Exotic molecular structures in highly-excited states of $^{12}$Be

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Abstract. The generalized two-center cluster model (GTCM), which can treat static structures and dynamical reactions in excited states, is applied to the light neutron-rich system, $^{12}$Be=$\alpha+\alpha+4N$. We discuss the change of the neutrons’ configuration around two $\alpha$-cores from the covalent structure to the ionic one. It is shown that, in the unbound region above particle-decay thresholds, the ionic configurations appear as the molecular resonances of $\alpha+^8$He, $^6$He+$^4$He and $^5$He+$^7$He. A new type of superdeformation is possible, and we find here the covalent superdeformation which has a hybrid configuration of the covalent and ionic ones. The excitation of these exotic structures through the two neutron transfer reaction is also discussed.

1. Introduction
It is well known that various deformed structures appear in excited states of nuclear systems. The strongly deformed states have been discussed from two different pictures so far; one is a deformation of the self-consistent mean field, while the other is a localization of strongly correlated sub-systems, clustering. The example of the former and latter cases are known as the superdeformed (SD) band [1] and the molecular resonances (MRs) [2], respectively. In $^{32}$S, for instance, some researchers try to clarify the relation between the SD bands and MRs [3]. Such study points out that the SD band generated by a deformed mean-field and the $^{16}$O+$^{16}$O MRs appear with a large energy interval, say about 10$\sim$20 MeV. In nuclei with $N=Z$, therefore, an interplay between the SD band and the MRs is not so prominent due to the large energy difference of these two structures.

In this report, we propose a new type of superdeformed structure based on a cluster picture in a light neutron-rich ($N>Z$) nucleus, and demonstrate that, in marked contrast with $N=Z$ systems, the proposed superdeformed state coexists with the MRs. The Be isotopes are the candidates manifesting such coexistence phenomena. These are typical examples of two-center superdeformed systems which build on an $\alpha+\alpha$ rotor of $^8$Be. The low-lying states of these systems can be described by the molecular orbitals (MO), such as $\pi^-$ and $\sigma^+$ orbitals associated with the covalent electrons of atomic molecules [4, 5, 6]. Here, the valence neutron(s) rotates around two centers simultaneously. Since the $\sigma^+$ orbital has an extended distribution along the $\alpha-\alpha$ axis, it enhances the $\alpha-\alpha$ distance to reduce neutrons’ kinetic energy [4]. This means that the large prolate-deformation with the two centers can be generated by this orbital. In $^{10}$Be, for example, the rotational band from the $0_2^+$ state with the configuration of $(\sigma^+)^2$ has a large moment of inertia and it has just been identified by the latest experiment [7]. Therefore, the
configurations associated with the $\alpha^+$ orbital should be called the “superdeformation with the covalent neutrons” (covalent SD), which is a foundation of a new type of the superdeformation proposed in the present study.

Furthermore, recent experiments on $^{12}$Be revealed the existence of many resonant states with small energy interval less than 1 MeV [8, 9, 10]. The observed resonances strongly decay into $^6$He$_{g.s.}$+$^6$He$_{g.s.}$ and $\alpha^+$$^6$He$_{g.s.}$, and similar resonances, decaying to He isotopes, have also been observed in $^{10}$Be [9] and $^{14}$Be [10]. These resonances are the candidates for the $^{3}$He$^+$$^3$He MRs ($X,Y=4,6,8$), where neutrons are trapped around one of the clusters analog to ionic electron configurations. Some of the states may be described by the MO picture [6], but it is impossible for the MO model to explain all the observed resonances. In Be isotopes, only small energy is required for the rearrangements between the covalent (MO) neutron structures and ionic ones due to the weakness of the $\alpha$ and neutron-neutron interactions. Therefore, above the threshold to decay into two He-fragments, the covalent SD and the MRs may coexist in the same energy region with a crucial interplay among them.

To investigate the coexistence phenomena, the intrinsic structures and its coupling to the scattering states should be treated in a unified manner, because the nucleus is an unbound system above the particle-decay thresholds. The ideal MO structures must be formed below the thresholds, which are realized as a bound system. However, in an unbound system, MO couples to the atomic orbital (AO) structures corresponding to the $^3$He$^+$$^3$He MRs [11, 12], because the decaying He-clusters shall be generated outside their contact distance. In studies of the unbound region of nuclei, therefore, theoretical model should cover both the MO and AO configurations.

We apply the generalized two-center cluster model (GTCM) [13, 14] to $^{12}$Be ($N=8,Z=4$) which is the typical example manifesting the coexistence phenomena in an unbound system. Our method covers the MO and AO model spaces and hence, it is possible to treat a scattering phenomena in the unbound states.

2. Framework

In GTCM, the total wave function of $^{12}$Be is given by the superposition of the basis $\{\Phi^J_{m,K}(S)\}$, where,

$$\Phi^J_{m,K}(S) = \hat{P}^J_K A \left\{ \psi_L(\alpha)\psi_R(\alpha) \prod_{j=1}^{4} \varphi_j(m_j) \right\} _S.$$  \hfill (1)

The $\alpha$-cluster $\psi_n(\alpha)$ ($n=L, R$) is expressed by the $(0s)^4$ configuration of the harmonic oscillator (HO) centered at left ($L$) or right ($R$) side with the relative distance of $S$ [15]. The single-particle wave function for the four valence neutrons localized around one of the $\alpha$ clusters is given by an atomic orbital (AO) $\varphi(p_k,i,\tau)$, 0$p$-orbitals $p_k$ ($k=x, y, z$) around $i$ (= $L$ or $R$) with the spin $\tau$ (= $\uparrow$ or $\downarrow$). Here, $\{m_j\}$ are indices of AO ($p_k,i,\tau$) and $m$ represents a set of AOs for the four neutrons, $m=(m_1,m_2,m_3,m_4)$. The intrinsic basis functions with the full anti-symmetrization $A$ are projected to the eigenstate of the total spin $J$, its intrinsic angular projection $K$ and the total parity $\pi$ by the projection operator $\hat{P}^J_K$.

The total wave function is finally given by taking the superposition over $S$, $m$ and $K$ as

$$\hat{\Psi}_\nu^J = \int dS \sum_{m,K} C^\nu_{mK}(S) \Phi^J_{m,K}(S).$$  \hfill (2)

The coefficients for the $\nu$-th eigenstate, $C^\nu_{mK}(S)$, are determined by solving a coupled channel GCM (Generator Coordinate Method) equation [15]. The present calculation is restricted to the axially symmetric ($K=0$) case, however we include all the possible AO configurations for the four valence neutrons within this approximation. Therefore, the model space of MO, where
each valence neutron rotates around two centers simultaneously, is also covered [13]. As for the nucleon-nucleon interaction, we use the Volkov No.2 and the G3RS for the central and spin-orbit parts, respectively. The parameters in the interactions and the size parameter of HO are the same as those applied in Ref. [14], which successfully reproduce the properties of $^{10}$Be. The adopted parameter set reasonably reproduce the threshold energies of $\alpha+^{8}$He$_{g.s.}$, $^{6}$He$_{g.s.}+^{4}$He$_{g.s.}$ and $^{4}$He$_{g.s.}+^{7}$He$_{g.s.}$. This is essentially important in the treatment of scattering phenomena.

3. Results

3.1. Structure of Adiabatic Energy surfaces

If we fix the distance parameter $S$ and diagonalize the Hamiltonian with respect to $m$ in Eq. (2), we obtain the energy eigenvalues as a function of $S$, which we call the adiabatic energy surfaces (AESs). In Fig. 1, we show the AESs for the $J^{π}=0^+$ states. There appear two lines (A and B) below the $\alpha+^{8}$He$_{g.s.}$ threshold with local minima around $\alpha\alpha$ distance $S \sim 3$ fm. Around these minima, each valence neutron rotates around both $\alpha$-clusters, and the MO structure is formed. The main configuration of the lowest line (A) is $(\pi_{3/2}^-)^2(\sigma_{1/2}^+)^2$, while the second one (B) has the dominant configuration of $(\pi_{3/2}^-)^2(\pi_{1/2}^-)^2$ for the four neutrons, which correspond to the $(0p)^2(sd)^2$ and $(0p)^4$ configurations at the limit of $S = 0$, respectively. The AESs show the interchange of the main components around $S \sim 3.2$ fm and hence, the strong mixing of these configurations occurs around the optimal $S$ value. Because of the mixing of $sd$-shell components, the $N=8$ magicy of the $p$-shell is broken in the ground state, which is consistent with the recent observation [16]. As the increase of $S$, these two surfaces are continuously changed to $\alpha+^{8}$He$_{g.s.}$ (triangles) and $^{5}$He$_{g.s.}+^{7}$He$_{g.s.}$ (double circles) configurations in the asymptotic region. When the two clusters are separated, neutrons cannot rotate around both clusters and are trapped around one of the clusters, which is the crossover from the MO structure to the AO one.

In the energy region above the threshold, there is another crossing of two AESs (C and D). Around the energy minimum point of the AES C, two of the valence neutrons are localized around individual $\alpha$ as $^{5}$He+$^{5}$He, which is the AO structure, and the remaining two neutrons occupy the $\sigma^+$ orbital and rotate around both clusters, which is the MO one. Because of the two neutrons in the $\sigma$-orbital, the clustering (the optimal $S$ value) is enhanced the same as in the second $0^+$ state of $^{10}$Be [4, 13, 14], thus the state is covalent SD state. However, here, other two neutrons have the ionic (AO) configuration, and the appearance of the hybrid configuration with both MO and AO characters is new feature in $^{12}$Be, which is not seen in our previous work for $^{10}$Be. The AES D has a specific character that the crossover from MO to AO occurs at small $\alpha\alpha$ distance. Up to $S \sim 2.4$ fm where the two $\alpha$-clusters almost overlap, this surface has a covalent (MO) configuration of $(\pi_{3/2}^-)^2(\pi_{3/2}^-)^2$. This is the one suggested in Ref. [6] as a cluster rotational band in the energy region above the threshold, but, in the present calculation, it is smoothly changed to the $^{6}$He$_{g.s.}+^{6}$He$_{g.s.}$ configuration at larger $S$ values and hence, the MO configuration cannot be stabilized.

3.2. Energy spectra and the $\alpha+^{8}$He $\rightarrow$ $^{6}$He+$^{6}$He reaction in $J^{π}=0^+$

The energy spectra of bound states are obtained not by the adiabatic approximation but by re-diagonalizing the original Hamiltonian with the basis of all the adiabatic states in Fig. 1. In addition, the coupling to the scattering continuum is taken into account when the system is excited above the threshold. This is achieved by the Kamimura’s method [17], where the total wave function is written as

$$\Psi^{Jπ(+)} = \sum_\nu b_\nu \hat{\Psi}^{Jπ} K=0 + \sum_\beta \varphi_\beta \chi^{(+)}_\beta .$$  \hspace{1cm} (3)

The first term stands for closed channels within the finite range of $S$, which is the linear combination of the solutions of Eq. (2) and describes the internal compound-states before
also shown. \(\alpha\)Kohn-Hulth \(\text{-}\)en-Kato variation method \([14, 17, 18]\). We consider three rearrangement channels, the shoulder region in \(\text{S}\) (iii) Covalent SD state. relative motion. \(\text{S}\) of the AES C in Fig. 1, which is the mixture of (\(\pi_{1/2}^-\)) and \(6\)He\(_{g.s.}\)\(+\)\(6\)He\(_{g.s.}\) are also shown.

There appear two bound states below the MO states. MO motion around the two \(\alpha\) cores (\(\pi_{3/2}^-\)\(2\)\(\sigma_{1/2}^+\)\(2\)) and (\(\pi_{3/2}^-\)\(2\))\(\pi_{1/2}^+\)\(2\)).

The obtained \(0^+\) states are classified into three categories. (i) MO states. There appear two bound states below the \(\alpha+g.s.\) threshold (\(0^+_1\) and \(0^+_2\)), which correspond to the lowest two local minima in the AESs A and B (Fig. 1). The energy difference is about 2 MeV and it agrees with the recent observation \([16]\). Here, the four neutrons are in MO motion around the two \(\alpha\) cores (\(\pi_{3/2}^-\)\(2\)\(\sigma_{1/2}^+\)\(2\)) and (\(\pi_{3/2}^-\)\(2\))\(\pi_{1/2}^+\)\(2\)). (ii) MR states. The resonance states, \(0^+_3\), \(0^+_4\), and \(0^+_5\) have the MR characters of corresponding threshold (\(\alpha+g.s.\), \(6\)He\(_{g.s.}\)\(+\)\(6\)He\(_{g.s.}\), and \(5\)He\(_{g.s.}\)\(+\)\(7\)He\(_{g.s.}\), respectively). They have large overlap with the AESs of A, B and D in Fig. 1; the \(0^+_4\) state largely overlaps with the AES D, while \(0^+_3\) and \(0^+_6\) overlap with the A and \(\beta\), respectively. The main components of the latter two states spread outside region of \(S>5\) fm where the AESs do not have any local minima but have shoulder-like shapes. This means that \(0^+_5\) and \(0^+_6\) are excitation modes of the clusters’ relative motion from the two bound states. Since the shoulder region in \(S\) just corresponds to crossover from MO to AO, their smooth connection with a variation of \(S\) is essentially important to describe MR states as excitations of clusters’ relative motion. (iii) Covalent SD state. The main component of \(0^+_4\) is the local minimum of the AES C in Fig. 1, which is the mixture of (\(\sigma^+\)\(2\)) (MO) and \(5\)He\(_{g.s.}\)\(+\)\(5\)He (AO). This state has

Figure 1. Adiabatic energy surfaces (AESs) for \(J^\pi=0^+\). The calculated threshold for the open channels, \(\alpha+g.s.\) (dotted line at the origin of the ordinate) and \(6\)He\(_{g.s.}\)\(+\)\(6\)He\(_{g.s.}\) are also shown.
a large clustering ($S \sim 5$ fm) due to the $(\sigma^+)^2$ formation.

![Figure 3](image_url)  

**Figure 3.** Rotational bands of $^{12}$Be. The shaded area represent the region where the resonances are observed [10], while the crosses and the triangles show the data in Refs. [9] and [16], respectively. The resonance energies of Refs. [9, 10] are measured from the calculated threshold of $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$.

The $0^+_1$ and $0^+_5$ states are strongly excited by the two neutron transfer reaction. In particular, the magnitude of the S-matrix reaches to unitarity limit, $|S_{f,i}|^2 \sim 1$, at the resonance position of $0^+_5$. This means that the exit channel of the resonance is limited to $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$. The covalent SD which is the main configuration of $0^+_5$ includes both components of $^6\text{He}^+ + ^6\text{He}$ and $^5\text{He}^+ + ^7\text{He}$, but the latter channel does not open at the resonance energy as shown in Fig. 2. Therefore, this resonance can decay only to $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$ and the S-matrix of the respective transition increases up to the maximum value.

### 3.3. Rotational band structures

We perform same kind of calculation for other $J^\pi$ states and identify the resonance energies, which are shown in Fig. 3. Six rotational bands are identified and the lowest two bands and their relative excitation modes are plotted by the same symbols (double circles and white ones). The maximum spin of the ground rotational band (double circles with the dashed line) reaches to $J^\pi=8^+$ because of the $(\sigma^+)^2$ nature of the neutrons, while the first excited band (white circles with the dashed line) has the component of closed $p$-shell configuration for the neutrons. Furthermore, there appear four rotational bands in the continuum region. We can see the overlapping behaviour of the $\alpha+^8\text{He}_{g.s.}$ band (double circles with the solid line) and $^4\text{He}_{g.s.} + ^6\text{He}_{g.s.}$ one (white squares) as the spin becomes high. This is because the coupling with the scattering continuum becomes strong in high spin region and hence, it becomes difficult to identify these two bands as the isolated states. In addition, the $^5\text{He}_{g.s.} + ^7\text{He}_{g.s.}$ molecular band (white circles with the solid line) appears with the comparable moment of inertia to those of the $\alpha+^8\text{He}_{g.s.}$ and $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$ bands. The SD band with covalent neutrons appears at the energy quite close to the $^4\text{He}^+ + ^\text{He}$ molecular bands. The estimated moment of inertia is larger than the ground rotational band. This covalent SD band is shown up to $J^\pi=4^+$, though we
can see some resonant behaviors in the S-matrix of $J^\pi=6^+$. The more accurate identification of the resonance poles could be done by imposing the absorbing boundary [18], which is a feature problem.

The present calculation well reproduces the energy-spin systematics of the experimental data shown by the crosses [9] and especially the shaded area where the resonance structures are fragmented [10]. In order to obtain the resonances with small energy interval, it becomes quite important to describe not only local minimum states of AESs but also crossover from MO to AO, which are generated as shoulder states in the outer region. In low-energy reactions, MRs with AO structures are strongly excited at this region. Our method covers both model spaces of MO and AO and hence, such fragmented phenomena of the resonances can be described.

4. Summary and future perspective

In summary, we have studied the exotic structures and the reaction dynamics of the highly excited states of $^{12}$Be as an unbound system by applying GTCM. We explored the structure of the adiabatic energy surfaces and showed the crossover from the neutrons’ covalent configuration to the ionic one. The rotational band structures are also investigated by solving the coupled channel GCM equation without any adiabatic approximations, in which coupling with all the possible neutron configurations and the open channels is explicitly taken into account. We found the superdeformation with covalent neutrons and the $^4$He+$^4$He molecular resonances coexist within small energy interval. The present results of the $\alpha+^4$He scattering will be directly compared with the future experiment which is planned at GANIL [19]. This is the first study pointing out the coexistence phenomena of molecular resonances and superdeformations, which shall be generally observed in light neutron-rich nuclei, and systematic studies are now proceeding.

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