by analyzing the single-particle wave functions to understand the role of the valence neutrons in the neutron-rich \(\text{Be}\) nuclei. The increase of the degree of the deformation along \(0^{+}\) and \(1^{-}\) states are sensitive to the strength of the spin-orbit force. The structures of \(0^{+}\) states are similar to the ones of the previous work with the simplest version of AMD \([12]\). The increase of the total spin due to the spin-orbit force. The reduction of the clustering structure is more rapid in the case of interaction \((2)\) with the stronger spin-orbit force and \(2^{+}\) states in the case \((2)\) interactions contain the dissociation of \(\alpha\). Regarding the dissociation of the \(\alpha\) cores, the structures of those states are sensitive to the strength of the spin-orbit force.

The \(2^{+}\) has the remarkably developed molecule-like structure with an exotic shape and belongs to the rotational band \(K = 0^{+}\). On the other hand, the lowest \(3^{+}\) state of \(10\text{B}\) is the ordinary state in terms of \(p\)-shell. The theory predicts a small value of the Gamow-Teller strength \(^{10}\text{B}(3^{+}) \rightarrow ^{10}\text{Be}(2^{+})\) because of the difference between the structures of the initial and final states.

### B. behavior of valence neutrons

Even though we did not assume the existence of any clusters in the model, we have found the \(2\alpha + 2n\) structures in most of the intrinsic states as mentioned above. We study the behavior of the valence neutrons surrounding \(2\alpha\) by analyzing the single-particle wave functions to understand the role of the valence neutrons in the neutron-rich \(\text{Be}\) nuclei. Considering that an intrinsic state is written by a Slater determinant \(\Psi_{AMD}\), the single-particle wave functions and the single-particle energies of an intrinsic state are determined by diagonalizing the single-particle Hamiltonian by the analogy with Hartree-Fock theory. First we transform the set of single-particle wave functions \(\varphi_i\) of an AMD wavefunction into an orthonormal base \(\tilde{\varphi}_\alpha\). The single-particle Hamiltonian can be constructed by use of the orthonormal base as follows \([3,12]\):
The density distribution of matter, protons and neutrons of the intrinsic states are shown at left, middle and right, respectively. The density is integrated along the axis perpendicular to adequate planes. The figures are for the results with the interactions case(1).

FIG. 2.
\begin{align}
\hat{h}_{\alpha\beta} &= \langle \hat{\psi}_{\alpha}|\hat{t}|\hat{\psi}_{\beta}\rangle + \sum_{\gamma} \langle \hat{\psi}_{\alpha}\hat{\psi}_{\gamma}|\hat{v}|\hat{\psi}_{\beta}\hat{\psi}_{\gamma} - \hat{\psi}_{\gamma}\hat{\psi}_{\beta}\rangle \\
&\quad + \frac{1}{2} \sum_{\gamma,\delta} \langle \hat{\psi}_{\alpha}\hat{\psi}_{\gamma}\hat{\psi}_{\delta}|\hat{v}_3|\hat{\psi}_{\beta}\hat{\psi}_{\gamma}\hat{\psi}_{\delta} + \hat{\psi}_{\delta}\hat{\psi}_{\beta}\hat{\psi}_{\gamma} + \hat{\psi}_{\gamma}\hat{\psi}_{\delta}\hat{\psi}_{\beta} - \hat{\psi}_{\beta}\hat{\psi}_{\delta}\hat{\psi}_{\gamma} - \hat{\psi}_{\gamma}\hat{\psi}_{\beta}\hat{\psi}_{\delta} - \hat{\psi}_{\delta}\hat{\psi}_{\gamma}\hat{\psi}_{\beta}\rangle \tag{20},
\end{align}

where the Hamiltonian operator is written by a sum of kinetic term, two-body interaction term and three-body interaction term; $H = \sum_i \hat{t} + \sum_{i<j} \hat{v}_2 + \sum_{i<j<k} \hat{v}_3$.

The single-particle energies in the $0^+_1$, $1^-$ and $0^+_2$ states are shown in Fig. 3. In each state the neutrons in the four orbits from the bottom correspond to the neutrons in the $2\alpha$ clusters. The level spacing of these four lower orbits becomes smaller in $1^-$ than in $0^+_1$ and smallest in the $0^+_2$ state with the increase of the distance between clusters. We consider the last two neutrons in the higher orbits as valence neutrons surrounding $2\alpha$ cores. We display the density distributions of single-particle wave functions for the two valence neutrons in the left column of Fig. 4. Figures in the middle and right columns of Fig. 4 are for the normalized density of the positive and the negative parity eigen states projected from the single-particle wave functions, respectively. By analyzing the single-particle wave functions it is found that two valence neutrons of the $0^+_1$ states contain the negative parity components more than 80% (the right column in figure 4) which seem to be $\pi$ bonds (Fig. 3(a)) in terms of molecular orbits. On the other hand in the case of $0^+_2$ band, the last 2 neutrons are predominantly in the positive parity orbits, which are analogous to the $\sigma$ bonds (Fig. 3(b)). In the $1^-$ band, each valence neutron contains both the positive parity component like $\sigma$ and the negative parity one similar to $\pi$. Since the parity of the total system is negative in the $1^-$ band, the states after the parity projection have one neutron in $\sigma$ orbit and the other neutron in $\pi$ orbit. Roughly speaking, the $0^+_1$, $1^-$ and $0^+_2$ states are understood as $2\alpha$ and two valence neutrons in $\pi^2$, $\sigma\pi$ and $\sigma^2$ orbits, respectively. The interesting point is that the valence neutrons play important roles to develop the clustering structure in the excited bands. We can argue that the clustering develops in the $1^-$ band and mostly in $0^+_2$ band owing to the $\sigma$ orbits of the valence neutrons, because the $\sigma$ orbit prefers the prolately deformed system as to gain its kinetic energy. This idea originates from the application of the two centers shell model to the dimer model for Be isotopes by W. von Oertzen and consistent with the argument in the work with the method of AMD+HF by Doté et al.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.pdf}
\caption{Single-particle energies in the intrinsic system of the $0^+_1$, $1^-$ and $0^+_2$ states. The energies of protons(neutrons) are displayed in the left(right) side in each figure.}
\end{figure}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{Single particle energy} & \textbf{MeV} & \textbf{0}^+_1 & \textbf{1}^- & \textbf{0}^+_2 \\
\hline
\textbf{MeV} & 0 & 0 & 0 & 0 \\
\hline
\textbf{0}^+_1 & | & | & | & | \\
\hline
\textbf{1}^- & | & | & | & | \\
\hline
\textbf{0}^+_2 & | & | & | & | \\
\hline
\end{tabular}
\caption{Table of single-particle energies.}
\end{table}

\section*{C. mechanism of clustering development}

As mentioned above, one of the viewpoints for the mechanism of the clustering development is the molecule-like orbits $\sigma$ and $\pi$. Here we try to understand the mechanism from the other viewpoint of the two-center clustering model.

The reason for the clustering development in the ordinary nuclei has been understood as the system gains the kinetic energy with the development of clustering although the potential energy losses. In order to understand the mechanism of clustering in light unstable nuclei, we think it is helpful to investigate the competition of the kinetic and the potential energies in the molecule-like states of $^{10}$Be.
FIG. 4. Density distribution of single-particle wave functions of the valence two neutrons in the intrinsic states of $0^+_1$, $1^-$ and $0^+_2$ (left column). The method to extract the single-particle wave functions are explained in the text. The middle and right columns are for the density of the positive parity and negative parity components projected from the single-particle wave functions, respectively. The wave functions projected into the parity eigen states are normalized for presentation.

FIG. 5. Schematic figures of the molecular orbits $\pi$ bond (a) and $\sigma$ bond (b) surrounding $2\alpha$ clusters.
In the density distribution of VAP results, the structures of the $0^+_1$, $1^−$ and $0^+_2$ states seem to be the two-center clustering structures which consist of $^6$He+$^6$He ($α$ $−$ $α$ for the $1^−$ state) and $0^+_2$ states. To estimate the dependence of the kinetic and potential energies on the degree of the spatial clustering development we represent the three kinds of configurations for the $^6$He+$α$ system corresponding to the $0^+_1$, $1^−$ and $0^+_2$ states of $^{10}$Be by the simplified AMD wave functions $Φ_{AMD}(Z)$ as follows. The intrinsic spin of the single-particle wave functions are fixed to be up or down for simplicity. For the $^6$He+$α$ system with the inter-cluster distance $d$ (fm), the centers of single-particle Gaussian wave functions are located around two points $\vec{a}_1 = (-3d/5\sqrt{2}, 0, 0)$ and $\vec{a}_2 = (2d/5\sqrt{2}, 0, 0)$. The three kinds of configurations of the centers for $0^+_1$, $1^−$ and $0^+_2$ states are shown in the right figures of Fig. 8. We put the centers for $p \uparrow$, $p \downarrow$, $n \uparrow$, $n \downarrow$ at the point $\vec{a}_1$ and $p \uparrow$, $p \downarrow$ at $\vec{a}_2$. The centers for the last 4 neutrons are located at the points very close to $\vec{a}_2$ as $\vec{a}_2 \pm \vec{δ}$ where enough small $\vec{δ}$ is chosen so that the angle $θ$ between $\vec{δ}$ and $\vec{a}_2$ is $θ = \pi/2, \pi/4$ and $0$ corresponding to the $0^+_1$, $1^−$ and $0^+_2$ states, respectively. For the parity eigen states projected from these three kinds of the simplified AMD wave functions $Φ_{AMD}(Z)$ we calculate the expectation values of total, kinetic and potential energies as the function of the inter-cluster distance $d$;

$$⟨H⟩ = \frac{⟨(1 ± P)Φ_{AMD}(Z)|H|(1 ± P)Φ_{AMD}(Z)⟩}{⟨(1 ± P)Φ_{AMD}(Z)|(1 ± P)Φ_{AMD}(Z)⟩} \quad \quad (21)$$

$$⟨T⟩ = \frac{⟨(1 ± P)Φ_{AMD}(Z)|T|(1 ± P)Φ_{AMD}(Z)⟩}{⟨(1 ± P)Φ_{AMD}(Z)|(1 ± P)Φ_{AMD}(Z)⟩} \quad \quad (22)$$

$$⟨V⟩ = \frac{⟨(1 ± P)Φ_{AMD}(Z)|V|(1 ± P)Φ_{AMD}(Z)⟩}{⟨(1 ± P)Φ_{AMD}(Z)|(1 ± P)Φ_{AMD}(Z)⟩} \quad \quad (23)$$

where we omit the spin-orbit and the Coulomb forces for simplicity. In Fig. 7 we present the total energy, the kinetic energy and the potential energy for the three kinds of clustering states $0^+_1$, $1^−$ and $0^+_2$ as the function of the distance $d$ between $^6$He and $α$ clusters. As shown in the figure for the total energy $⟨H⟩$, the optimum distances indicate that the clustering structure develops in the system for the $1^−$ state and is most remarkable in the state for $0^+_1$, which is consistent with the present results of VAP calculations. The shift of the minimum point of the total energy is understood by the energetically advantage of the kinetic part as follows. It is found that the kinetic energies in the small $d$ region are sensitive to the configurations, while in the case of the potential energies significant differences are not seen in the three configurations. When the cluster approaches each other the kinetic energy in the configuration for the $1^−$ state becomes larger than $0^+_1$ by $1/2\hbarω$ (about 7 MeV for $ν = 0.17$), because all the neutrons in $0^+_1$ are in $0s$ and $0p$ shells, while in the negative parity state for $1^−$ one valence neutron must rise to the higher $sd$ shell in the small $d$ region. Since in the small $d$ limit the wave function is almost same as the harmonic oscillator shell model wave function due to the antisymmetrization, the kinetic energy of the $sd$ shell is larger than by $1/2\hbarω$ than the one of $p$ shell. Thus the system for $1^−$ loses as to the kinetic energy in the small distance $d$, as a result, the minimum point of total energy shift to the larger $d$ region than the one in the $0^+_1$ state. In the case of the linear configuration for the excited $0^+_2$ state, the two valence neutrons occupy the $sd$ orbit in the small $d$ limit and the kinetic energy is larger than $0^+_1$ by $\hbarω$. That is why the optimum point $d$ in $0^+_2$ is the largest of the three. In other words, when the cluster approaches each other, the system feels the repulsive force in kinetic part because of the Pauli principle. That is the reason why the clustering structure remarkably develops in the $0^+_2$ state. In the analysis with this simplified two cluster model, we can conclude that the clustering develops so as to gain the kinetic energy. It is compatible with the viewpoint of the molecular $σ$ orbit.

VI. SUMMARY

We studied the structures of excited states of $^{10}$Be by performing variational calculations after the spin-parity projection in the framework of antisymmetrized molecular dynamics (AMD). We explained the formulation of the variation after projection and the method to construct the higher excited states with AMD.

The excitation energies of many levels of $^{10}$Be were reproduced by AMD calculations with the finite range interactions. The theoretical results well agree to the experimental data of $E1$, $E2$ transition strength. The results successfully describe the new data of $B(GT)$ for the $β$ transition strength reduced from the $0^0$ angle cross sections of the charge exchange reactions $^{10}$Be($^{3}$He,$^4$He)$^{10}$Be$^\ast$.

We discuss the structures of excited states. By analyzing the intrinsic structures it is found that the excited levels are classified into the rotational bands as $K^\pi = 0^+_1$, $2^+, 0^+_{2}$ and $1^−$. Although the $α$ clusters are not assumed in the model, the theoretical results show that the $2α + 2n$ structures appear in most of the states. Particularly the molecular-like states with the developed $2α$ structure constructs the rotational bands $K^\pi = 0^+_{2}$ and $1^−$ in which the
level spacing is small because of the large deformations. The molecule-like structure develops more largely in $K^\pi = 1^-$ than in $K^\pi = 0^+_1$ and most remarkably in $K^\pi = 0^+_2$.

We extracted the single-particle wave functions to discuss the behavior of the valence neutrons. In the analysis of the intrinsic states of $0^+_1$, $1^-$ and $0^+_2$ states (the band heads of the rotational bands $K^\pi = 0^+_1$, $1^-$, $0^+_2$), we found that the two valence neutrons are in the molecular orbits surrounding $2\alpha$. The positive and negative parts of the orbits are analogous to the $\sigma$ and $\pi$ bonds in terms of the electron orbits in molecules. Roughly speaking, the $0^+_1$ states, $1^-$ and $0^+_2$ bands is regarded as the states with the two valence neutrons in $\pi^2$, $\sigma\pi$ and $\sigma^2$ orbits, respectively. The neutrons in the $\sigma$ orbit plays as important role for the development of clustering because $\sigma$ orbit profits from the kinetic energy in the prolately deformed system.

In order to understand the mechanism of the clustering development in the excited states of $^{10}\text{Be}$, we analyze the kinetic and the potential parts of the total energies with the simplified model of the two-center $^6\text{He}+\alpha$ cluster model. In the $1^-$ and $0^+_2$ states, when the distance between clusters becomes small the systems feel the repulsive kinetic energy because the valence neutrons must rise into higher orbits. Because of the repulsive kinetic energy in the small inter-cluster distance the clustering structure develops in the excited states $1^-$ and $0^+_2$ to gain as to the kinetic energy.

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FIG. 7. Total, kinetic and potential energies as the distance between clusters in the simplified $^6\text{He}+\alpha$ cluster models for the excited states of $^{10}\text{Be}$. The adopted interaction is the MV1 force with $m = 0.62$, and the spin-orbit and the Coulomb forces are omitted. The distance $d$ between clusters and the configuration for the $0^+_1$, $1^-$ and $0^+_2$ states are defined in the text. The true lines, the dashed lines and the dot-dashed lines correspond to the energies in the system for $0^+_1$, $1^-$ and $0^+_2$ states of $^{10}\text{Be}$, respectively.
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