

## Coexistence of Covalent Superdeformation and Molecular Resonances in an Unbound Region of $^{12}\text{Be}$

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

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Since the superdeformed (SD) rotational band has been discovered in  $^{152}\text{Dy}$  [1], the observation of the SD band has been extended to the light mass region up to  $^{36}\text{Ar}$ , and its existence in  $^{32}\text{S}$  has been discussed quite recently. For systems lighter than  $^{32}\text{S}$ , strongly deformed states have been discussed from the view point of the so-called "molecular resonances" (MRs) for a long time [2]. Recent study points out that the SD band with a deformed mean field structure and the  $^{16}\text{O} + {}^{16}\text{O}$  MRs corresponding to a binary cluster structure appear with a large energy interval of about 10 ~ 20 MeV [3]. Therefore, coexistence of the SD band and the MRs is being discussed in the  $A \sim 30$  region; however, in nuclei with  $N = Z$ , the interplay is not so prominent due to the large energy difference between these two structures.

In further light systems, there appear a great variety of strongly deformed structures which build on clusters if valence neutrons are added. For instance, a molecular orbital (MO) structure, where a valence neutron rotates around clusters simultaneously, is found to appear in light neutron-rich ( $N > Z$ ) systems [4,5]. The MO is quite different from the MRs. The MO states are realized at the local energy minima with a definite deformation parameter; hence, the MO is similar to the SD state of the deformed mean field. However, no definite intercluster distance for the MRs exist since the MRs are barrier-top resonances. In this Letter, we propose a new type of *superdeformed* structure based on the MO picture in a light  $N > Z$  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 isotopes are typical examples of two-center superdeformed systems which build on an  $\alpha + \alpha$  rotor of  ${}^8\text{Be}$ . The low-lying states of these systems can be described by the MO such as  $\pi^-$  and  $\sigma^+$  orbitals associated with the covalent electrons of atomic

molecules. Since the  $\sigma^+$  orbital has an extended distribution along the  $\alpha - \alpha$  axis, it enhances the  $\alpha - \alpha$  distance to reduce the neutrons' kinetic energy [4]. This means that the large prolate deformation with the two centers can be generated by this orbital. In  $^{10}\text{Be}$ , for example, the rotational band from the  $0_2^+$  state with the configuration of  $(\sigma^+)^2$  has a large moment of inertia, which has just been identified by the latest experiment [6]. Therefore, the configurations associated with the  $\sigma^+$  orbital should be called a "superdeformation with covalent neutrons" (covalent SD), which is the foundation for a new type of the superdeformation proposed in this Letter.

Furthermore, recent experiments on  $^{12}\text{Be}$  revealed the existence of many resonant states with small energy spacings of less than 1 MeV [7–9]. The observed resonances strongly decay into  ${}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$  and  $\alpha + {}^8\text{He}_{g.s.}$ , and similar resonances, decaying to He isotopes, have also been observed in  $^{10}\text{Be}$  [8] and  $^{14}\text{Be}$  [9]. These resonances are the candidates for  ${}^X\text{He} + {}^Y\text{He}$  MRs ( $X, Y = 4, 6, 8$ ) analog to ionic electron configurations, where neutrons are trapped around one of  $\alpha$  cores. Some of the states may be described by the MO picture [5], but the MO model cannot explain all the observed resonances. In Be isotopes, only a small amount of energy is required for the rearrangements between the covalent (MO) neutron structures and the ionic ones due to the weakness of the  $\alpha - N$  and neutron-neutron interactions. Therefore, above the particle-decay thresholds into two He-fragments, the covalent SD and the MRs may coexist in the same energy region with a crucial interplay among them.

In order to investigate the coexistence phenomena, the intrinsic structures and their 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  $^X\text{He} + ^Y\text{He}$  MRs [10,11] because the decaying He clusters are generated outside their contact distance. In studies of the unbound region of the nuclei, therefore, a theoretical model should cover both the MO and AO configurations.

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

In the generalized two-center cluster model (GTCM), the total wave function of  $^{12}\text{Be}$  is given by the superposition of the basis  $\{\Phi_{\mathbf{m}}^{J^\pi K}(S)\}$ , where,

$$\Phi_{\mathbf{m}}^{J^\pi K}(S) = \hat{P}_K^{J^\pi} \mathcal{A} \left\{ \psi_L(\alpha) \psi_R(\alpha) \prod_{j=1}^4 \varphi_j(m_j) \right\}_S. \quad (1)$$

The  $\alpha$  cluster  $\psi_n(\alpha)$  ( $n = L, R$ ) is expressed by the  $(0s)^4$  configuration of the harmonic oscillator (HO) centered at the left ( $L$ ) or right ( $R$ ) side with the relative distance  $S$  [14]. The single-particle wave function for the four valence neutrons localized around one of the  $\alpha$  clusters is given by an atomic orbital (AO)  $\varphi(p_k, i, \tau)$ , and  $0p$  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  $\mathbf{m}$  represents a set of AOs for the four neutrons,  $\mathbf{m} = (m_1, m_2, m_3, m_4)$ . The intrinsic basis functions with the full antisymmetrization  $\mathcal{A}$  are projected to the eigenstate of the total spin  $J$ , its intrinsic angular projection  $K$ , and the total parity  $\pi$  by the projection operator  $\hat{P}_K^{J^\pi}$ .

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

$$\hat{\Psi}_\nu^{J^\pi} = \int dS \sum_{\mathbf{m}, K} C_{\mathbf{m}, K}^\nu(S) \Phi_{\mathbf{m}}^{J^\pi K}(S). \quad (2)$$

The coefficients for the  $\nu$ th eigenstate,  $C_{\mathbf{m}, K}^\nu(S)$ , are determined by solving a coupled channel GCM (generator coordinate method) equation [14]. 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 [12]. 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. [13], which successfully reproduce the properties of  $^{10}\text{Be}$ . The adopted parameter set reasonably reproduces the threshold energies of  $\alpha + ^8\text{He}_{g.s.}$ ,  $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$ , and  $^5\text{He}_{g.s.} + ^7\text{He}_{g.s.}$ . This reproduction is essential in the treatment of scattering phenomena.

If we fix the distance parameter  $S$  and diagonalize the Hamiltonian with respect to  $\mathbf{m}$  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  $J^\pi = 0^+$  states. There appear two (green and pink) lines below the  $\alpha + ^8\text{He}_{g.s.}$  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 green line is  $(\pi_{3/2}^-)^2(\sigma_{1/2}^+)^2$ , while the pink line has the dominant configuration of  $(\pi_{3/2}^-)^2 \times (\pi_{1/2}^-)^2$  for the four neutrons, corresponding to the  $(0p)^2 \times (sd)^2$  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; hence, the strong mixing of these configurations occurs around the optimal  $S$  value. Because of the mixing of the  $sd$ -shell components, the  $N = 8$  magicity of the  $p$  shell is broken in the ground state, which is consistent with recent observation [15]. As  $S$  increases, these two surfaces are continuously changed to  $\alpha + ^8\text{He}_{g.s.}$  (green circles) and  $^5\text{He}_{g.s.} + ^7\text{He}_{g.s.}$  (pink 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 a crossover from the MO structure to the AO one.

In the energy region above the threshold, there is another crossing of two AESs (red and blue). Around the energy minimum point of the red curve, two of the valence neutrons are localized around individual  $\alpha$  as  $^5\text{He} + ^5\text{He}$ , which is the AO structure, and the remaining two neutrons occupy the  $\sigma^+$  orbital and rotate around both clusters, which represents the MO character. Because of the two neutrons in the  $\sigma^+$  orbital, the clustering (the optimal  $S$  value) is enhanced in the same way as in the second  $0^+$  state of  $^{10}\text{Be}$  [4,12,13]. Thus, the state is the covalent SD state. However, in this Letter, two other neutrons have the

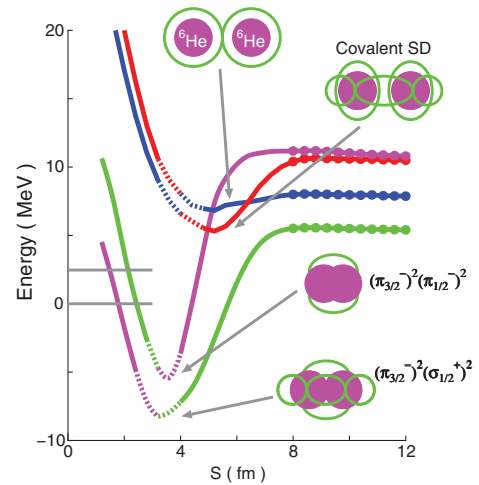


FIG. 1 (color). Adiabatic energy surfaces (AESs) for  $J^\pi = 0^+$ . The calculated threshold for the open channels,  $\alpha + ^8\text{He}_{g.s.}$  (origin of the ordinate) and  $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$  are also shown.

ionic (AO) configuration, and the appearance of the hybrid configuration with both MO and AO characters is a new feature in  $^{12}\text{Be}$ , which has not been seen in our previous work on  $^{10}\text{Be}$ . The blue surface has a specific character such 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 configuration is the one suggested in Ref. [5] as a cluster rotational band in the energy region above the threshold, but it is smoothly changed to the  ${}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$  configuration at larger  $S$  values.

The energy spectra of bound states are obtained not by the adiabatic approximation, but by re-diagonalizing the original Hamiltonian on 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 Kamimura's method [16]. In this method, we solve the coupling between the closed channels expressed by the linear combination of the discrete solutions of Eq. (2) with the finite range of  $S$  and the binary open channels on which the scattering boundary condition is explicitly imposed [13,17]. We consider three rearrangement channels,  $\alpha + {}^8\text{He}_{g.s.}$ ,  ${}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$ , and  ${}^5\text{He}_{g.s.} + {}^7\text{He}_{g.s.}$  as the open channels, in which  ${}^5,7\text{He}$  are described by the HO wave functions.  ${}^5,7\text{He}$  are unbound nuclei, but this treatment gives rise to no serious problems if we discuss the reactions between the former two channels.

By imposing the appropriate boundary conditions, we obtain whole energy spectra from the bound states to the unbound ones as shown in Fig. 2 ( $J^\pi = 0^+$ ). In this figure, the scattering matrix ( $S$  matrix) for the two-neutron

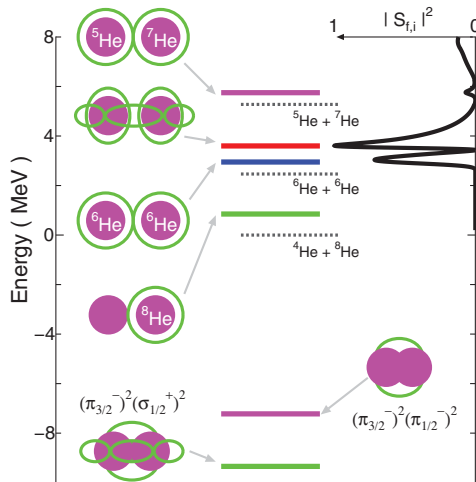


FIG. 2 (color). Energy spectra for  $J^\pi = 0^+$ . The solid curve at the right side shows the squared magnitude of the  $S$  matrix for  $\alpha + {}^8\text{He}_{g.s.} \rightarrow {}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$  with a respective scale at the top-right corner. The dotted lines represent the threshold energy of the open channels considered in the calculation.

transfer reactions,  $\alpha + {}^8\text{He}_{g.s.} \rightarrow {}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$ , is also shown. The resonance energies are identified by checking the anticlockwise behavior of the  $S$  matrix in the complex plane. The obtained  $0^+$  states are classified into three categories:

(i) *MO states*.—Two bound states appear below the  $\alpha + {}^8\text{He}_{g.s.}$  threshold ( $0_1^+$  and  $0_2^+$  shown by green and pink, respectively), which correspond to the lowest two local minima in Fig. 1. The energy difference is about 2 MeV and this difference agrees with recent observation [15]. 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,  $0_3^+$  (green),  $0_4^+$  (blue), and  $0_6^+$  (pink) have the MR characters of the corresponding threshold ( $\alpha + {}^8\text{He}$ ,  ${}^6\text{He} + {}^6\text{He}$ , and  ${}^5\text{He} + {}^7\text{He}$ , respectively). The resonance states have large overlap with the AESs shown by the respective colors in Fig. 1; the  $0_4^+$  state largely overlaps with the blue curve, while  $0_3^+$  and  $0_6^+$  overlap with the green and pink AESs, respectively. The main components of the latter two states spread outside the region of  $S > 5$  fm where the AESs do not have any local minima, but have shoulderlike shapes. This spreading means that  $0_3^+$  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 the crossover from MO to AO, their smooth connection with a variation of  $S$  is essentially important in describing MR states as excitations of the clusters' relative motion.

(iii) *Mixed symmetry state*.—The main component of  $0_5^+$  (red) is the local minimum of the red curve in Fig. 1, which is the mixture of  $(\sigma^+)^2$  (MO) and  ${}^5\text{He} + {}^5\text{He}$  (AO). This state has a large clustering ( $S \sim 5$  fm) due to the  $(\sigma^+)^2$  formation.

The  $0_4^+$  and  $0_5^+$  states are strongly excited by the two-neutron transfer reactions. In particular, the magnitude of the  $S$  matrix reaches the unitary 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 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.

We performed the same kind of calculations for other  $J^\pi$  states and identified the resonance energies, which are shown in Fig. 3. Six rotational bands are identified and they are plotted by the same colors as the band heads shown in Fig. 2. The maximum spin of the ground rotational band (green squares) reaches to  $J^\pi = 8^+$  because of the  $(\sigma^+)^2$  nature of the neutrons, while the second band (pink squares) has the component of a closed  $p$ -shell configuration for the neutrons. Furthermore, there appear four rotational bands in the continuum region. We can see the overlapping behavior of the  $\alpha + {}^8\text{He}_{g.s.}$  band (green

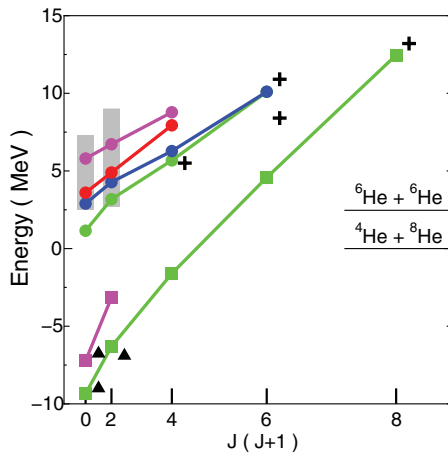


FIG. 3 (color). Rotational bands of  $^{12}\text{Be}$ . The shaded area represents the region where the resonances are observed [9], while the crosses and the triangles show the data in Refs. [8,15], respectively. The resonance energies of Refs. [8,9] are measured from the calculated threshold of  ${}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$ .

circles) and  ${}^6\text{He}_{g.s.} + {}^6\text{He}_{g.s.}$  one (blue) as the spin becomes high. This behavior is because coupling with the scattering continuum becomes strong in the high-spin region; hence, identifying these two bands as isolated states becomes difficult. In addition, the  ${}^5\text{He}_{g.s.} + {}^7\text{He}_{g.s.}$  molecular band (pink circles) appears with a moment of inertia comparable 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 (red) appears quite close to the  ${}^X\text{He} + {}^Y\text{He}$  molecular bands. The estimated moment of inertia is larger than that of the ground state. This covalent SD band is shown up to  $J^\pi = 4^+$ , though we can see some resonant behaviors in the  $S$  matrix of  $J^\pi = 6^+$ . By imposing the absorbing boundary [17], which is a feature problem, a more accurate identification of the resonance poles can be done.

The present calculation reproduces well the energy-spin systematics of the experimental data shown by the crosses [8] and especially the shaded area where the resonance structures are fragmented [9]. In order to obtain the resonances with small energy spacings, it becomes quite important to describe not only the local minimum states of AESs, but also the crossovers 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 phenomena of fragmented resonances can be described.

In summary, we have studied the exotic structures and the reaction dynamics of the highly excited states of  $^{12}\text{Be}$  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 have also been 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  ${}^X\text{He} + {}^Y\text{He}$  molecular resonances coexist within a small energy interval. The present results of the  $\alpha + {}^8\text{He}$  scattering will be directly compared with a future experiment, which is planned at GANIL [18]. This is the first study pointing out the coexistence phenomena of molecular resonances and superdeformations, which would be generally observed in light neutron-rich nuclei, and systematic studies are now proceeding.

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