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Molecular-orbital structure in neutron-rich Be and C isotopes

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Abstract. The structure of Be and C isotopes are investigated based on the molecular-orbit (MO) model. The low-lying states are characterized by several configurations of valence neutrons, which are constructed as combinations of basic orbits. In ^{10}Be, all of the observed positive-parity bands and the negative-parity bands are described within the model. The second 0^+ state of ^{10}Be has a large α-α cluster structure, and this is characterized by a $(1/2^+_\sigma)^2$ configuration. An enlargement of the α-α distance due to two-valence neutrons along the α-α axis makes their wave function smooth and reduces the kinetic energy drastically. Furthermore, the contribution of the spin-orbit interaction due to coupling between the $S_z = 0$ and the $S_z = 1$ configurations, is important. In the ground state of ^{12}Be, the calculated energy exhibits similar characteristics, that the remarkable α clustering and the contribution of the spin-orbit interaction make the binding of the state with $(3/2^-_\pi)^2(1/2^+_\sigma)^2$ configuration properly stronger in comparison with the closed p-shell $(3/2^-_\pi)^2(1/2^-_\pi)^2$ configuration. This is related to the breaking of the $N = 8$ (closed p-shell) neutron magic number. Also, the molecule-like structure of the C isotopes is investigated using a microscopic α+α+α+n+n+$\cdots$ model. The combination of the valence neutrons in the π- and the σ-orbit is promising to stabilize the linear-chain state against the breathing and bending modes, and it is found that the excited states of ^{16}C are the most promising candidates for such structure.

PACS. 21.10.-k Properties of nuclei; nuclear energy levels – 21.60.Gx Cluster models

1 Introduction

Numerous experiments using unstable nuclear beams have succeeded in extending the observed neutron drip line, and various features of β-unstable nuclei have been revealed [1,2]. To discover new isotopes and exotic properties of weakly bound nuclei requires drastic changes in our understanding of the nuclear structure. For example, neutron halo structures in ^{6}He, ^{11}Li, ^{11}Be, ^{14}Be, ^{17}B and ^{19}C suggest a breaking of the density saturation due to weakly bound neutrons [3]. Anomalous is not only the halo structure of weakly bound neutrons, but also the change of the shell structure. Experimental results show that the number of neutrons in the drip line isotopes of p-shell nuclei Be and B go beyond the magic number $N = 8$ (^{14}Be, $N = 10$ and ^{19}B, $N = 14$). In these nuclei, neutrons occupy orbits in higher shells (sd-shell for Be). Since nuclei near to the drip line are weakly bound systems, energy gaps between the shells become small. Recently, contributions of such higher shells were analyzed in $N = 8$ nuclei. A calculation based on the shell model has shown that the slow β-decay of ^{12}Be to ^{12}B can be explained by an admixture of the sd-shell in ^{12}Be ($N = 8$) in which the closed p-shell component must be less than 30% [4]. This shows that the concept of magic numbers is vague in ^{12}Be.

In the case of light nuclei, it has been shown that cluster structure appears in the vicinity of a threshold energy [5,6]. This model is an important candidate for explaining shell-structure anomalies. In Be and B region, α-α structure is well established, and especially in ^{9}Be, a microscopic α+α+n model has reproduced the properties of low-lying states [7,8]. In ^{10}Be, the microscopic α-cluster model has also been applied [9,10], and a developed cluster structure in the excited states was considered. According to this analysis of ^{9}Be, the α-α cluster structure of the core can reproduce not only natural parity states, but also the famous anomalous parity $1/2^+$ state at low energy [7,8]. It has been shown that the density of the $1/2^+$ state is polarized along the α-α axis, so that there is a strong mixing of the s-wave and the d-wave component. The ratio of the spectroscopic factors $S^{1/2^+}[s_{1/2} \times {}^8\mathrm{Be}\ (0^+)]$ and $S^{1/2^+}[d_{5/2} \times {}^8\mathrm{Be}\ (2^+)]$ is 0.79 : 0.30 [8]. This polarization of the neutron density due to the α-α core is an important mechanism to make the $1/2^+$ state low lying. This strong-coupling feature of the $1/2^+$ state can be qualitatively interpreted in terms of deformed models as the [220] expression in the Nilsson diagram.

The intention of the present work was to analyze the structure of Be isotopes systematically beyond $N = 8$ and

to understand recent experimental data, including excited states based on the molecular-orbit (MO) model [11,12]. There have been pioneering studies for Be isotopes based on the MO model [9,10,13], where the properties of the low-lying states were qualitatively described, including the development of the α-α cluster structure in the excited states. However, to perform a systematic analysis of the structure of Be isotopes quantitatively over a wide energy range ($\sim$ 10 MeV), it is necessary to thoroughly improve the models. Here, we present a new framework in which the model space for valence neutrons are vastly extended.

Furthermore, the molecule-like structure of the C isotopes is investigated using a microscopic α+α+α+n+n+... model. Recently, the discussions of the well-developed cluster structure are extended to the neutron-rich nuclei, and the role of valence neutrons which stabilize the linear-chain structure has been pointed out. For example, von Oertzen has extended his analyses for the molecular structure in Be isotopes [14] to C isotopes, and the linear-chain state consisting of 3α and valence neutrons around it has been speculated. Even if the 3α-system without valence neutrons (^{12}C) does not have a linear-chain structure, the valence neutrons around it are expected to increase the binding energy and stabilize the linear-chain state.

2 Models

The total wave function of a microscopic α+α+n+n... model for the Be isotopes is fully antisymmetrized and expressed by a superposition of basis states centered to different relative distances between the α-clusters (d) with various configurations of the valence neutrons ($c1$, $c2$ ...) around the α-clusters:

$$\Phi^J_{MK} = \sum_{d,c1,c2\cdot\cdot} P^J_{MK}\mathcal{A}[\phi_1^{(\alpha)}\phi_2^{(\alpha)}(\phi_1^{c1}\chi_1)(\phi_2^{c2}\chi_2)\cdot\cdot]. \quad (1)$$

The projection to the eigenstates of angular momentum (P^J_{MK}) is performed numerically. Each α-cluster consisting of four nucleons is described by Gaussians ($G_{\alpha i}$) centered at $R_{\alpha i}$ and spin-isospin wave function(χ):

$$\phi_i^{(\alpha)} = G^{p\uparrow}_{R_{\alpha i}}G^{p\downarrow}_{R_{\alpha i}}G^{n\uparrow}_{R_{\alpha i}}G^{n\downarrow}_{R_{\alpha i}}\chi_{p\uparrow}\chi_{p\downarrow}\chi_{n\uparrow}\chi_{n\downarrow}, \qquad i=1,2 \quad (2)$$

$$G_R = \left(\frac{2\nu}{\pi}\right)^{\frac{3}{4}}\exp[-\nu(\mathbf{r}-\mathbf{R})^2], \qquad \nu = 1/2\beta^2, \quad (3)$$

where, the oscillator parameter (β) is equal to 1.46 fm. For the linear-chain state, the values of $\{R_{\alpha i}\}$ are $-d/2$ and $+d/2$ on the z-axis. Each valence neutron ($\phi_i^{ci}\chi_i$) around the α-α core is expressed by a linear combination of local Gaussians:

$$\phi_i^{ci}\chi_i = \sum_j g_j G_{R_j}\chi_i. \quad (4)$$

These valence-neutron orbits are classified according to the MO picture [13]. The orbit of the valence neutron perpendicular to the z-axis of the α-α core is called π-orbit, and one along the z-axis is called σ-orbit. The antisymmetrization imposes the forbidden space for the valence neutrons; the π-orbit must have at least one node perpendicular to the z-axis, and the σ-orbit must have at least two nodes since two α-clusters along the z-axis already occupy the orbitals with $n_z = 0, 1$.

In the present framework, each valence-neutron orbit is introduced to have a definite K^π value at the zero limit of centers of local Gaussians ($\{R^j\}$) describing the spatial distribution of the orbit. The precise positions of $\{R^j\}$ are determined variationally before the angular-momentum projection. Since the values of $\{R^j\}$ are optimized to be finite, the orbits are not exactly the eigenstate of K^π, and are labeled as $\bar{K}^\pi$. For the π-orbit with $\bar{K}^\pi = 3/2^-$ ($|3/2^-_\pi\rangle$), the spatial part and the spin part of $\bar{K}$ are defined to be parallel ($rY_{11}|n\uparrow\rangle$), for which the spin-orbit interaction acts attractively. At the same time, $|3/2^-_\pi\rangle$ is described as a linear combination of two orbits centered at the right- and left-hand side of the system based on the MO picture:

$$|3/2^-_\pi\rangle = \frac{1}{\sqrt{N_\pi}}\{(p_x+ip_y)_{+a}+(p_x+ip_y)_{-a}\}|n\uparrow\rangle, \quad (5)$$

$$(p_x)_{\pm a} = G_{\pm a\mathbf{e}_z+b\mathbf{e}_x} - G_{\pm a\mathbf{e}_z-b\mathbf{e}_x}, \quad (6)$$

$$(p_y)_{\pm a} = G_{\pm a\mathbf{e}_z+b\mathbf{e}_y} - G_{\pm a\mathbf{e}_z-b\mathbf{e}_y}. \quad (7)$$

Here, $(p_x+ip_y)_{\pm a}$ denotes the orbit centered at $\pm a$ on the z-axis, and these variational parameters a and b are optimized by using the Cooling Method in antisymmetrized molecular dynamics (AMD) [15–17] for each basis state. Furthermore, the $|1/2^-_\pi\rangle$ orbit, where the spin-orbit interaction acts repulsively, can also be defined by changing the spin direction of $|3/2^-_\pi\rangle$, where the spatial part and the spin part of $\bar{K}$ are antiparallel ($rY_{11}|n\downarrow\rangle$):

$$|1/2^-_\pi\rangle = \frac{1}{\sqrt{N_\pi}}\{(p_x+ip_y)_{+a}+(p_x+ip_y)_{-a}\}|n\downarrow\rangle. \quad (8)$$

The distribution of the σ-orbit is just along the α-α axis, then it is introduced to have two nodes. $|1/2^+_\sigma\rangle$ is represented as a linear combination of two orbits with $\bar{K} = 1/2$, whose centers are $+a$ and $-a$ on the z-axis:

$$|1/2^+_\sigma\rangle = \frac{1}{\sqrt{N_\sigma}}\{(p_z)_{+a}-(p_z)_{-a}\}|n\uparrow\rangle, \quad (9)$$

$$(p_z)_{\pm a} = G_{a\mathbf{e}_z+b\mathbf{e}_z} - G_{a\mathbf{e}_z-b\mathbf{e}_z}\,. \quad (10)$$

These three orbits ($|3/2^-_\pi\rangle$, $|1/2^-_\pi\rangle$ and $|1/2^+_\sigma\rangle$) are the basic building blocks for the molecular-orbital structure. Also, $|-3/2^-_\pi\rangle$, $|-1/2^-_\pi\rangle$ and $|-1/2^+_\sigma\rangle$ orbits are introduced by taking the time reversal of $|3/2^-_\pi\rangle$, $|1/2^-_\pi\rangle$, and $|1/2^+_\sigma\rangle$ orbits, respectively.

For C isotopes, MOs are introduced around 3α-clusters, and in this case, the σ-orbit must have at least three nodes since three α-clusters along the z-axis already occupy the orbitals with $n_z = 0, 1, 2$.

The Hamiltonian and the effective nucleon-nucleon interaction are the same as in refs. [11,12], and parameters of Volkov No. 2 [18] for the central part and the G3RS

spin-orbit term [19] for the spin-orbit part are determined from the $\alpha + n$ and $n + n$ scattering phase shifts, and the binding energy of deuteron is also reproduced with these parameters.

3 Results

3.1 Molecular structure in Be isotopes

In this subsection, we present the results for the Be isotopes. The basis states are combined using the Generator Coordinate Method (GCM). The energy levels of ^{10}Be are calculated with the bound-state approximation. Three 0^+ states appear. Their dominant valence neutron components are $(3/2^-_\pi)^2$ for the ground state, $(1/2^+_\sigma)^2$ for the second 0^+ state, $(1/2^-_\pi)^2$ for the third 0^+ state. The total energy of the ground state is calculated to be -61.4 MeV, which corresponds to -7.3 MeV with respect to $\alpha+\alpha+n+n$ threshold (the experimental value is -8.4 MeV). The 0^+_2 state and the 0^+_3 state are obtained at excitation energies of 8.1 MeV and 11.6 MeV, respectively. From the ground and the second 0^+ states, the $K^\pi = 0$ rotational bands are formed as i) 0^+_1 (0.0 MeV)–2^+_2 (3.3 MeV)–4^+_1 (10.7 MeV) and ii) 0^+_2 (8.1 MeV)–2^+_3 (9.5 MeV)–4^+_2 (12.5 MeV). The level spacing of 0^+_1–2^+_1 is 3.3 MeV, which nicely corresponds to the experimental value in ^{10}Be (3.37 MeV), which is almost comparable with the case of ^{8}Be (~ 3 MeV). On the contrary, the second 0^+ band has a very large moment of inertia, more than twice that of the ground state. The second 2^+ state at 5.8 MeV (exp. 6.0 MeV) and the 3^+ state at 9.6 MeV consist mainly of $K^\pi = 2^+$ components, and the 1^+ state at 10.1 MeV and 2^+_4 state at 11.2 MeV are dominantly the $K^\pi = 1^+$ (spin-triplet) components.

The experimentally observed levels clearly be reassigned to the ground-state rotational band (0^+_1, 0.0 MeV–2^+_1, 3.4 MeV–4^+_1, 11.3 MeV). For the second 0^+ band, the 0^+_2 and the 2^+_3 states are observed at 6.3 MeV and 7.5 MeV respectively, and a candidate for the 4^+ state of this band, whose cluster structure is recently discussed [21], is 10.2 MeV. All of these observed levels have a nice correspondence with the present calculated results.

The second 0^+ state has a much larger charge radius (2.93 fm, proton radius 0.813 fm is used) than the ground state (2.51 fm), which is a signature of the developed α-α structure. As for the configuration of this state, the result based on the shell model supports that valence neutrons occupy not the p-orbit, but the sd-orbit. In the Cohen-Kurath model [20], where all the configurations in the p-shell are taken into account, the excitation energies of the first and the second 2^+ states almost agree with the experimental values (2^+: 3.7 MeV and 2^+: 5.4 MeV, experimentally 3.4 MeV and 6.0 MeV, respectively). However, the second 0^+ state is put at 12.35 MeV. This energy is about twice the observed excitation energy of 0^+_2 (6.263 MeV). This result implies that the 0^+_2 state (band head of cluster band) cannot be understood within the p-shell and the contributions of sd-shells are required.

The negative-parity states are also calculated. In addition to reproducing the four observed states (1^-, 2^-, 3^- and 4^-), we predict a second 2^- state and a second 3^- state. The presence of two states for each J^π is due to a coupling effect between two bands: $K^\pi = 1^-$ and $K^\pi = 2^-$. In the $K^\pi = 1^-$ band, a valence neutron for the π-orbit and one for the σ-orbit have opposite spin directions ($S_z = 0$), and in the $K^\pi = 2^-$ band, they have the same spin direction ($S_z = 1$). Since the energies of these two bands are close and the coupling between them is strong, there is no clear band structure for the negative-parity states.

Both the calculated and the experimental results reflect this K-mixing effect, and the level spacing between the 1^- state and the 2^- state is very small. If we restrict ourselves to only $K = 1$, 1^- is found at -53.0 MeV and 2^- at -52.0 MeV. The level spacing is more than 1 MeV. However, for the 2^- state, the band head of the $K = 2^-$ band is at -51.6 MeV, and the coupling is very strong. Therefore, when we perform K-mixing, the level spacing between these two states becomes much smaller (-53.4 MeV for 1^-, -53.5 MeV for 2^-). Since $K = 2$ is a spin-triplet, this 2^- state has a strong admixture of the $K = 1$ component and the $K = 2$ component, just like in the so-called spin vibrational state.

We must notice that the spin-orbit interaction is shown to strongly contribute for the second 0^+ state, when spin-triplet states for the valence neutrons are included among the basis states. If the $1/2^+$ orbit is the pure s-orbit, naturally there is no contribution of the spin-orbit interaction. In Be isotopes, the orbit is not spherical but it contains the d-orbit component. However, the spin-orbit interaction again vanishes, when the two valence neutrons occupy along the α-α axis, since two neutrons with the same spatial distribution construct only the spin-singlet state. This has been the situation in traditional MO models [9, 10]. When one of the valence neutrons deviates from the α-α axis, the spin-triplet state can be constructed, and the spin-orbit interaction strongly acts between this state and the original $(1/2^+_\sigma)^2$ configuration with spin-singlet. The calculated second 0^+ energy shows that the smaller is the α-α distance, the larger is the contribution of the coupling with the spin-triplet state. When the α-α distance is 5 fm, the coupling of $S = 1$ to the original $(1/2^+_\sigma)^2$ increases the binding energy by about 3 MeV, however, when the α-α distance is 3 fm, the coupling increases the binding energy by about 4.5 MeV. Therefore, the coupling with the spin-triplet becomes stronger as the α-α distance becomes small.

Next, the large contribution of this spin-orbit interaction is discussed concerning ^{12}Be. In ^{12}Be, four valence neutrons rotate around two α-clusters and, mainly, two configurations are important for the 0^+ ground state. One is $(3/2^-_\pi)^2(1/2^-_\pi)^2$ for the four valence neutrons, which corresponds to the closed p-shell configuration of the neutrons at the zero limit of the α-α distance. The other configuration is $(3/2^-_\pi)^2(1/2^+_\sigma)^2$, where two of the four valence neutrons occupy the σ-orbit. We compare the energy of these two configurations as a function of the α-α distance. When

it is small, for example 2 fm, the dominant configuration of the four valence neutrons is $(3/2^-_\pi)^2(1/2^-_\pi)^2$ for the ground state. On the other hand, the $(3/2^-_\pi)^2(1/2^+_\sigma)^2$ configuration for the four valence neutrons becomes lower as the α-α distance is increased. Due to the spin-orbit coupling, the energy is almost the same as that of $(3/2^-_\pi)^2(1/2^-_\pi)^2$, corresponding to the closed p-shell configuration. Furthermore, the energy of $(3/2^-_\pi)^2(1/2^+_\sigma)^2$ is suggested to become even lower than $(3/2^-_\pi)^2(1/2^-_\pi)^2$ when the pairing effect between $(3/2^-_\pi)^2$ and $(1/2^-_\pi)^2$ is taken into account. These effects play crucial roles in accounting for breaking of the $N = 8$ magic number.

3.2 Molecular structure in C isotopes

In this subsection, the MO approach introduced for the Be isotopes is applied to a study of C isotopes. The stability of the linear-chain states (α-α-α linear configuration) against the breathing-like path and the bending-like path are shown to be increased by adding valence neutrons around a 3α-core.

We show the calculated results for the stability of the linear-chain state for various configurations. The isotopes and configurations which we take into account are ^{12}C, $^{14}\mathrm{C}(3/2^-_\pi)^2$ (two n's in the π-orbits), $^{14}\mathrm{C}(1/2^-_\sigma)^2$ (two n's in the σ-orbits), $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\pi)^2)$ (four n's in the π-orbits) and $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ (two n's in the π-orbits and two n's in the σ-orbits). Two variational paths are introduced corresponding to the breathing-like and the bending-like degrees of freedom. The parameters d and θ stand for the α-α distance and the bending angle of the 3α-core, respectively.

Firstly, we show the 0^+ energy curves for the linear-chain structure against the breathing path. It is found that the energy pocket around $d = 3$ fm (parameter d describes the α-α distance) becomes deeper as the increase of number of valence neutrons in the π-orbit (^{12}C $\rightarrow$ $^{14}\mathrm{C}(3/2^-_\pi)^2$ $\rightarrow$ $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\pi)^2)$). The 3α-system (^{12}C) has minimal energy around $d = 3.5$ fm, however, this is too shallow to conclude the stability of the linear-chain state. On the contrary, in $^{14}\mathrm{C}(3/2^-_\pi)^2$, there appears evident minimal energy around $d = 3$ fm. The energy (~ -82 MeV) is lower than ^{12}C by 11 MeV and the energy pocket is much deeper. This energy corresponds to the excitation energy of 18 MeV from the ground state calculated with an equilateral-triangle configuration for the 3α-core. $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\pi)^2)$ is most stable among these states and it has an energy pocket of ~ -86 MeV, and the corresponding α-α distance is $d = 2.5$ fm, shorter than ^{12}C and $^{14}\mathrm{C}(3/2^-_\pi)^2$. Therefore, the π-orbit is found to stabilize the linear-chain structure as the increase of valence neutrons and to prevent a breathing-like break-up of the system.

Next, we discuss the case where the valence neutrons occupy the σ-orbit. $^{14}\mathrm{C}(1/2^-_\sigma)^2$ has an excitation energy higher by about 14 MeV in comparison with $^{14}\mathrm{C}(3/2^-_\pi)^2$. It is rather surprising that the difference is only 14 MeV in spite of the fact that $3/2^-_\pi$ has only one node and $1/2^-_\sigma$ has three nodes. This is because the σ-orbit is along the α-α-α core: The higher nodal orbits along the symmetry axis become low lying as a result of the clustering of the core. The σ-orbit enhances the prolonged shape of the 3α-core, and the optimal d-value is $\sim$3.5 fm. However, the $^{14}\mathrm{C}(1/2^-_\sigma)^2$ case has no deep pocket enough to be stabilized against the breathing-like path. When two more valence neutrons occupy the π-orbit, although this minimal energy is higher by 5 MeV than that of $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\pi)^2)$, $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ has the minimal 0^+ energy of ~ -81 MeV. The calculated energy pocket is deep enough to guarantee the stability for the breathing-like path.

Finally, the stability of these linear-chain states against the bending-like path is examined (parameter θ describes the bending angle of α-α-α). Except for the case of the $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ configuration, the curvature of these states is rather monotonic and the energy minimum does not clearly appear. However, the $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ case shows a sharp increase of the 0^+ energy as the increase of the bending angle and is found to be stable against the bending-like path. This feature is much different from ^{12}C, $^{14}\mathrm{C}((3/2^-_\pi)^2)$, $^{14}\mathrm{C}((1/2^-_\sigma)^2)$, and $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\pi)^2)$ cases.

$^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ is found to be only the case which is stable against both the breathing- and the bending-like path. The 0^+ energy increases by 15.7 MeV from $\theta = 0^\circ$ (exact linear-chain) to $\theta = 30^\circ$, in which the kinetic energy part is 10.3 MeV. To understand the energy increase with the increase of the bending angle θ of this case, we calculate and compare the overlap between the wave functions with $\theta = 0^\circ$ and $\theta = 30^\circ$ for various configurations. In ^{12}C, the wave functions with $\theta = 0^\circ$ and $\theta = 30^\circ$ have the squared overlap of 0.91, and $^{14}\mathrm{C}((3/2^-_\pi)^2)$ has almost the same value. $^{14}\mathrm{C}((3/2^-_\sigma)^2)$ has the value of 0.85, smaller than $^{14}\mathrm{C}((3/2^-_\pi)^2)$ by only 6%, and $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\pi)^2)$ has almost the same value as the $^{14}\mathrm{C}((1/2^-_\sigma)^2)$ case. This result shows that the overlaps additionally decrease a little for the σ-orbital neutrons, and also for the π-orbital neutrons as the increase of the valence neutrons. In spite of these, the overlap between $\theta = 0^\circ$ and $\theta = 30^\circ$ for the $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ case, shows a significantly large decrease to 0.60. $^{16}\mathrm{C}((3/2^-_\pi)^2(1/2^-_\sigma)^2)$ is only the configuration which shows drastic decrease of the overlap between $\theta = 0^\circ$ and $\theta = 30^\circ$.

As discussed in following part, it can be known that the drastic decrease as the increase of the bending angle is due to the increase of the overlap between two neutrons in the π-orbit and two neutrons in the σ-orbit. When the overlap between them increases, the overlap component in the total wave function is diminished due to the Pauli exclusion principle, that is, the so-called Pauli blocking. Therefore, the physical state can be expressed by the modified wave function which is made by subtracting the overlap component from the original wave function. Since the energies of the π- and the σ-orbits discussed here are relatively low, the modified wave function involves larger components of higher excitation energy in comparison with the wave function at $\theta = 0$ free from the Pauli blocking. As a result, the Pauli blocking due to the increase of the over-

lap between four valence neutrons is considered to bring the increase of the energy proportional to the decrease of the squared overlap. This is a possible explanation for the rapid increase of the energy against the bending angle.

4 Conclusion

The structure of Be isotopes has been investigated using the α+α+n+$n\cdots$ model, where the orbits for the valence neutrons have been introduced based on the molecular-orbit (MO) model. All of the low-lying positive- and negative-parity states of ^{10}Be have been clearly described by combinations of three basic orbits for the valence neutrons around the two α-clusters. These orbits originate from the low-lying $3/2^-$, $1/2^+$ and $1/2^-$ states in ^{9}Be. We have studied the behavior of the α-α core for each configuration of the valence neutrons.

In ^{10}Be, the ground state and the third 0^+ state are characterized by the π-orbit of the valence neutrons. The second 0^+ state has a large α-α distance, which is characterized by the σ-orbit. The two valence neutrons stay along the α-α axis (the $1/2^+$ orbit) and reduce the kinetic energy by enhancing the α-α distance. A large $E2$ transition probability between states which belong to a rotational band (0_2^+, 2_3^+, 4_2^+) is a signature for the presence of such states.

The binding mechanism of the second 0^+ state other than the enlargement of α-α distance has also been discussed. The contribution of the spin-orbit interaction due to the coupling between the $S_z = 0$ and the $S_z = 1$ configurations is important for the state.

This coupling between the spin-singlet and the triplet basis states is also important in the case of ^{12}Be. Without the spin-triplet basis state, the energy of the configuration $(3/2^-_\pi)^2(1/2^+_\sigma)^2$ is much higher than that of the closed p-shell configuration ($(3/2^-_\pi)^2(1/2^-_\pi)^2$) by 4 MeV. However, the energy of $(3/2^-_\pi)^2(1/2^+_\sigma)^2$ is drastically decreased by coupling with the spin-triplet states. This is because the effect becomes stronger as the α-α distance becomes shorter, and ^{12}Be has an optimal α-α distance around 3 fm, which is smaller than the second 0^+ state of ^{10}Be by 1 fm. The study shows that an energy of $(3/2^-_\pi)^2(1/2^+_\sigma)^2$ is almost the same as $(3/2^-_\pi)^2(1/2^-_\pi)^2$, or even lower. This effect is suggested to play a crucial role in accounting for the dissipation of the $N = 8$ magic number in ^{12}Be. It is an interesting subject to analyze the binding mechanism and properties of the ground state by taking into account the pairing mixing among states with configurations of $(3/2^-_\pi)^2(1/2^-_\pi)^2$, $(3/2^-_\pi)^2(1/2^+_\sigma)^2$, and $(1/2^-_\pi)^2(1/2^+_\sigma)^2$. A detailed analysis is going to be performed not only for this state, but also for excited states where new states with cluster structure have been recently observed.

In C isotopes, the stability of the linear-chain state (α-α-α linear configuration) has been examined. It is summarized that only the ^{16}C($(3/2^-_\pi)^2$)($(1/2^-_\sigma)^2$) configuration has the simultaneous stabilities for the breathing-like break up path and for the bending-like path up to ^{16}C. A combination of the π- and the σ-orbits occupied by four neutrons plays doubly important roles to make a deep energy pocket for breathing-like path and to prevent the bending-like free motion of the α-α-α linear chain. The band head energy is calculated to be around 25 MeV in excitation, and is expected to form a rotational band with an energy slope of $\frac{\hbar^2}{2I} = 150$ keV.

As further studies, we intend to confirm the stability of the linear-chain configuration by superposing states based on generator coordinate method. Also, we are interested in the similar structure in ^{18}C.

References

1. I. Tanihata, T. Kobayashi, O. Yamakawa, S. Shimoura, K. Ekuni, K. Sugimoto, N. Takahashi, T. Shimoda, H. Sato, Phys. Lett. B **206**, 592 (1988).
2. *Proceedings of the International Symposium on Physics of Unstable Nuclei, Niigata*, Nucl. Phys. A **588**, (1995); *Proceedings of the Fourth International Conference on Radioactive Nuclear Beam, Omiya*, Nucl. Phys. A **616**, (1997).
3. I. Tanihata, J. Phys. G: Nucl. Part. Phys. **22**, 157 (1996).
4. T. Suzuki, T. Otsuka, Phys. Rev. C **56**, 847 (1997); 279 (1992).
5. D. Brink, *Proceedings of the International School of Physics "Enrico Fermi", Course XXXVI*, edited by C. Bloch (Academic Press, New York, London, 1966) p. 247.
6. Y. Fujiwara, H. Horiuchi, K. Ikeda, M. Kamimura, K. Katō, Y. Suzuki, E. Uegaki, Prog. Theor. Phys. Suppl. **68**, 60 (1980).
7. S. Okabe, Y. Abe, H. Tanaka, Prog. Theor. Phys. **57**, 866 (1977); S. Okabe, Y. Abe, Prog. Theor. Phys. **59**, 315 (1978).
8. S. Okabe, Y. Abe, Prog. Theor. Phys. **61**, 1049 (1979).
9. H. Furutani, H. Kanada, T. Kaneko, S. Nagata, H. Nishioka, S. Okabe, S. Saito, T. Sakuda, M. Seya, Prog. Theor. Phys. Suppl. **68**, 193 (1980).
10. M. Seya, M. Kohno, S. Nagata, Prog. Theor. Phys. **65**, 204 (1981).
11. N. Itagaki, S. Okabe, Phys. Rev. C **61** 044306, (2000).
12. N. Itagaki, S. Okabe, I. Ikeda, Phys. Rev. C **62**, 34301 (2000).
13. Y. Abe, J. Hiura, H. Tanaka, Prog. Theor. Phys. **49**, 800 (1973).
14. W. von Oertzen, Z. Phys. A **354**, 37 (1996); **357**, 355 (1997).
15. Y. Kanada-En'yo, H. Horiuchi, A. Ono, Phys. Rev. C **52**, 628 (1995).
16. A. Ono, H. Horiuchi, T. Maruyama, A. Ohnishi, Prog. Theor. Phys. **87**, 1185 (1992); Phys. Rev. Lett. **68**, 2898 (1992).
17. Y. Kanada-En'yo, H. Horiuchi, A. Doté, Phys. Rev. C **60**, 064304 (1999).
18. A.B. Volkov Nucl. Phys. **74**, 33 (1965).
19. N. Yamaguchi, T. Kasahara, S. Nagata, Y. Akaishi, Prog. Theor. Phys. **62**, 1018 (1979).
20. S. Cohen, D. Kurath, Nucl. Phys. **73**, 1 (1965).
21. N. Soić *et al.*, Eurohys. Lett, **34**(1), 7 (1996).