Alpha-cluster Structure from No-Core Monte Carlo Shell Model

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Abstract

Owing to recent computational and methodological advancements, *ab initio* approaches in nuclear structure physics have been largely developed. The no-core Monte Carlo shell model (MCSM) is one of these methods to investigate nuclear structure in light nuclei. With this method, it is currently capable to calculate physical observables up to around lower *sd*-shell region. As one of physics investigations with the no-core MCSM, the α-cluster structure of Be isotopes and ^{12}C nucleus is focused on and qualitatively discussed from an *ab initio* point of view.

Keywords: *Alpha-cluster structure; Monte Carlo shell model; no-core shell model*

1 Introduction

Nowadays, there are many approaches to solve nuclear many-body problems. One of successful methods is the shell-model approach [1–3]. The shell-model calculations have provided much of theoretical understanding of nuclear structure based on the single-particle picture. In these calculations, the energy eigenvalues and eigenfunctions are obtained by the diagonalization of sparse real symmetric matrices using the Lanczos method to describe several low-lying states. The limitation of this approach is directly related to the size of Hamiltonian matrices to be diagonalized. In the case of no-core shell model, the current limit is around 10^{10} M-scheme dimensions [4]. The dimension of Hamiltonian matrices in the single-particle truncation is illustrated in Fig. 1. Now the mass region of interest has been extended to heavier and/or neutron-rich nuclei to investigate various exotic phenomena, and is located at the area beyond the scope of this standard approach with the Lanczos method.

Under these circumstances, there are some variants of shell-model approaches aiming to go beyond the standard approach. One of them is the Monte Carlo shell model (MCSM) [5–7]. Here, we provide a brief overview of the MCSM, especially for the no-core calculations, and the study on the α-cluster structure using this method. The outline of this contribution is as follows. In Section 2, the formulation of the

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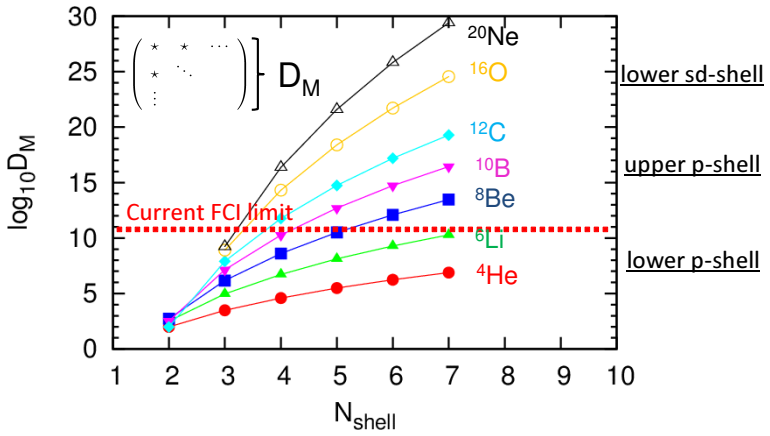

Figure 1: The M-scheme dimensions as a function of the size of basis space for several light nuclei.

MCSM is briefly introduced. In Section 3, the current status of the MCSM for no-core calculations is shown. As one of physics investigations by the no-core MCSM, we discuss α-clustering phenomena in Be isotopes and ^{12}C nucleus in Section 4. The summary is given in Section 5.

2 Monte Carlo Shell Model

In the Monte Carlo shell model (MCSM), the Hamiltonian comprises one- and two-body terms, and is written in the second quantized form as

$$\hat{H} = \sum_{ij} t_{ij} \hat{c}_i^\dagger \hat{c}_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k, \tag{1}$$

with the creation and annihilation operators, $\hat{c}^\dagger$ and $\hat{c}$, respectively. The indices, i, j, k, and l, stand for the single-particle states. The one- and two-body matrix elements are described as t_{ij} and $\bar{v}_{ijkl}$. Here, the two-body matrix elements are antisymmetrized as $\bar{v}_{ijkl} = -\bar{v}_{jikl} = -\bar{v}_{ijlk} = \bar{v}_{jilk}$.

With this Hamiltonian, the MCSM wave function is expressed as a linear combination of total-angular-momentum- and parity-projected deformed Slater determinants,

$$|\Psi^{(N_b)}_{IM\pi}\rangle = \sum_{n=1}^{N_b} \sum_{K=-I}^{I} f^{(N_b)}_{nK} \hat{P}^{I\pi}_{MK} |\phi_n\rangle, \tag{2}$$

with the total-angular-momentum- and parity-projection operator, $\hat{P}^{I\pi}_{MK} = \hat{P}^I_{MK}\hat{P}^\pi$. The number of deformed Slater determinants is N_b. The amplitude $f^{(N_b)}_{nK}$ is the coefficient of each basis function. The deformed Slater determinant reads

$$|\phi\rangle = \prod_{\alpha=1}^{N_f} \sum_{i=1}^{N_{sp}} D_{i\alpha} \hat{c}_i^\dagger |-\rangle, \tag{3}$$

with the numbers of nucleons N_f and single-particle states N_{sp}. Note that the particle vacuum is described as $|-\rangle$. The complex matrix D characterizes the deformation from the spherical harmonic-oscillator Slater determinants.

In Eq. (3), the matrix elements of D are determined by minimizing the energy eigenvalues in stochastic and deterministic ways following the variational principle. The stochastic sampling of bases is done in a way similar to the auxiliary-field Monte Carlo technique, introducing auxiliary fields by the Hubbard–Stratonovich transformation. Candidates of basis function are generated by the imaginary-time evolution. Among these generated candidates, we take the one which gives the lowest energy eigenvalue. Then, we further minimize the energy eigenvalue by optimizing the matrix D in a deterministic way with the conjugate gradient method.

Concerning the actual computational procedure, we start with one basis, usually the Hartree–Fock basis. We increase the number of bases by repeating the basis search in stochastic and deterministic ways as described above until the energy eigenvalues sufficiently converge. The typical number of bases becomes finally around 100, so that we reduce the diagonalization problem of a large and sparse Hamiltonian matrix into a dense Hamiltonian matrix with about 100 linear dimension. At each step of the basis search, the energy eigenvalues E and coefficients of eigenvector f_{nK} are obtained by solving the following generalized eigenvalue problem,

$$\sum_{nK}\langle\phi_m|\hat{H}\hat{P}^{I\pi}_{MK}|\phi_n\rangle f_{nK} = E\sum_{nK}\langle\phi_m|\hat{P}^{I\pi}_{MK}|\phi_n\rangle. \tag{4}$$

In order to evaluate the energy eigenvalues more precisely, we also compute the energy variance and extrapolate our MCSM results towards vanishing energy variances where the exact eigenvalue of original Hamiltonian matrix exists. For more details, see the reviews of MCSM in Refs. [5–7].

3 *Ab initio* no-core MCSM

One of the major challenges in nuclear physics is to understand nuclear structure and reactions from the first principles. For this purpose, a number of *ab initio* studies have become actively done these days, mainly due to a rapidly growing computational power and refinement of *ab initio* techniques for quantum many-body calculations (see review articles, for example, Ref. [8] and references therein).

In the *ab initio* approaches, all nucleon degrees of freedom are activated and nuclear forces from two- and three-nucleon interactions fitted to NN-scattering data and deuteron properties (applying some soften procedures of original interactions) are used as an input of many-body calculations. Typically, the cost for these calculations tends to be computationally expensive. Therefore, an alternate way to reduce the computational cost is awaited. For instance, in the case of no-core shell model, a couple of methods have been proposed and are providing new insights into *ab initio* nuclear structure calculations, such as the importance-truncated no-core shell model [9, 10] and symmetry-adapted no-core shell model [11]. The no-core MCSM is one of the variants pursuing this direction [12, 13].

For the application of the no-core MCSM, we have employed the JISP16 NN interaction due to the limitation of handling explicit $3N$ interactions at present. This is the J-matrix inverse scattering potential (JISP), one of the realistic nonlocal NN

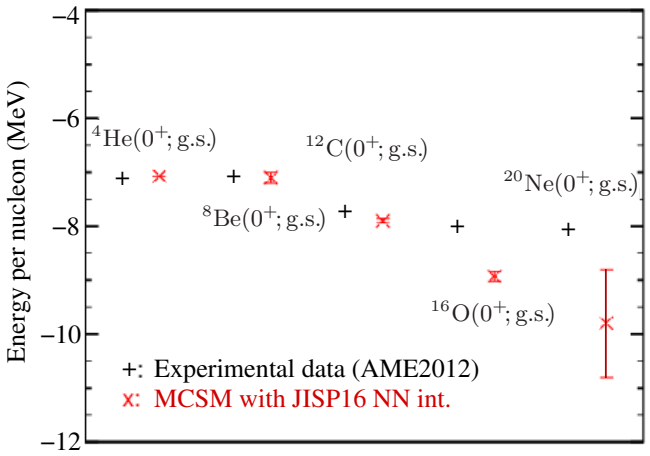

Figure 2: Comparison of binding energies for light nuclei between MCSM calculations and experimental data. The error bars denote estimated uncertainties for the extrapolation of MCSM results.

interactions constructed through phase-equivalent transformations [14]. This interaction is fitted not only to the two-nucleon scattering data and deuteron properties but also to the properties of light nuclei up to ^{16}O. Although we treat only NN interactions in the calculations, it is sufficient to prove the capability of the MCSM technique for no-core shell-model calculations.

With the JISP16 NN interaction, we have calculated the ground-state energies and root-mean-square point-nucleon radii of ^{4}He, ^{8}Be, ^{12}C, ^{16}O and ^{20}Ne nuclei as shown in Figs. 2 and 3, respectively, including the nuclei in which the standard no-core shell-model calculations are hardly performed to obtain converged results due to huge dimensionality of Hamiltonian matrices. From our recent no-core MCSM computation on the K computer, the JISP16 NN interaction provides the binding energies consistent with experimental data up to around ^{12}C, but overbinds nuclei as A increases. In a similar way, the radii are consistent with experiment up to around $A \sim 8$, but are clearly underestimated for A larger than 12. Our results infer the necessity of explicit inclusion of $3N$ potentials for heavier nuclei above the upper p-shell region even with a non-local potential such as the JISP16 NN interaction.

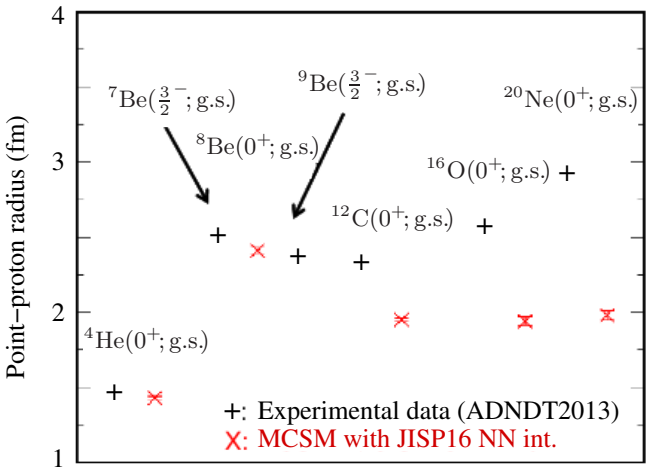

Figure 3: Comparison of radii for light nuclei between MCSM calculations and experimental data. Note that the experimental data for neighboring Be isotopes are plotted as a reference of the MCSM calculation for ^{8}Be.

However, a new non-local NN interaction, the Daejeon16 NN, is expected to give better results than those with the JISP16 NN interaction [15, 16]. It is interesting to see how well the results of no-core MCSM calculations can be improved with this interaction and to what extent the off-shell properties of such kind of nonlocal NN interactions can absorb the effects of explicit $3N$ interactions beyond the p-shell region.

4 Alpha-cluster structure from the no-core MCSM

For physics applications of the no-core MCSM, the α-cluster structure has been recently investigated focusing on two- (three-) α-cluster structure of Be (C) isotopes. The α-cluster structure in light nuclei is one of the fundamental aspects in nuclear many-body system, and has been studied intensively for a long time. Up to present, there are a number of studies on α-cluster physics from the first principles as well as those based on cluster models. The purpose for the investigation by the no-core MCSM is to understand the mechanism of appearance and disappearance of α-cluster structures in the intrinsic density of nuclei utilizing the nature of deformed Slater determinants in the MCSM wave functions.

As an exploratory study, a proof-of-principle calculation by the no-core MCSM has been done for the low-lying states of ^{10,12}Be nuclei with the AV18 and N3LO χEFT NN potentials transformed by the unitary correlation operator method [17]. Physical observables of low-lying states of ^{10}Be are reasonably well reproduced. Following this exploratory study of Be isotopes, the no-core MCSM has been further applied to the study of intrinsic shape of these exotic nuclei [18–21]. The no-core MCSM calculations with JISP16 NN interaction have been performed to construct intrinsic densities of ground and some excited states in Be isotopes in order to better understand the α-cluster and molecular-orbital structure of Be isotopes. For a visualization of intrinsic structure of nuclei, we superpose the deformed Slater determinants in the MCSM wave function before the angular-momentum and parity projections so as to obtain the density distribution in the body-fixed frame by aligning the orientation of each deformed Slater determinant in terms of quadrupole deformation.

From our investigation, we have obtained some promising results as shown in Fig. 4. First, we have observed the emergence of two-α-cluster structure in the ^{8}Be ground state without any assumption of the α-cluster structure. This fact indicates that the α clusters can be described efficiently with deformed Slater determinants. Second, we can identify in the ground and first excited 0^+ states of ^{10}Be nuclei the molecular-orbital structures formed by two valence neutrons (equal to the total number of neutrons minus the number of protons) on top of two α clusters. For the ground state (the first excited 0^+ state), two valence neutrons give π- (σ-) orbit of molecular orbital states. In addition, we can observe four valence neutrons forming some mixture of the π- and σ-orbital structures in the ^{12}Be ground state. Third, we can see the fading of intrinsic shape of the α clusters as the number of neutrons increases. This structure change cannot be obtained by cluster models, which assume the α cluster as a fundamental degree of freedom. This finding implies a way to investigate the deformation of α clusters.

In addition to the investigation of intrinsic structure of Be isotopes, we also extend our analysis to three α clusters in the ^{12}C nucleus. In the analysis of the intrinsic shape of ^{12}C, we introduce the cluster analysis in the statistics. We define the distance

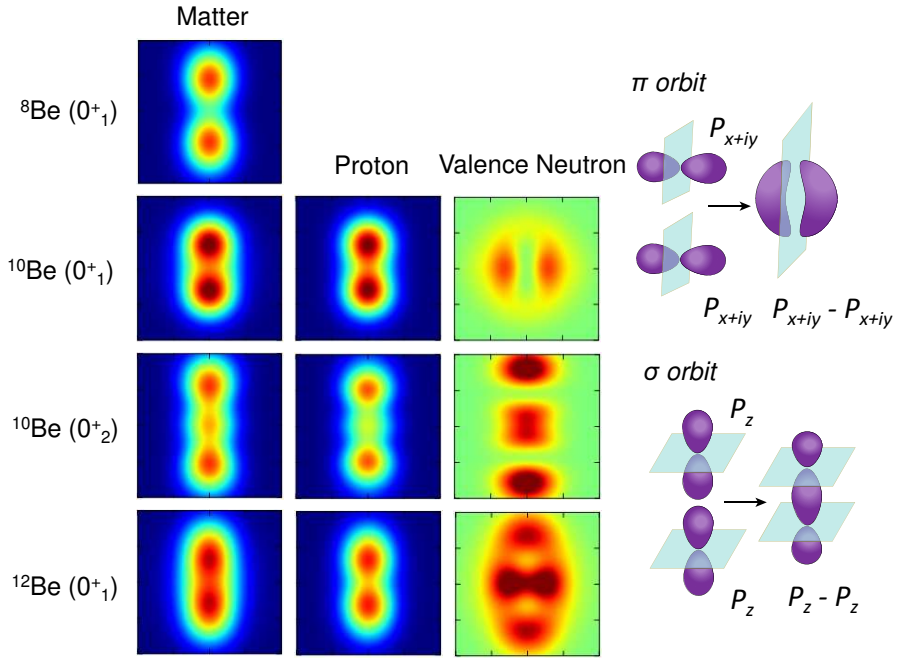

Figure 4: Schematic intrinsic density illustrating the α-cluster and molecular-orbital structure of Be isotopes obtained by the no-core MCSM.

measured in the Euclidean space which gauges the similarity of densities and categorize the groups of similar shape. For the first application, we divide our deformed Slater determinants, which amount around 100 basis states, into 15 groups. By separating the deformed Slater determinants into these groups, we have calculated overlap probability of deformed Slater determinants in each group with the total MCSM wave function. The results are shown in Fig. 5. From this analysis, we have obtained the 0^+ ground state of ^{12}C mainly composed by the group of the compact (shell-model-like) shape and that of three α clusters. For the second 0^+ state, the overlap probability is distributed among all 15 groups on an equal footing. It indicates that this state is a gas-like state, which is proposed by the study with the THSR wave functions [22] as the Bose–Einstein condensation of the α gas.

5 Summary

We shortly outlined the Monte Carlo shell model (MCSM) from its formalism to some numerical results, focusing on recent application of this method to *ab initio* no-core calculations. The essence of the MCSM is the importance truncation. The size of the original large sparse Hamiltonian matrix spanned by harmonic-oscillator Slater determinants is reduced to a smaller dense one spanned by stochastically selected bases. With this method, one can perform large-scale shell-model calculations even in the case that the standard shell-model approaches with the Lanczos method cannot handle. Most of the physics of interest usually lies on the forefront of and even beyond the current computational limit.

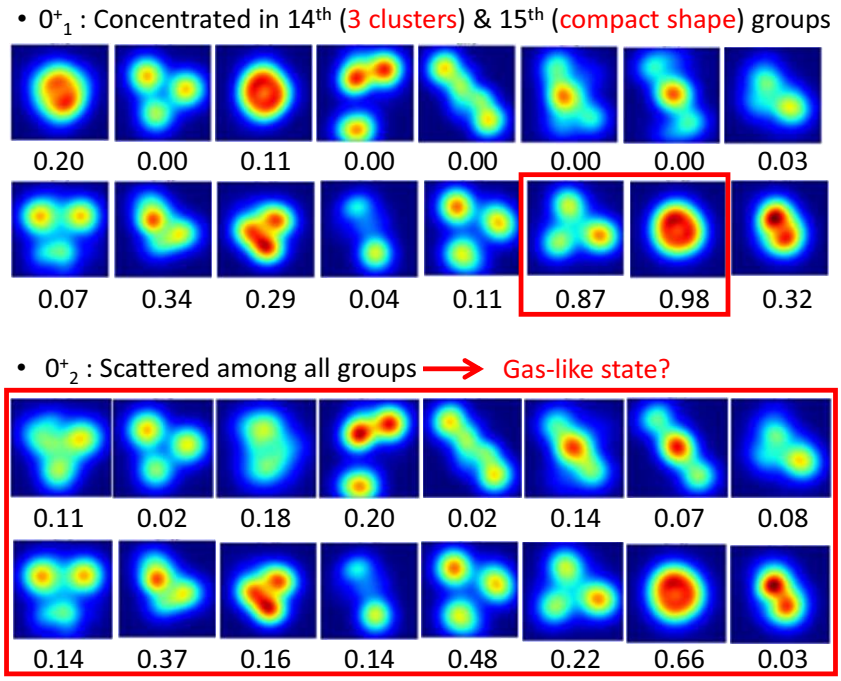

Figure 5: Cluster analysis of the ^{12}C nucleus in the no-core MCSM.

In this contribution, the MCSM has been presented focusing on the no-core shell-model calculations. It is found that the no-core MCSM results for light nuclei up to $A \leq 20$ with a NN potential can be extrapolated to the limit of infinite basis space and provide *ab initio* solutions with evaluated theory uncertainties. The JISP16 NN interaction gives good agreement with experimental data up to around 12-nucleon system even without handling explicit three-nucleon interactions. As one of physics applications, an exploratory study of the α cluster phenomena has been provided with the visualization of intrinsic density obtained from the MCSM wave functions before spin- and parity-projections. We found the emergence of two-α-cluster structure in the ^{8}Be ground state without any assumption of α clusters. We also identified the molecular orbital states of valence neutrons in neutron-rich Be isotopes. The deformation of α clusters was seen in the ground states of Be isotopes with increasing the number of neutrons. Following the study of the Be isotopes, the analysis of the intrinsic shape of ^{12}C was briefly discussed. The intrinsic density of the ground state of ^{12}C is mainly composed of compact shell-model-like and three-α-cluster shapes, while the overlap probability for the second 0^+ state is distributed among various configurations which indicates a gas-like state.

For future perspectives, the no-core MCSM calculations with the Daejeon16 NN interaction are necessary for providing some insights on how far such kind of nonlocal NN interactions can be applied to a heavier mass region. Also, a quantitative analysis of the α-cluster structures based on intrinsic densities is expected to be done in the near future.

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