Application of the generalized two-center cluster model to $^{10}\text{Be}$

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A generalized two-center cluster model (GTCM), including various partitions of the valence nucleons around two $\alpha$-cores, is proposed for studies on the exotic cluster structures of Be isotopes. This model is applied to the $^{10}\text{Be}=\alpha+\alpha+n+n$ system and the adiabatic energy surfaces for $\alpha-\alpha$ distances are calculated. It is found that this model naturally describes the formation of the molecular orbitals as well as that of asymptotic cluster states depending on their relative distance. In the negative-parity state, a new type of the $\alpha+{^4}\text{He}$ cluster structure is also predicted.

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Recent experiments by Freer et al. [1] revealed the existence of the interesting resonant states, which dominantly decay to $^6\text{He}_{g.s.} + ^6\text{He}_{g.s.}$ and $\alpha + ^8\text{He}_{g.s.}$ channels in the 10 to 25 MeV excitation energy interval of $^{12}\text{Be}$. Similar resonant states, decaying to He-isotopes such as $^6\text{He}$ and $^4\text{He}$, have also been observed in other Be isotopes of $^{10}\text{Be}$ [1] and $^{14}\text{Be}$ [2]. These experiments strongly suggest the existence of exotic cluster states consisting of the respective He-isotope clusters.

Theoretically, Kanada-En'yo and her collaborators [3] have studied a wide range of light nuclei within the anti-molecular orbital model (MOM), Itagaki et al. has extensively studied the low-lying states of Be isotopes to clarify the roles of valence neutrons on a development of clusterization. The molecular orbitals, such as $\pi$ and $\sigma$ orbitals associated with the covalent binding of atomic molecules, have been shown to give a good description for the low-lying states of Be-isotope clusters.

On the other hand, Descouvemont and Baye [4] have applied a traditional cluster model ($^6\text{He}+^6\text{He})+(\alpha+^8\text{He})$, assuming the substructures of $^6\text{He}_{g.s.}$ and $^8\text{He}_{g.s.}$, to illustrate the resonances observed in $^{12}\text{Be}$. However, it is plausible to assume $^6\text{He}$ and $^8\text{He}$ nuclei to be stable and frozen clusters because the energy for two-neutrons separation is quite small in both nuclei. Thus, it is properly considered that the valence neutron of $^6\text{He}$ and $^8\text{He}$ are associated with companion clusters when they approach each other, which is similar to the covalent binding of valence neutrons in the low-lying states.

The purpose of this letter is to study the molecular structures in low-lying and high-lying states in a unified way by taking into account couplings between a valence neutron’s motion and a relative motion of the $\alpha$ clusters. To achieve this purpose, we propose a new framework of a generalized two-center cluster model (GTCM) where we can describe atomic-orbital motions of valence neutrons around individual $\alpha$ clusters on the same footing with molecular orbitals, being a single-particle motion around two $\alpha$-cores. We apply this model to the $^{10}\text{Be}=\alpha+\alpha+n+n$ and discuss its applicability to studies of the molecular structure in both the low-lying and high-lying states.

The basis functions of GTCM for $^{10}\text{Be}$ are given as

$$\Phi^{J^T}_{K}(^{10}\text{Be};\ S)$$
$$= \hat{P}^{J}_{K}A \left\{ \psi_{L}(\alpha) \psi_{R}(\alpha) \sum_{m,n} d_{m}^{J^T_{K}} \varphi(m) \sum_{n} d_{n}^{J^T_{K}} \varphi(n) \right\} = \sum_{m,n} C_{m,n}^{J^T_{K}}(S) \Phi_{m,n}^{J^T_{K}}(S), \quad (1)$$
$$\Phi_{m,n}^{J^T_{K}}(S)$$
$$= \hat{P}^{J}_{K}A \left\{ \psi_{L}(\alpha) \psi_{R}(\alpha) \varphi(m) \varphi(n) \right\} \equiv \hat{P}^{J}_{K} \Phi_{m,n}^{\pi}(^{10}\text{Be};\ S), \quad (2)$$

where $C_{m,n}^{J^T_{K}}(S)$ means the product of $d_{J^T_{K}}^{m}$, $d_{J^T_{K}}^{n}$. The $\alpha$-cluster wave function $\psi_{i}(\alpha) (i=L, R)$ is given by the $(\theta b)^4$ configuration in the harmonic oscillator (HO) potential with the relative distance-parameter $S$. The position of an $\alpha$-cluster is explicitly specified as the left (L) or right (R) side. A single-particle state for valence neutrons around one of $\alpha$ clusters is given by an atomic orbitals, $\varphi(i, p_n, \tau)$ with the subscripts of a center $i (=L$ or $R$), a direction $p_n$ ($n=x, y, z$) of $0p$-orbitals and a neutron spin $\tau$ (= $\uparrow$ or $\downarrow$). In Eq. (2), the index $m(n)$ is an abbreviation of the atomic orbital $(i, p_n, \tau)$. The basis function $\Phi_{m,n}^{\pi}(^{10}\text{Be}; S)$ with the parity $\pi$ is projected to the eigenspace of the total spin $J$ and its intrinsic angular projection $K$ by the projection operator $\hat{P}^{J}_{K}$. Various linear combinations of $\Phi_{m,n}^{J^T_{K}}(S)$ can be shown to reproduce not only molecular orbital configurations but also cluster-model states of $^6\text{He}+^6\text{He}$ and $^4\text{He}+^8\text{He}$.

First, we illustrate that the molecular-orbital configuration of $(\sigma^+)^2$ can be constructed from a linear combination of the basis function for instance. Since $\sigma^+$ orbital
is expressed as $\varphi(L, p_z, \tau) - \varphi(R, p_z, \tau)$, the wave function of $^{10}$Be with $(\sigma^+)^2$ of valence neutrons are written as follows:

$$\hat{\Phi}^{(+)}_{10\text{Be}; S} = \mathcal{A}\{\psi_L(\alpha)\psi_R(\alpha)$$

$$\times(\varphi(L, p_z, \uparrow) - \varphi(R, p_z, \uparrow)) \cdot (\varphi(L, p_z, \downarrow) - \varphi(R, p_z, \downarrow))\}$$

$$= \mathcal{A}\{\psi_L(\alpha)\varphi(L, p_z, \uparrow)\varphi(L, p_z, \downarrow) \cdot \psi_R(\alpha)$$

$$- \psi_L(\alpha)\varphi(L, p_z, \uparrow) \cdot \psi_R(\alpha)\varphi(R, p_z, \downarrow)$$

$$- \psi_L(\alpha)\varphi(L, p_z, \downarrow) \cdot \psi_R(\alpha)\varphi(R, p_z, \uparrow)$$

$$+ \psi_L(\alpha) \cdot \psi_R(\alpha)\varphi(R, p_z, \uparrow) \varphi(R, p_z, \downarrow)\}. \quad (3)$$

This expression means that a $^{10}$Be wave function with the molecular orbitals can be described by a linear combination of various kinds of molecular orbitals. The valence neutrons are localized at one of $\alpha$-cores. For instance, $0p_{3/2} \downarrow \downarrow \uparrow \uparrow$ is expressed as $\{\varphi(i, p_z, \uparrow) - i\varphi(i, p_z, \uparrow)\}$. Thus, the $3/2^+ \downarrow$ states of $^6$He with the $0p_{3/2}$ neutron is written as $\sum_n \mathcal{A}\{\psi_i(\alpha) \cdot \varphi(n)\} = \mathcal{A}\{\psi_i(\alpha) \cdot \varphi_i(\uparrow, \uparrow)\} - \mathcal{A}\{\psi_i(\alpha) \cdot \varphi_i(\uparrow, \downarrow)\}$. Similarly, the $^6$He($I^\pi$) clusters with a definite intrinsic spin-parity $I^\pi$, such as $[0p_{3/2}^2]^{0+}$, can be constructed from a certain linear combination of $\sum_n \mathcal{A}\{\psi_i(\alpha) \cdot d_m \varphi(m) \cdot d_n \varphi(n)\}$. Therefore, the wave function of Eq. $\mathfrak{1}$ can describe the cluster-model states of $[\alpha \otimes ^6\text{He}(I^\pi)]$ and $[^6\text{He}(I^\pi_1) \otimes ^6\text{He}(I^\pi_2)]$.

The wave function of $^{10}$Be is finally given by taking a superposition over the relative distance-parameter $S$ and the intrinsic angular projection $K$ as

$$\Psi^{J^\pi}(^{10}\text{Be}) = \int dS \sum_K \Phi^{J^\pi}_{K}(^{10}\text{Be}; S)$$

$$= \int dS \sum_{K} C_{\beta K}^{J^\pi}(S) \Phi^{J^\pi}_{K}(S) \quad (4)$$

with $\beta \equiv (m, n)$. The coefficients $C_{\beta K}^{J^\pi}(S)$ are determined by solving a coupled channel GCM (Generator Coordinate Method) equation $\mathfrak{2}$:

$$\int dS \sum_{\beta K} C_{\beta K}^{J^\pi}(S)$$

$$\times \left\{\Phi_{\beta K}^{J^\pi}(S') \mid H - E^{J^\pi} \mid \Phi_{\beta K}^{J^\pi}(S)\right\} = 0. \quad (5)$$

To see the coupling properties, we solve Eq. $\mathfrak{5}$ in a step by step. First, we solve Eq. $\mathfrak{3}$ at a fixed $S$. Namely, we solve

$$\sum_{\beta K} C_{\beta K}^{J^\pi}(S)$$

$$\times \left\{\Phi_{\beta K}^{J^\pi}(S') \mid H - E^{J^\pi} \mid \Phi_{\beta K}^{J^\pi}(S)\right\} = 0. \quad (6)$$

The eigenvalue $E^{J^\pi}(S)$ is a function of the relative distance-parameter $S$, and then we call the solutions of energies and wave functions “adiabatic energy surfaces” and “adiabatic eigenstates”, respectively. The calculated adiabatic energy surfaces for the $J^\pi=0^+$ state are shown by open circles in Fig. $\mathfrak{1}$. Here, for the nucleon–nucleon interaction, we adopted the Volkov No.2 with the Majorana parameter $m=0.576$ and without the Bartlett and Heisenberg exchanges. Due to the reduction of the Majorana parameter, the total binding energy is gained and it becomes easy to see the continuum states. We also employed the G3RS interactions for the spin-orbit parts. The radius parameter $b$ of HO wave functions for $^{\alpha}$ clusters and valence neutrons is taken as 1.44 fm.

At the asymptotic distance ($S \to \infty$), where two $\alpha$-cores are completely separated, we can define the asymptotic channels such as $[^4\text{He}+^{6}\text{He}(I)]_L$ and $[^6\text{He}(I_1)+^{4}\text{He}(I_2)]_{1L}$, in which individual clusters have intrinsic spins $(I_1, I_2)$ and coupled with the channel spin $I=(I_1+I_2)$ and the relative one $L$. We call the coupling scheme of these asymptotic channels as “a cluster-coupling scheme”. The solid and dotted curves shown in the right part of Fig. $\mathfrak{1}$ are the expectation values $\langle H \rangle$ of the $[^4\text{He}+^{6}\text{He}(I)]_L$ and $[^6\text{He}(I_1)+^{4}\text{He}(I_2)]_{1L}$ clustering schemes, respectively.

From Fig. $\mathfrak{1}$ we can see that in $S \geq 6$ fm, the calculated energy surfaces are completely the same as those of cluster-coupling wave functions. This means that, in this region, the valence neutrons are localized at one of $\alpha$-cores and rotation of two clusters is de-coupled to each other. At the asymptotic region, therefore, each nucleus keeps its isolated states and weakly coupled to each other. On the other hand, in $S \leq 6$ fm, the energies for the cluster-coupling scheme deviate from the adiabatic energy surfaces.

We study the adiabatic eigenstates in an internal region ($S \lesssim 4$ fm) in the view of the molecular orbital formation. As shown in an example of $(\sigma^+)^2$ in Eq. $\mathfrak{3}$, the wave function of molecular orbitals is expressed by a linear combination of different kinds of cluster-wave functions, where each cluster has no good angular momenta. In the molecular orbitals, the valence neutrons are moving around two $\alpha$-cores with a specific direction in respect to the $\alpha-\alpha$ axis. Such a configuration of the system is called as “a strong-coupling scheme”. The overlap of the adiabatic eigenstates with the wave functions of molecular orbitals identifies the dominant components in the adiabatic eigenstates as shown in Fig. $\mathfrak{1}$. The adiabatic eigenstates connected by the thin-solid curves at the internal region have the common dominant-components of various kinds of molecular orbitals.
The lowest adiabatic surface A of Fig. 1. In up-most row, the distances of the calculated eigenstates are shown. The distance parameter of $S=6 \text{ fm}$ corresponds to the “intermediate-coupling region”. Thus, the eigenstate has “an intermediate coupling”.

Finally, the GCM equation (5) is solved by employing the basis states ranging from $S=1 \text{ fm}$ to $S=9 \text{ fm}$ with the mesh of 0.5 \text{ fm}. We obtain the result that the lowest three GCM solutions have energy gains of about 1−2 \text{ MeV}, and the dominant amplitudes around the respective local minimums in the adiabatic energy surfaces A, B and C. Therefore, these solutions of the $0^+_1$, $0^+_2$ and $0^+_3$ states are concluded to have the molecular-orbitals configuration of $(\pi_3/2)^2$, $(\alpha^+_1/2)^2$ and $(\sigma^+_1/2)^2$, respectively.

Similarly, we calculate the $J^\pi=1^-$ state. The calculated energy surfaces are shown in Fig. 2. We focus on the lowest five surfaces and investigated their intrinsic structure, because there is no definite local-minimums in higher surfaces. As shown by two vertical dotted-lines in Fig. 2, we find the dynamical transition from the strong-coupling scheme to the cluster-coupling one in the adiabatic surfaces. However, the first excited surface connected by a thick curve has an almost pure-component of the $[\alpha+6^6\text{He}(0^+_1)]_{J'=1^-}$ channel. Thus, this excited surface is made by the pure cluster-coupling state of this channel in a wide range of the $\alpha-\alpha$ distance.

The energy gain of the lowest three solution due to GCM is about 1−3 \text{ MeV} depending on the states. In the lowest and the third $1^-$ states, we find that the wave functions distribute around the respective local minimums of the adiabatic surfaces. Thus, the intrinsic struc-
structures of the $1^-_1$ and $1^-_3$ states are explained with the molecular orbitals of $(\pi_{3/2}\sigma_{1/2})^{\pm}_K=1$ and $(\pi_{1/2}\sigma_{1/2})^{\pm}_K=1$, respectively. The $1^-_2$ state has the main components of the first excited surface in Fig. 2 which is interpreted in terms of the cluster-coupling states of $\{a^6\text{He}(0^+_1)\}_{L=1}$. To see band structures in $^{10}$Be, we solve GCM Eq. (5) for the higher spins with a natural parity $(-1)^J$. The calculated bands are shown in Fig. 3 with an inset showing the respective observed states. The moment of inertia of individual bands is well reproduced. Furthermore, our model predicts the existence of the higher spin states which were suggested by a recent experiment. In the $(\sigma_{1/2}^\pm)^2$ band shown by the white circles, we find the enhancement of the $\{a^6\text{He}(2^+_1)\}_{L=4}$ state at a maximum spin (solid circle). In the present calculation, all the excitation energies is higher than those of the observed states. This can be improved by optimizing the nucleon-nucleon force and the radius $b$ to reproduce the cluster’s threshold energies. The reproduction of threshold energies is quite important for the study on the decay width. The quantitative analysis including the decay width will be given in forthcoming papers.

In summary, we proposed a generalized two-center cluster model (GTCM) and discussed its application to the $^{10}$Be=$\alpha+\alpha+n+n$ system with $J^p=0^+$ and $1^-$. The adiabatic energy surfaces depending on the $\alpha-\alpha$ distance were calculated. The adiabatic eigenstates have the molecular orbital configuration at an internal region, while they becomes the cluster-coupling states at an external one. The middle distances correspond to the transitional region having an intermediate coupling-scheme between the internal regions and the external ones. It should be noticed that, in our model, both schemes of the molecular-orbitals and cluster-coupling schemes can be naturally described in an equal footing without any difficulty relevant to the double-projection procedure.

Finally, we solved the coupling between the relative motions of clusters and the intrinsic motion of valence neutrons. The low-lying $0^+$ states and the lowest $1^-$ one have the respective molecular-orbital configurations, which are consistent with previous studies based on MOM [4] and AMD [5]. In addition, our model predicts the possible appearance of the $\{a^6\text{He}(2^+_1)\}_{L=4}$ cluster-structures in the lowest $6^+$ state. Furthermore, we theoretically obtain the second $1^-$ state with the $\{a^6\text{He}(0^+_1)\}_{L=1}$ structure and expect to observe it experimentally. To see correspondence with experiments, it is necessary to analyze resonant states above threshold energies. We are now going to tackle this problem.

In conclusion, we can say that GTCM well describes the low-lying molecular orbitals obtained by other theoretical models [4, 5, 8]. Furthermore, this model naturally reproduce the asymptotic cluster-coupling states which are described by the traditional cluster model [6] in an equal footing. These results indicate that the present GTCM is applicable to the study of low-lying and high-lying states in $^{10}$Be. Since the $\alpha+\alpha+2n$ model for $^{10}$Be is a special case (x=2) of a general $\alpha+\alpha+x\gamma$ model, it is very easy to apply GTCM to systematic studies of resonances observed in excited Be-isotopes as well as their low-lying states. In particular, its application to $^{12}$Be $=\alpha+\alpha+4n$ is very interesting because of their accumulated experimental results [1-2]. A direct extension to the $\alpha+\alpha+4n$ model for $^{12}$Be is is now under progress.

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