Density profiles in the intrinsic frame of light nuclei obtained from Monte Carlo shell model calculation

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Abstract. The wave functions of the ground states for 8,10Be which are obtained from the Monte Carlo shell model (MCSM) are investigated. A method to define an intrinsic state in the MCSM is discussed. The appearance of two-α-cluster structure in 8Be and the property of the valence neutrons in 10Be are discussed.

1. Introduction
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 conventional 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 = 12), shell model calculations without assuming an inert core can be performed. On the other hand, α-cluster configuration exists in light nuclei, which has an important role to determine the transition strength at the α-breakup-threshold-energy region. The appearance of α-cluster structure has been studied for a few decades [1].

Recently, ab initio calculations have been started for the lightest part. One example is the Green’s function Monte Carlo (GFMC) [2] approach. In its analysis of A = 8 nuclei, the two-α-cluster shape emerges in a priori from the density distribution. In order to estimate the transition properties, it is important to confirm the existence of the cluster configuration by calculating the density distribution of light nuclei 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 α-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 no core full configuration (NCFC) approach [3].

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Another approach is the Monte Carlo shell model (MCSM) [4] method which has been applied to the various nuclei by using the recent parallel computer with sophisticated energy-minimum search where the conjugate gradient method and energy-variance extrapolation [5, 6] 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 the proceedings, we show the density profiles of 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 $^8_{\text{Be}}$, $^{10}_{\text{Be}}$ which are expected to have the two-α-cluster configuration. In $^{10}_{\text{Be}}$, the density for the valence neutrons is discussed.

2. Formulation

In this section, we show how to obtain the intrinsic structure for the no-core-MCSM wave function. 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

$$|\phi_n\rangle = \prod_{\alpha=1}^{N_p} \sum_{i=1}^{N_{sp}} c_i^{\dagger} D_{\text{ia}}(n)|-\rangle,$$

(1)

where $|-\rangle$ is a vacuum state and the $c_i^{\dagger}$'s are creation operators on the single-particle orbit, $i$. The resultant wave function is given by a superposition of the angular-momentum-projected Slater determinants,

$$|\Psi\rangle = P_{MK}^{J_{\pi}}|\Phi\rangle, \quad |\Phi\rangle = \sum_{n=1}^{N_{\nu}} f_n |\phi_n\rangle.$$

(2)

In this study, we use the values, $\pi = +$, $J = 0$, $M = 0$ and $K$-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 [7].

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

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

(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 the 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, 

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

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

3. Result

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 the alignment (the left panel) becomes vaguer because of the mixture of different directions of principal axes of the basis states. On the other hand, the intrinsic densities (the right panel) 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 structure. Since the number of particles 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].

![Figure 1](image)

Figure 1. $^8\text{Be}$ proton densities before alignment of principal axes of unprojected basis states, $| \Phi \rangle$ (left panel) and of intrinsic state, $| \Phi^{\text{intr}} \rangle$ (right panel) for various $N_b$ and slices along $yz$ plane. The numbers of basis states are $N_b = 1, 10$ and 100 for the lower, middle and upper figures, respectively. Slices along $yz$ plane are $x = 0 \text{ fm}$ plane (left) or $x = 1 \text{ fm}$ plane (right) for each panel. The size of each box is $8 \text{ fm} \times 8 \text{ fm}$. The model space and harmonic oscillator energy are $N_{\text{shell}} = 4$ and $h\omega = 20 \text{ MeV}$, respectively.

We perform the same analysis for the ground state of $^{10}\text{Be}$. We depict the densities as shown in Fig. 2. The valence-neutron density is estimated by subtracting the proton density from the neutron density. We can see that the valence neutrons are located mainly around the node of $^8\text{Be}$-like core. This picture is consistent with the behavior of $\pi$-orbit in the molecular orbital model of $^{10}\text{Be}$ [8].
Figure 2. The densities of the $0^+$ ground state for $^{10}$Be are shown. The number of basis states is $N_b = 1, 20$ and $30$ (lower, middle and upper, respectively). The model space and harmonic oscillator energy are $N_{\text{shell}}=4$ and $\hbar \omega=25$ MeV, respectively. The intrinsic densities for proton, neutron and valence neutrons are shown (left, middle and right, respectively).

In summary, we analyse the density distribution of the $0^+$ ground state of $^{8,10}$Be. We use the 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 for the $0^+$ ground state of $^8$Be. In the analysis for the $0^+$ ground state of $^{10}$Be, we see the two-$\alpha$-cluster shape and $\pi$-orbit-like configuration of the valence neutrons. This corresponds to the result of the $\alpha$ cluster model. However, it is necessary to clarify whether the present analysis is valid with larger model spaces, with Coulomb interaction and without contamination of spurious center of mass motion as a future study.

Acknowledgements
This work has been supported by the SPIRE Field 5 from MEXT, and the CNS-RIKEN joint project for large-scale nuclear structure calculations. The numerical calculations were performed on the T2K Open Supercomputers at the University of Tokyo and Tsukuba University.

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