Cluster structure in Monte Carlo shell model

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Abstract. The wave function of ⁸Be, which is obtained from the Monte Carlo shell model (MCSM), is discussed. A method to define an intrinsic state in the MCSM is proposed. The appearance of two-α-cluster structures in ⁸Be is demonstrated.

1. Introduction
One of the purposes of theoretical nuclear physics is to understand the physical observables of nuclei in the large region of the nuclear chart. So far, nuclear density functional theory is the only method able to describe them across the whole nuclear chart. If we go beyond the theory in terms of the accurate description for the excited states and the reliability for nuclear interactions, we need to select a specific model to understand the properties of nuclei at each region. The shell model calculation is usually suited for the study of the medium mass region. In the large region of the nuclear chart, the shell model picture is essential to understand the nuclear magic numbers related to the single-particle motion of a nucleon.

The shell model calculation enables us to take all relevant degrees of freedom of nucleon motion into account when the particles are set to be in the valence shell on top of the core nucleus. For the lightest part of the nuclear chart (mass number lower than A = 14), shell model calculations without assuming an inert core can be performed. The model space without the core is important for the accurate prediction of the properties of light nuclei.

On the other hand, α cluster configuration exists in light nuclei, which has an important role at the α-breakup-threshold-energy region. In this picture, the four nucleons (spin-up proton, spin-down proton, spin-up neutron and spin-down neutron) become an ingredient of the subsystem, ⁴He (α particle). The subsystem is so stable that one α cluster has possibility to exist separately from the remaining nucleus especially for the excited states near α-breakup thresholds.

The appearance of α cluster structure has been studied for a few decades. In the early stage of the study, phenomenological (e.g. α cluster model) calculations have been performed [1]. Recently, ab initio calculations have been started for this region. One example is the Green’s function Monte Carlo (GFMC) [2] approach and another is the lattice effective field theory [3, 4]. In their analyses of A = 8 and 12 nuclei, the two and three-α-cluster shapes emerge a priori. It is important to confirm the existence of the cluster configuration by calculating the density distribution of ⁸Be from shell-model side. However, it is difficult to discuss α-cluster configuration in view of intrinsic shape utilizing shell model calculations. This is because
the single-particle orbit of the shell model is expanded around the one center of the harmonic oscillator potential.

Recently, the size of the model space which is tractable in the shell model calculation has been increased due to the development of parallel computers and methodology of shell model calculations. Therefore, it is natural to expect that \( \alpha \)-cluster configurations are included in the single-particle orbit of the shell model if the model space is large enough. In fact, the deformation and cluster-like shape for Li isotopes have been investigated by using the no core full configuration (NCFC) approach [5].

Another approach is the Monte Carlo shell model (MCSM) [6] method which has been applied to the various nuclei by using modern parallel computers with sophisticated energy-minimum search where the conjugate gradient method and energy-variance extrapolation [7, 8, 9] are combined. The MCSM is expected to be applicable toward the large region of the nuclear chart both with and without the inert core (no-core MCSM). In this work, we show the density profiles of the wave function obtained in the no-core-MCSM calculation. For this purpose, we define the intrinsic state from the no-core-MCSM wave function in the following section. We focus on the ground state of \( ^8\text{Be} \) which is expected to have the two-\( \alpha \)-cluster configuration.

2. Formulation
In this section, we show how to obtain the intrinsic structure for \( ^8\text{Be} \). In order to investigate the cluster-like state, it is important to extract the intrinsic state from the wave function whose angular momentum is a good quantum number in the no-core MCSM.

In the no-core-MCSM calculation, the wave function is projected to the state which has a good angular momentum quantum, \( J \). We use a Slater determinant, \( |\phi_n\rangle \), to describe a basis state which is defined as
\[
|\phi_n\rangle = \prod_{\alpha=1}^{N_p} \sum_{i=1}^{N_{\text{sp}}} c_{i\alpha}^\dagger D^{(n)}_{i\alpha} |-\rangle,
\]
where \(|-\rangle\) is a vacuum state and \( c_{i\alpha}^\dagger \)'s are creation operators of the single-particle orbit, \( i \). It is specified by coefficients of the harmonic oscillator state. The resultant wave function is given by a superposition of the angular-momentum-projected Slater determinants,
\[
|\Psi\rangle = P_{MK}^{J_\pi} |\Phi\rangle,
\]
where \( |\Phi\rangle = \sum_{n=1}^{N_b} f_n |\phi_n\rangle \).

In this study, we use the values \( \pi = +, J = 0, M = 0 \) and therefore \( K \)-quantum number \( K = 0 \). The coefficients \( f_n \)'s are determined by diagonalizing the Hamiltonian matrix, \( \langle \phi_i | H | \phi_j \rangle \). In the no-core-MCSM procedure, we tune the value of \( D^{(n)} \) for each Slater determinant by the conjugate gradient method in order to minimize the expectation value of the Hamiltonian with \( J \)-projected wave functions. Here, we use the JISP16 \( NN \) interaction which reproduces \( NN \) scattering data and properties of deuteron and other light nuclei [10].

In this \( J \)-projected wave function, the cluster-like structure is difficult to be visualized. To analyse the wave function in detail, we go back to the wave function before the angular momentum projection, \( |\Phi\rangle \), which is the linear combination of the unprojected basis states. However, this state is not considered as an intrinsic state because the principal axis of a basis state, \( |\phi_i\rangle \), is not necessarily in the same direction as the other basis states. The directions are rather randomly distributed after the energy-minimum search in the MCSM procedure. As a result, intrinsic structures such as cluster configurations may be hidden.

In order to extract the wave function of the intrinsic state, we rotate each basis state so that its diagonalized Q-moment is aligned along the z-axis, following the concept of the intrinsic state.
in the GFMC [2]. The intrinsic wave function $|\Phi^{\text{intr}}\rangle$ is defined as

$$|\Phi^{\text{intr}}\rangle = \sum_n f_n R(\Omega_n)|\phi_n\rangle,$$

(3)

with the transformed basis state $|\phi_n^R\rangle$. Here, $R(\Omega_n)$ is the rotation operator with an Euler angle $\Omega_n$, which is determined by the condition, $\langle \phi_n^R|Q_{i,j}|\phi_n^R\rangle = \delta_{i,j} q_i$, where $Q_{i,j}(=x,y,z)$ are the operators of Q-moment. We note that this state, $|\Phi^{\text{intr}}\rangle$, exactly has the same energy after the angular momentum projection. After that, it is probable that these aligned basis states have large overlap with each other and make a distinct principal axis toward the $z$-axis when the condition $q_z > q_y > q_x$ is set. The intrinsic density is obtained by the expectation value of the one-body-density operator,

$$\rho^{\text{intr}}(r) = \langle \Phi^{\text{intr}}|\sum_i \delta(r - r_i)|\Phi^{\text{intr}}\rangle,$$

(4)

where $r_i$ denotes the position of the $i$-th nucleon.

### 3. Results

Figure 1 shows the proton densities for the $0^+$ ground state of $^8\text{Be}$. Here, the densities of the wave function $\Phi$ (before alignment) are shown in the left panel. The intrinsic densities of the wave function $\Phi^{\text{intr}}$ are shown in the right panel. As shown in the results of $N_b = 1$, a clear deformation and its neck structure to be called dumbbell shape appear. We can see that as the number of the Slater determinants ($N_b$) increases, the densities before alignment become vaguer because of the mixture of different directions of principal axes of the basis states. On the other

![Figure 1](image-url)
hand, the intrinsic densities have clearer dumbbell-like structure for each $N_b$. In addition, the density distribution of the intrinsic state is almost unchanged with respect to $N_b$. This result indicates the appearance of cluster structures. We see that the neck of the dumbbell shape is more enhanced in $N_{\text{shell}} = 4$ than in $N_{\text{shell}} = 3$. Since the number of particles appeared in the density distribution for opposite sides of the principal axis are almost the same, this state can be considered as two $\alpha$ clusters. This result is similar to that of the GFMC [2].

In summary, we analyse the density distribution of the $0^+$ ground state of $^8\text{Be}$. We use a method by which one can extract the intrinsic structure from the wave function in the no-core MCSM. We show that the neck shape indicating the two $\alpha$ clusters emerges within a relatively small number of the harmonic oscillator quanta. We notice that the shape which appears in the no-core MCSM has the similar property in the GFMC in terms of the density. However, it is necessary to clarify - in future studies - whether the present analysis is valid with larger model spaces, with Coulomb interaction and without contamination of spurious center of mass motion.

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