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Molecular Structures and monopole excitations in light neutron-excess systems

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Abstract. The generalized two-center cluster model (GTCM), which can treat covalent, ionic and atomic configurations in general systems with two inert cores plus valence nucleons, is formulated on the basis of the microscopic cluster model. In this model, the covalent configurations constructed by the molecular orbital (MO) method and the atomic (or ionic) configuration obtained by the valence bonding (VB) method can be handled in a consistent manner. GTCM is applied to the light neutron-rich system, ^{12}Be $= \alpha + \alpha + 4N$. The energy spectra are characterized in terms of the excitation degrees of freedom, such as the the excitation of two α relative motion and the neutrons' single particle excitation. A large enhancement in a monopole transition from a ground MO state to the excited states is found, which seems to be consistent to a recent observation. The systematics of the 0^+ states in even Be isotopes over a wide range of the excitation energy is also discussed.

1. Introduction

In the last two decades, developments of experiments with secondary RI beam have extensively advanced the studies on light neutron-rich nuclei. In particular, much efforts have been devoted to the investigation of molecular structure in Be isotopes. The Be isotopes can be considered as typical examples of two-center superdeformed systems which build on an $\alpha + \alpha$ rotor of ^{8}Be. Theoretically, molecular orbital (MO), such as the π^- and σ^+ orbitals associated with the covalent bonding in molecular systems, have been successful in understanding the low-lying states of Be isotopes as well as B isotopes [1, 2, 3].

There is a long history in the MO model, and the MO picture has been extended to various systems beyond the Be and B isotopes [4, 5]. The MO model can describe many kinds of characteristic properties of Be and B isotopes, but they are mainly limited to the analysis on low-lying bound states, and theoretical studies on the highly excited states above the particle-decay threshold is still open area. In contrast to the situation of theoretical studies, recent experiments on ^{12}Be revealed the existence of many resonant states [6, 7], which strongly decay into ^{6}He$_{g.s.}$+^{6}He$_{g.s.}$ and α+^{8}He$_{g.s.}$. These resonances are expected to have the structures similar to the ionic or valence bonding (VB) structure in molecular physics, in which electrons are trapped in one of ions and generate the exchange force due to the anti-symmetrization effect.

In the present study, we investigate the exotic molecular structures appearing in an unbound region of ^{12}Be and even Be isotopes. In order to do a unified study of the ionic VB structures in a continuum and the low-lying MO structures, the traditional MO model [1, 2] must be extended because the MO structures do not satisfy the asymptotic boundary condition of the scattering states in a continuum, which are described by the ionic VB structures. Therefore, the MO and VB structures are combined to each other for the study of various molecular structures, appearing from bound states to continuum states.

For this purpose, we have formulated the generalized two-center cluster model (GTCM) [8]. In this model, the covalent MO configuration can be smoothly connected to the atomic or ionic VB configuration, in which valence neutrons are localized around one of the α cores. Furthermore, it becomes possible to describe both the formation of the covalent MO structures and the reaction process induced by the collision of the ionic VB state. In ^{12}Be for instance, this model can handle the formation of an atomic structure of ^{6}He+^{6}He, ionic structures of α+^{8}He and ^{5}He+^{7}He, and covalent MO structures in a consistent manner. In this report, we investigate the exotic molecular structures based on two α cores plus excess neutrons in ^{12}Be, which appears in the continuum energy region. In addition, we also discuss the monopole excitation in ^{12}Be. The monopole excitation is considered to be a candidate of a sign to identify the molecular structure [9, 10]. Finally, the application of GTCM is extended to even Be isotopes, and the systematic analysis of even Be isotopes are presented.

2. Theoretical Framework

The detailed explanation of GTCM has already been published in Refs. [8, 9], and we briefly explain its formulation in the following. In this model, the basis function of Be = $\alpha + \alpha + \mathrm{X}N$ is given by the $\{\Phi^{J^\pi K}_{\mathbf{m}}(S)\}$, where,

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

The α-cluster $\psi_n(\alpha)$ (n=L, R) is expressed by the $(0\mathrm{s})^4$ configuration of the harmonic oscillator (HO) centered at the left(L)- or right(R)- side with the relative distance S. The single-particle wave function for the valence neutrons localized around one of the α 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 τ (= $\uparrow$ or $\downarrow$).

Here, $\{m_j\}$ are indices of AO (p_k, i, τ) and $\mathbf{m}$ represents a set of AOs for the valence neutrons, $\mathbf{m}$=$(m_1 \sim m_X)$. The intrinsic basis functions with the full anti-symmetrization $\mathcal{A}$ are projected to the eigenstate of the total spin J, its intrinsic angular projection K, and the total parity π by the projection operator $\hat{P}^{J^\pi}_K$.

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

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

The coefficients for the ν-th eigenstate, $C^\nu_{\mathbf{m}K}(S)$, are determined by solving a coupled-channel GCM (Generator Coordinate Method) equation [11]. The present calculation is restricted to the J=K=0 case; however, we include all the possible AO configurations for the excess neutrons within this approximation. Therefore, the MO structures, where each valence neutron rotates around two centers simultaneously, and the VB structures with the ionic configuration of the excess neutrons, can be handled in a consistent manner [8, 9].

As for the nucleon-nucleon interaction, we use the Volkov No.2 [12] and the G3RS [13] 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 Refs. [8, 9], which successfully reproduce the properties of ^{10,12}Be. The adopted parameter set reasonably reproduces the threshold energies of ^{x}He+^{y}He in respective Be isotopes.

The unified treatment of the formation of the intrinsic states, which have the MO or VB structures, and their coupling to the scattering continuum can be achieved by the combined method of GTCM [8, 9] and the closed state method [14, 15]. In this method, the total wave function is given by the following linear combination

$$\Psi^{J^\pi(+)} = \sum_\beta \varphi_\beta \, \chi_\beta^{(+)} + \sum_\nu b_\nu \hat{\Psi}_\nu^{J^\pi} \quad . \tag{3}$$

The first term stands for the "open channels" labeled by β, on which the scattering boundary condition is explicitly imposed [8, 9]. Here, φ_β and $\chi_\beta^{(+)}$ denote the internal and relative wave-functions of the two scattering nuclei, and the whole nucleons included in the scattering nuclei are completely anti-symmetrized. In the calculation of the ^{12}Be $= \alpha + \alpha + 4N$ system, for instance, we consider three rearrangement channels, such as α+^{8}He$_{g.s.}$, ^{6}He$_{g.s.}$+^{6}He$_{g.s.}$ and ^{5}He$_{g.s.}$+^{7}He$_{g.s.}$, as open channels.

The second term stands for the "intrinsic states" confined within the interaction region, which is a linear combination of the solutions in Eq. (2). The solutions in Eq. (2) are simply calculated by the diagonalization procedure. Therefore, the basis of the intrinsic states, $\hat{\Psi}_\nu^{J^\pi}$ labeled by an eigenvalue number ν, is damped in the asymptotic region. The second term describes the closed compound states formed before decaying into the binary open channels.

3. Results

3.1. Classification of the levels according to the excitation degrees of freedom

The energy levels of ^{12}Be are calculated under the appropriate boundary conditions; the bound state boundary condition and the scattering boundary condition. The internal MO states, $(\pi_{3/2}^-)^2(\sigma_{1/2}^+)^2$ in 0_1^+ and $(\pi_{3/2}^-)^2(\pi_{1/2}^-)^2$ in 0_2^+, appear in the bound region. In addition to bound MO states, we newly identified the four resonant states with a various structures: α+^{8}He$_{g.s.}$ in 0_3^+, ^{5}He$_{g.s.}$+^{7}He$_{g.s.}$ in 0_6^+, ^{6}He$_{g.s.}$+^{6}He$_{g.s.}$ in 0_4^+, $\tilde{\varphi}(L)\tilde{\varphi}(R)(\sigma_{1/2}^+)^2$ in 0_5^+.

The excitation schemes of these six 0^+ states are explained in Ref. [8], and they are classified in Fig. 1. We briefly summarized the excitation schemes as follows: (1) Molecular orbital (MO) excitation: The excited states with a different type of the covalent MO structures corresponds to the MO excitation from the ground states. For example, the excitation of $0_1^+ \rightarrow 0_2^+$ can be interpreted in terms of the MO excitation with $(\sigma_{1/2}^+)^2 \rightarrow (\pi_{1/2}^-)^2$. In the similar manner, the 0_2^+ and 0_5^+ states are characterized by the MO excitation from the ground 0_1^+ state. These excitations involve the pair rearrangements of the neutrons: $(\sigma_{1/2}^+)^2 \rightarrow (\pi_{1/2}^-)^2$ for 0_2^+ and $(\pi_{3/2}^-)^2 \rightarrow \tilde{\varphi}(L)\tilde{\varphi}(R)$ for 0_5^+, in which $\tilde{\varphi}(i)$ denotes the atomic orbit localized at the center i $(=L, R)$. The MO excitations involves the change in the mean distance of two α cores.

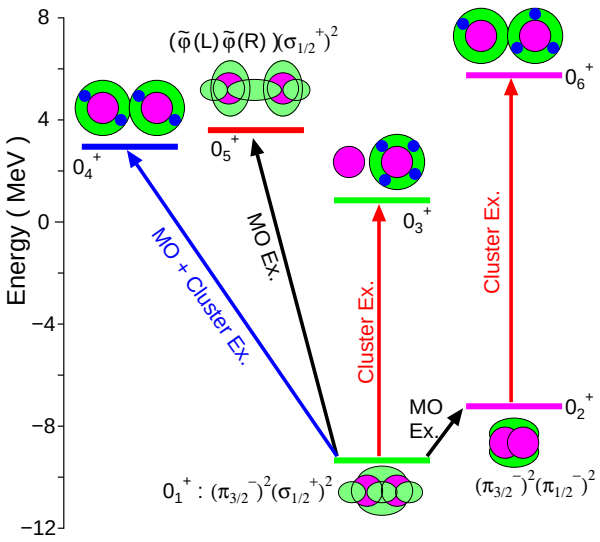

Figure 1. Energy spectra classified by the excitation degrees of freedom in ^{12}Be (J^π=0^+). See text for details.

(2) Cluster excitation: The 0_3^+ state has a
dominant amplitude of $\alpha + {}^8\mathrm{He}_{g.s.}$, and this state is realized as a result of the excitation of the $\alpha - \alpha$ relative wave function from the 0_1^+ state. Specifically, the 0_3^+ state corresponds to the higher nodal state of the 0_1^+ state. In a similar classification, the 0_6^+ state with ${}^5\mathrm{He}_{g.s.} + {}^7\mathrm{He}_{g.s.}$ corresponds to the excited state of the two α relative motion from the 0_2^+ state.

(3) Double excitation: The main component of 0_4^+ is a linear combination of the MO configuration of $(\pi_{3/2}^-)^2(\pi_{3/2}^+)^2$ and the VB configuration of ${}^6\mathrm{He}_{g.s.}+{}^6\mathrm{He}_{g.s.}$. The mixture of these two configurations is generated by the double excitations in the $\alpha - \alpha$ relative motion and the excitation of the MO motion of the excess neutrons.

The ^{12}Be nucleus is constructed by adding four excess neutrons to the unbound two α cores of ^{8}Be. This means that, in ${}^{12}\mathrm{Be} = \alpha + \alpha + 4N$, the ground state contains two degrees of freedom by nature: the $\alpha - \alpha$ relative motion and the single particle motion of the four excess neutrons. All the excited states are realized by activating these two degrees of freedom although these degrees of freedom are not strongly activated in the ground state.

3.2. Monopole transition in ^{12}Be

It is very interesting to consider the dynamical excitation of the static structures summarized in Fig. 1 in realistic experiments. We consider the monopole excitation, which is a direct transition from the ground 0_1^+ to the excited 0^+ states. The monopole transition is expected to be an important key to identify the excitation degrees of freedom [8, 10]. The monopole operators for the isoscalar transition ($\hat{\mathcal{M}}(IS)$) and isovector transition ($\hat{\mathcal{M}}(IV)$) are given by

$$\hat{\mathcal{M}}(IS) \;=\; \sum_{i=1}^{A} \xi_i^2, \quad \hat{\mathcal{M}}(IV) \;=\; \sum_{i=1}^{A} \xi_i^2 \tau_{3i} \;\;, \tag{4}$$

where ξ_i is a coordinate of i-th nucleon measured from the center of mass in the total system. Both the operators in Eqs. (4) are composed of the squared radius operators for composite nucleons and hence, monopole excitations are sensitive to the (transition) density distribution of a nucleus; specifically, the isoscalar operator strongly sensitive to a total density distribution of a nucleus, while the isovector operator strongly responds to a difference of the neutron and proton distributions.

Here we focus on the case of ^{12}Be and discuss the ratio of the monopole matrix elements, such as

$$\left|\tilde{M}(T)\right| \;\equiv\; \left|\frac{M(T)}{M^{s.p.}}\right|, \;\; T \;=\; IS, IV \;\;. \tag{5}$$

Here $M(T)$ denotes the monopole matrix elements defined by

$$M(T) \;= < 0_\nu^+ |\, \hat{\mathcal{M}}(T) \,|\, 0_1^+ > \quad (\nu = 2 \sim 6) \tag{6}$$

with $T = IS$ or IV, while $M^{s.p.}$ represents the single particle limit of the monopole strength [9].

In table 1, the ratio of the monopole strength for the isoscalar (IS) and isovector (IV) are shown. All the isoscalar strength ($|\tilde{M}(IS)|$) are comparable to or a few times larger than the single particle strength. In a recent experiment [7], the IS monopole matrix element for the 0_3^+ state, corresponding to the band head of $\alpha + {}^8\mathrm{He}_{g.s.}$, has been measured [7]. The observed $|\tilde{M}(IS)|$ strength is about 2.08, which is consistent to the GTCM calculation, $|\tilde{M}(IS)| = 3.53$, shown in table 1. The isovector ($|\tilde{M}(IV)|$) strength is weaker than the isoscalar strength, but all the magnitudes are still comparable to the single-particle limit value of $M^{s.p.}$. Thus, the monopole strength comparable to the single particle strength appears at $E_x \leq 20$ MeV in the present system.

State	$\lvert\tilde{M}(IS)\rvert$	$\lvert\tilde{M}(IV)\rvert$
0_2^+	2.59	0.98
0_3^+	3.53	0.75
0_4^+	0.92	0.69
0_5^+	1.48	0.90
0_6^+	1.76	0.57

Table 1. The ratios of the various monopole strength and the single particle strength in the $1p$-shell. Individual strength $\tilde{M}$ are defined by $\tilde{M}(T) \equiv M(T)/M^{s.p.}, T = IS, IV$.

The results shown in table 1 are in marked contrast to a naive mean field picture. In a naive mean field picture, a $2\hbar\omega$ ($\sim$ 35 MeV) jump is needed for monopole excitations because a monopole excitation of a single particle wave function involves one higher nodal excitation. The present calculations predict that the monopole strength comparable to the mean-field model appears in much lower energy region than the region expected in a naive mean-field picture.

3.3. Systematics in even Be isotopes

The systematics of the 0^+ energy levels in even Be isotopes is shown in Fig. 2. The systems becomes the bound states (discrete levels) and continuum states (continuous reaction probabilities) below and above the lowest He decay threshold energy, respectively. We can observe the formation of intruder 0^+ states along the levels connected by the dashed lines. In ^{8}Be, a well developed $\alpha + \alpha$ state exists just above the α threshold. This unbound two-α state becomes a bound 0_2^+ state at $E_x \sim 6$ MeV in ^{10}Be with two extra neutrons. The extra neutrons form the MO configuration of $(\sigma^+)^2$ around two α cores. The 0_2^+ state in ^{10}Be becomes the ground 0_1^+ state in ^{12}Be, which also has the MO configuration of $(\pi^+)^2(\sigma^+)^2$, and the systematics of ^{8,10,12}Be nicely reproduce the experimental observation. The energy of the intruder 0^+ state becomes high as a system goes to the neutron drip-line nuclei, ^{14,16}Be.

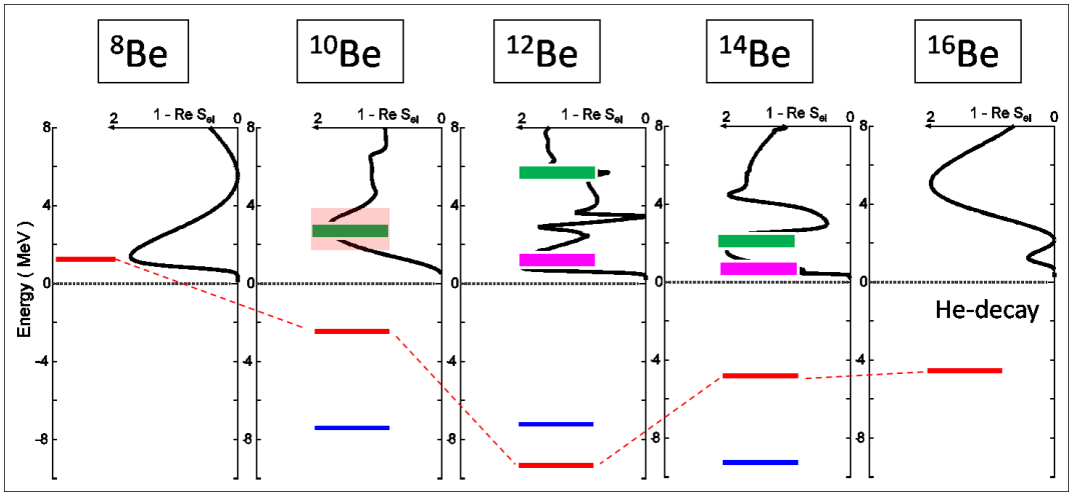

Figure 2. Systematics of the $J^\pi = 0^+$ energy levels for even Be isotopes. The lowest He-decay thresholds are taken to be zero energy point. The solid curves above the threshold represent the total reaction probabilities for the central collision. See text for details.

Above the He-decay threshold (dotted lines at zero energy), the several resonances are identified, and some of them are plotted by the solid lines in Fig. 2. The resonant levels mainly

have the VB structure of ^{x}He + ^{y}He, such as ^{10}Be = α + ^{6}He, ^{12}Be = α + ^{8}He and ^{14}Be = ^{6}He + ^{8}He. In ^{10,12,14}Be, the resonant VB levels are realized as the excitation of the $\alpha - \alpha$ relative motions from the bound 0^+_1 and 0^+_2 states. On the contrary, the 0^+_2 state corresponds to the excited states of the neutrons' MO motion from the ground 0^+_1 state. Therefore, the excited states in Be isotopes are generated by the excitations of two degrees of freedom: the $\alpha - \alpha$ relative motion and neutrons' MO motion. This results means that a ground states of Be isotopes have a hybrid structure of two α-cores and extra neutrons, and various excited states are generated by the excitation of these two degrees of freedom.

4. Summary

In summary, we have studied the exotic molecular structure in ^{12}Be and even Be isotopes from bound states to a continuum. To achieve the unified studies of the molecular orbit (MO) structure in a bound region and the valence bonding (VB) structure in a continuum, we have applied the generalized two-center cluster model (GTCM) [8, 9]. The energy levels are calculated under the appropriate boundary conditions. Various molecular structures appear in the excited states, and these molecular structures are classified in terms of the excitation degrees of freedom; the 2α excitations and the excitation of excess neutrons.

The isoscalar and isovector monopole strengths are investigated. We have found that all the energy levels have the monopole strengths comparable with or larger than the respective single-particle strength. As a consequence, in the ^{12}Be nucleus, strong monopole transitions can be observed in the lower energy region than the region expected from a naive mean-field picture. The magnitude of the monopole strength is consistent with recent observations [7].

The application of GTCM has been extended to even Be isotopes, and the energy levels of the 0^+ state are shown over a wide range of the excitation energy. In the bound region below the lowest He decay threshold, the covalent MO structures appears, while the ionic VB structures, such as ^{x}He+^{y}He, are realized in the unbound region. These two kinds of configurations are generated by the two α excitation and excitation of the excess neutrons. Therefore, the coupling of the α clusters and the excess neutrons is essential in the formation of the excited states.

The α cluster structure is not peculiar in Be isotopes but generally appear in the excited states in light $N = Z$ systems, such as ^{12}C = 3α, ^{16}O = α + ^{12}C and ^{20}Ne = α + ^{16}O, for example. Therefore, such the wide variety induced by the α cluster and the excess neutrons is expected to be general in the light nuclear systems, and the systematic studies is interesting. The application of GTCM to other cluster systems is now under progress.

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