Appearance of $\alpha$-cluster structure in Be isotopes based on Monte Carlo shell model

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Abstract. Properties of Be isotopes are investigated by using Monte Carlo shell model (MCSM). The structure of $^{10}$Be is studied through the intrinsic density. With this density, the appearance of the $\alpha$-cluster structure and molecular orbits of low-lying states is discussed. Excitation energies for the $2^+$ states are compared with experiments and other theoretical calculations.

1. Introduction

In light nuclei, the appearance of the $\alpha$-cluster structure has been studied from many aspects [1]. For instance, the structure of the developed $\alpha$ cluster has been investigated by using phenomenological $\alpha$-cluster models near $\alpha$-cluster thresholds. Recently, $ab$ $initio$ calculations have started to reveal the properties of light nuclei and their cluster nature. The analysis of $A = 8$ nuclei based on the Green’s function Monte Carlo (GFMC) [2] has been one of the milestones. In the study, the two-$\alpha$-cluster shape has been found to emerge $a$ $priori$ in the density distribution without assuming any cluster configurations. After that, the $ab$ $initio$ calculations have been associated with the cluster structure in some cases [3,4]. For $p$-shell nuclei, calculations based on the shell model without assuming an inert core have been performed. When the model space is large enough, it is natural to expect that the shell model is able to describe the cluster configuration. The example is the investigation by using the translationally invariant density based on the No-Core Full Configuration (NCFC) [5]. In fact, the deformation and cluster-like shape for Li isotopes have been investigated. Here, the wave functions are not assumed to have any cluster structure $a$ $priori$. As another approach, the Monte Carlo shell model (MCSM) has been developed [6,7]. The MCSM without assuming an inert core has an advantage in the applicability for the variety of light nuclei [8]. The use of MCSM wave functions is also beneficial for extracting the intrinsic structure. Here, only the wave function before the angular-momentum projection is needed. In this study, we focus on the properties of Be isotopes. In Be isotopes, observables such as $E0$ and $E2$ transition strengths have been studied [9–15]. Recently, the shell model calculations based on NCFC [16] have well reproduced the physical quantities for Be isotopes such as the $2^+_1$ energies and $B(E2)$ values. There are also studies of Be isotopes based on MCSM [17]. In this MCSM calculation, the truncation of the model space
has been \( N_{\text{shell}} = 4 \), which means that all single-particle orbits below \( pf \) shell are taken into account. In their study, the harmonic oscillator parameter has been treated empirically. We investigate the properties of the \( 0^+ \) states of \(^{10}\text{Be}\) with the model space \( N_{\text{shell}} = 4 \). Here, the appearance of the \( \alpha \)-cluster structure and molecular orbits have been discussed. When we calculate the \( 2_1^+ \) energies of Be isotopes, we increase the size of the model space from \( N_{\text{shell}} = 4 \) to \( 6 \). The contents of the proceedings are as follows. In Sect. 2, we show the formulation of MCSM, the numerical setup and the definition of the intrinsic state. In Sect. 3, we discuss the \( 0^+_1 \) and \( 0^+_2 \) states of \(^{10}\text{Be}\). We also show the theoretical results of the \( 2_1^+ \) energies of \(^{8,10,12}\text{Be}\). Finally, we make conclusions and comments for future plans.

2. Formulation

2.1. Calculations of the MCSM wave function

The basis state of the MCSM wave function is described by a Slater determinant, \(|\phi_n\rangle\), which is given as

\[
|\phi_n\rangle = \prod_{i=1}^{N_p} \sum_{i=1}^{N_{sp}} c_i^n D_{ia}^{(n)} |\rangle,
\]

(1)

where, \(|\rangle\) shows a vacuum state and the \( c_i^n \) is a creation operator for a single-particle orbit, \( i \). Here, \( i \) is specified by \( t, n, l, j \) (denoting quanta for the isospin, radial node, orbital angular momentum and total angular momentum, respectively). \( N_p \) and \( N_{sp} \) denote the numbers of nucleons and single-particle orbits, respectively. The resultant wave function is given by a superposition of the \( N_b \) Slater determinants as follows,

\[
|\Psi(J^\pi)\rangle = \sum_{K=-J}^{J} P_{MK}^{J\pi} |\Phi_K\rangle, \quad |\Phi_K\rangle = \sum_{n=1}^{N_b} g^K_n f_n |\phi_n\rangle.
\]

(2)

Here, \( P_{MK}^{J\pi} \) is the parity and angular-momentum projection operator. This superposition has been obtained iteratively by increasing \( N_b \). The coefficients, \( g^K_n \) and \( f_n \), are determined by diagonalizing the Hamiltonian and norm matrices \( \langle \phi_i | H |\phi_j \rangle \) and \( \langle \phi_i | P_{KK'}^{J\pi} |\phi_j \rangle \), respectively. For the \( n \)-th step of the iteration, the coefficients, \( D_{ia}^{(n)} \), are optimized by the conjugate gradient method to minimize the sum of the energy eigenvalues of the desired states.

As for the interaction, we use the JISP16 non-local \( NN \) interaction which reproduces two-nucleon scattering data and properties of deuteron and other light nuclei without using three-body interactions explicitly [18]. In the present work, the Coulomb interaction is neglected for simplicity. The contamination of the center of mass motion is factorized approximately by the Lawson’s procedure [19], namely adding the Hamiltonian of the center of mass motion, \( H_{cm} \), to the original Hamiltonian, \( H_0 \). The Hamiltonian to be diagonalized is given as

\[
H = H_0 + \beta \left( H_{cm} - \frac{3}{2} \hbar \omega \right).
\]

(3)

In the present study, the coefficient is fixed to \( \beta \frac{\hbar \omega}{\omega} = 1 \).

2.2. Setup for numerical calculations

The numerical calculation of \( P_{MK}^{J\pi} \) includes the integration of the Euler angles, \( \Omega = (\alpha, \beta, \gamma) \). For the computations of the integral, we need to discretize these angles. We use about 20,000 mesh points for \( N_{\text{shell}} = 4 \) and about 50,000 mesh points for \( N_{\text{shell}} = 6 \). The number of the Slater determinants, \( N_b \), is set around 100. For efficient calculations of the matrix elements, OpenMP+MPI hybrid parallelization is applied. The computations were performed on the K computer (RIKEN AICS), FX10 (the University of Tokyo) and T2K Open Supercomputers (the University of Tokyo and University Tsukuba).
2.3. Definition of the intrinsic state

In the \(J^\pi\)-projected wave function, the cluster-like structure is difficult to be visualized. To investigate the wave function in detail, we go back to the wave function before the angular-momentum projection, \(|\Phi_K\rangle\), which is a linear combination of the unprojected basis states. However, this state is difficult to be interpreted as an intrinsic state. The reason is that the principal axes of the basis states, \(|\phi_n\rangle\), do not have the same direction one another. As a result, the intrinsic structure such as cluster configurations may be hidden. In order to extract the wave function of the intrinsic state, we rotate all basis states so that their diagonalized q-moments are aligned along the z-axis, following the concept of the intrinsic state defined in the GFMC [2]. The formula is already applied on MCSM in the previous study [20]. The intrinsic wave function \(|\Phi_{\text{intr}}\rangle\) is defined as

\[
|\Phi_{\text{intr}}\rangle \equiv \sum_n f_n R(\Omega_n) |\phi_n\rangle = \sum_n f_n |\phi_n^{R}\rangle,
\]

with the rotational operator \(R(\Omega_n)\) and the transformed basis state \(|\phi_n^{R}\rangle\).

3. Results

In this section, we investigate the properties of \(^8\)Be, \(^{10}\)Be, and \(^{12}\)Be based on MCSM and compare them with the experiments and other theoretical calculations. We need to confirm which \(\hbar\omega\) value to use, since the physical values may strongly depend on it. For this purpose, we focus on the \(\hbar\omega\) dependence of \(0^+\) states of \(^{10}\)Be.

In Fig. 1(a), we depict the energy curve with respect to \(\hbar\omega\). Here, we optimize the two lowest \(0^+\) states. In Fig. 1(b), the expectation values of the Hamiltonian of the center of mass motion are shown. The contamination of the center of mass motion is larger than that for the ground state. Since all values in the figure are small, the approximate factorizations of the center of mass motion are obtained well both for \(N_{\text{shell}} = 4\) and 6. The energy minimum of the curve for \(N_{\text{shell}} = 4\) is around \(\hbar\omega = 25\) MeV for both \(0_1^+\) and \(0_2^+\). We investigate the properties of the two states at \(\hbar\omega = 25\) MeV and \(N_{\text{shell}} = 4\).

In Fig. 2, the intrinsic densities of the \(|\Psi(0_1^+)\rangle\) and \(|\Psi(0_2^+)\rangle\) for \(^{10}\)Be are shown. The density distributions of the proton and matter indicate the existence of two-\(\alpha\) cluster states, which has been already discussed based on MCSM for the \(0_1^+\) state [7,20]. The density of the valence
Figure 2. Density distributions of $^{10}\text{Be}$. The upper (lower) figures show the $0^+_1$ ($0^+_2$) state for the matter (left), proton (middle) and valence neutron (right). The parameters of the MCSM are $N_{\text{shell}} = 4$ and $\hbar \omega = 25$ MeV. The number of the basis states is $N_b \sim 100$.

neutron is defined by the difference between the neutron and proton densities. For the $0^+_1$ state, the orbits of the valence neutrons show a node at the center of the two-$\alpha$ clusters. The density is located outside the z-axis which is along the two-$\alpha$ clusters. For the $0^+_2$ state, the density of the valence neutrons is located mainly at the center of two-$\alpha$ clusters. These valence neutrons mainly occupy the $p$ and $sd$ shells for the $0^+_1$ and $0^+_2$ states, respectively. These two specific features of the $0^+_1$ and $0^+_2$ states correspond to the picture of the $\pi$ and $\sigma$ orbits in the molecular orbit model [21], respectively. As for the eigenenergy, the model space is enlarged from $N_{\text{shell}} = 4$ to $N_{\text{shell}} = 6$. For $N_{\text{shell}} = 6$, the energy minima for the $0^+_1$ and $0^+_2$ states are located around $\hbar \omega = 25$ and 20 MeV, respectively. For simplicity, we fixed $\hbar \omega = 20$ MeV. The excitation energies of the $0^+_2$ state are 19.0 and 12.7 MeV for $N_{\text{shell}} = 4$ and 6, respectively. These values are larger than the experimental one, 6.1793(7) MeV. However, they are in a reasonable region when we consider that the energy convergence with respect to $N_{\text{shell}}$ has some remaining effects.

In Fig. 3, $2^+_1$ energies for Be isotopes are shown. In the MCSM calculation, we optimize two states for the $0^+$ states and one state for the $2^+$ state. Here, the MCSM, NCFC, GFMC and experimental results are shown. As the red open diamonds show, there are discrepancies between the MCSM results before the extrapolation and the other results. The value for $^8\text{Be}$ is consistent with NCFC. Even though the discrepancy increases as the neutron number increases, we can still see the tendency to have a kink at neutron number $N = 8$ similar to the other methods. Since the number of the Slater determinants is far below the dimension of the model space defined by the $N_{\text{shell}}$, the calculated eigenenergies give the upper limit of the exact one.
Figure 3. Excitation energies for the $2^+_1$ state of Be isotopes for the experiments (black closed circles), GFMC [2] (blue open squares), NCFC [16] (brown triangle), MCSM without the extrapolation (red open diamond) and MCSM with the extrapolation (red triangle). The parameters of the MCSM are $N_{\text{shell}} = 6$ and $\hbar \omega = 20$ MeV.

To estimate the exact eigenenergy, we apply the extrapolation method [7, 22, 23]. After the extrapolation, we find a good agreement between the two for $^{8,10}\text{Be}$ (red triangle). We notice that the deviation of the energies before the extrapolations is mainly due to the larger energy variance of the $2^+_1$ states than those of the $0^+_1$ states. For $^{12}\text{Be}$, there are still uncertainties in the extrapolation. This is due to the limited number of the basis states for the extrapolation.

4. Conclusions
We investigate the properties of Be isotopes based on no-core MCSM. For the $0^+_1$ states of $^{10}\text{Be}$ with $N_{\text{shell}} = 4$, the molecular orbits appear. Their features of the molecular orbits are consistent with those derived from another phenomenological model. For the study of the $2^+_1$ state of $^{8,10,12}\text{Be}$, the model space is set to $N_{\text{shell}} = 6$. Even though the number of the basis states in the MCSM before the extrapolation is limited, the tendency of the excitation energies is similar to the results obtained from the NCFC and experiments. However, there is a certain amount of disagreement. The improvement is obtained by the extrapolation method for $^{8,10}\text{Be}$. To perform the extrapolation for $^{12}\text{Be}$, we need further investigations in terms of the model space.

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