Cluster-orbital shell model approach and developments for study of neutron-rich systems

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Abstract
We develop an m-scheme approach of the cluster-orbital shell model (COSM). By using the Gaussian as the radial part of the basis function, components of the unbound states are correctly taken into account. We apply the m-scheme COSM to oxygen isotopes and study the energies and r.m.s.radii.

1 Introduction

Innovation both on experimental techniques and theoretical approaches enables us to study nuclei for wider area than ever. Now the front line of the research field has reached to the neutron and proton drip-lines not only in light mass region but also in the middle mass region [1]. For example, the abrupt increase of the r.m.s.radius at ^{23}O has been observed as one of the typical phenomena of nuclei in the drip-line region [1].

For the theoretical study, however, it is not so straightforward to reproduce such the abrupt increase [2–4]. In the drip-line regions, it is important to include the components of unbound states. The continuum shell model [5] and the Gamow shell model [6] are one of the practical solutions to solve such the problem for inclusion of the unbound states in the shell model picture.

The cluster-orbital shell model (COSM) approach has been developed to study light neutron rich nuclei [7]. Using COSM with the Gaussian basis set, many-body resonant states can be exactly calculated by making use of the complex scaling method [8]. As shown in Ref. [8], the COSM formalism with the Gaussian basis can describe the halo structure, which is a typical property of the weakly bound system. We propose an extension of the COSM approach to treat the dynamics of the core [9] and showed the importance of the modification of the radius of the core nucleus. We also discussed the role of the unbound states in the COSM approach [10]. In Ref. [10], we investigated the contribution of the continua and resonant poles in the helium isotopes and compared those obtained by the GSM approaches.

In this paper, we propose an m-scheme approach of COSM to overcome the limitation on the number of valence nucleons in the practical calculation. As the example of the neutron-rich nuclei, we study oxygen isotopes and calculate binding energies and r.m.s.radii. In Sect. 2, we briefly show the formalism of our m-scheme COSM and the model for interaction and wave functions. In Sect. 3, we show the calculated results for oxygen isotopes. In Sect. 4, summary and discussion are given.

2 Formalism and interaction

2.1 Cluster-orbital shell model

We briefly explain the formalism of the cluster-orbital shell model (COSM) [7]. In COSM, the coordinates of the valence nucleons are spanned from the center of mass of the core nucleus, and the kinetic energy of the center of mass motion $\hat{T}_G$ is subtracted from the total A-body Hamiltonian. Hence, the the total Hamiltonian of COSM is described as follows:

$$\hat{H} = \sum_{i=1}^{A} \hat{t}_i - \hat{T}_G + \sum_{i<j}^{A} \hat{v}_{ij}$$

$$= \hat{H}_C + \sum_{i\in V}(\hat{t}'_i + \hat{V}'_i) + \sum_{i<j\in V}(\hat{T}_{ij} + \hat{v}_{ij})\,. \tag{1}$$

Here, $\hat{t}'_i$ is a one-particle kinetic energy operator between the core and the ith valence nucleon. The index "V" in the sum in Eq.(1) stands for the nucleons in the valence nucleons part. $\hat{H}_C$ is the Hamiltonian for nucleons in the core, and $\hat{T}_{ij}$ is the two-body kinetic operator, $\hat{T}_{ij} = (\hbar^2/m)\nabla_i \cdot \nabla_j$, which comes from the subtraction of the center of mass motion. The potential between the core and the ith valence nucleon is defined by taking the sum for the nucleons in the core part as $\hat{V}'_i \equiv \sum_{k\in C}\hat{v}_{ik}$.

The core and valence wave functions, $|\Phi_C\rangle$ and $|\Phi_V\rangle$ are anti-symmetrized for nucleons in each part. The total wave function $|\Psi\rangle$ is constructed by the core and valence parts as follows:

$$|\Psi\rangle = \mathcal{A}'\Big\{\,|\Phi_C\rangle\,|\Phi_V\rangle\Big\}\,, \tag{2}$$

where $\mathcal{A}'$ stands for the anti-symmetrization between two nucleons; one nucleon in $|\Phi_C\rangle$ and other one in $|\Phi_V\rangle$. Therefore, the wave function $|\Psi\rangle$ is totally anti-symmetrized.

In the study of oxygen isotopes, we fix the lowest configuration of the harmonic oscillator wave functions for the core part; $|\Phi_C\rangle$, and the size parameter of the harmonic oscillator is determined so as to reproduce observed value of the r.m.s.radius of ^{16}O.

For the valence nucleons, on the other hand, the radial function is taken as the products of the Gaussian functions as follows:

$$F(r_1,\cdots,r_N) \equiv g_1(r_1)\cdots g_N(r_N)\,, \tag{3}$$

where $g_i(r_i)$ is the Gaussian function for the ith valence nucleon with the normalization N_i and the width parameter a_i as $g_i(r_i) = N_i\exp(-\frac{1}{2}a_i r_i^2)$. In order to describe the correct property of the asymptotic behavior of weakly bound systems, it is necessary to include the components of the unbound states. Therefore, the valence part is constructed by a superposition of the Gaussian functions,

$$\begin{aligned}\Phi_V &= \sum_m c^{(m)}\Phi^{(m)}_{JMTM_T} \\ &= \sum_m c^{(m)}\mathcal{A}\Big\{F^{(m)}(r_1,\cdots,r_N)\cdot|JMTM_T\,^{(m)}\rangle\Big\}\,.\end{aligned} \tag{4}$$

In the above equation, m stands for the index of the basis functions. In each basis function, the Gaussian width parameter a_i, angular momenta j_i and l_i are the parameters in the calculation, and optimized in a variational way [11, 12]. We discussed the advantages of the Gaussian basis functions [9]. It has been shown that the superposition of the Gaussian correctly describes the halo structure [8] and includes components of the unbound states [10].

2.2 M-scheme COSM

We employ the basis set so that the z-components of the total angular momentum and total isospin are fixed: $|MT_z\rangle = \{\phi_{\alpha_1}\phi_{\alpha_2}\cdots\phi_{\alpha_N}\}_{M,\,M_T}$. Here, $\{\cdots\}_{MT_z}$ indicates that the z-component of the total spin and isospin; M and T_z are fixed. α_i are spin and isospin for ith nucleon, j_i, l_i, s_i, t_i and their z-components.

Hence, the wave function for the valence part becomes as follows:

$$\begin{aligned}\Phi_V &= \sum_m c^{(m)}\Phi^{(m)}_{MM_T} \\ &= \sum_m c^{(m)}\mathcal{A}\Big\{F^{(m)}(r_1,\cdots,r_N)\cdot|MM_T\,^{(m)}\rangle\Big\}\,.\end{aligned} \tag{5}$$

If the basis size is sufficiently large, the eigen vectors have a good quantum number of the total spin and isospin, and the coefficients $c^{(m)}$ play the role of the Clebsh-Gordan coefficients. Furthermore, the lowest eigen value becomes the lowest-energy state with the possible spin and isospin, for having the z-components of M and M_T.

2.3 Model and Interaction

We construct the interaction between the core and a valence nucleon, by taking into account the structure of the core and the exchange effect with an approximated way.

$$\hat{V}_i'|\Phi_V\rangle \equiv \sum_{k\in C} \left\langle \Phi_C \;\middle|\; \hat{v}_{i\,k} \;\middle|\; \mathcal{A}' \left\{ |\Phi_C\rangle\,|\Phi_V\rangle \right\} \right\rangle \simeq \hat{V}_i^d + \hat{V}_i^{ex} \,. \tag{6}$$

The interaction is constructed by folding the nucleon-nucleon interaction with the core wave function. The direct part of the folding procedure gives the $\hat{V}_i^d$ term. For taking the anti-symmetrization between the nucleons in the core and valence parts, we introduce the approximation, which is proposed by Kaneko et al. in Ref. [13], in which the recoil effect and other exchange kernels except for the knock-on exchange term are omitted [13], which gives the $\hat{V}_i^{ex}$ term.

Due to the Pauli principle between the nucleons in the core and a valence nucleon, it is necessary to eliminate the spurious states for the valence nucleon system. We use the orthogonality condition model (OCM) [14] in order to treat the Pauli principle and eliminate the spurious states. As a conventional method, we introduce a pseudo potential $\lambda\hat{\Lambda}_i = \lambda|F.S.\rangle\langle F.S.|$ to the Hamiltonian of the valence nucleons. $|F.S.\rangle$ is the projection operator to the occupied states in the core, in other words, the forbidden states. For the ^{16}O core wave function, these states are $(0s_{1/2})$, $(0p_{3/2})$ and $(0p_{1/2})$. By taking $\lambda \to \infty$ in the diagonalization of the matrix of the Hamiltonian, the forbidden states $|F.S.\rangle$ are effectively eliminated. Furthermore, we introduce an effective LS-potential $\hat{V}_i^{ls}$ to reproduce the spin-orbit partners in ^{17}O, $5/2_1^+$ and $3/2_1^+$. The strength parameter of the LS-potential is adjusted to reproduce the energies of the above states.

To summarize, the Hamiltonian for the ith valence nucleon, $\hat{h}_i$ becomes as follows:

$$\hat{h}_i = \hat{t}_i' + \hat{V}_i^d + \hat{V}_i^{ex} + \hat{V}_i^{ls} + \lambda\hat{\Lambda}_i \,. \tag{7}$$

And the parameters in the potentials are adjusted to reproduce three states, $5/2_1^+$, $1/2_1^+$ and $3/2_1^+$, as the single-particle states of the ^{16}O+n system; $0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$.

For the nucleon-nucleon interaction, we use the Volkov No.2 [17] and Minnesota [18] interactions.

3 Results

In this section, we show calculated results for energies and r.m.s.radii of the oxygen isotopes from ^{17}O to ^{26}O. In the calculations, we take the maximum angular momentum for each partial wave as $L_{\max} = 2$. Therefore, $s_{1/2}$, $p_{3/2}$,$p_{1/2}$, $d_{5/2}$ and $d_{3/2}$ partial waves are included in the calculation. As shown in the calculation of the single neutron separation energies, the binding energy becomes over-binding for heavier oxygen isotopes, which is shown in Fig. 1. The calculated radii are almost on the empirical $A^{1/3}$-line and much smaller than the experimental values. Especially, for ^{23}O and ^{24}O, the discrepancy of calculated radii from the experiments is more than 0.2 (fm).

We consider that the small r.m.s.radii in neutron-rich oxygen isotopes is caused by the strong attraction of the nucleon-nucleon interaction near drip-line. Hence, we perform other calculations using the Minnesota potential [18] (MN) with the exchange parameter $u = 0.95$, which has a weaker attraction than that of VN2. Calculated energy of ^{18}O by using the Minnesota potential shows slightly under binding, ~ 1.9 (MeV). Even though the attraction of the Minnesota potential is weaker than the Volkov one, ^{25}O and ^{26}O are still bound nuclei, and the drip-line is not reproduced.

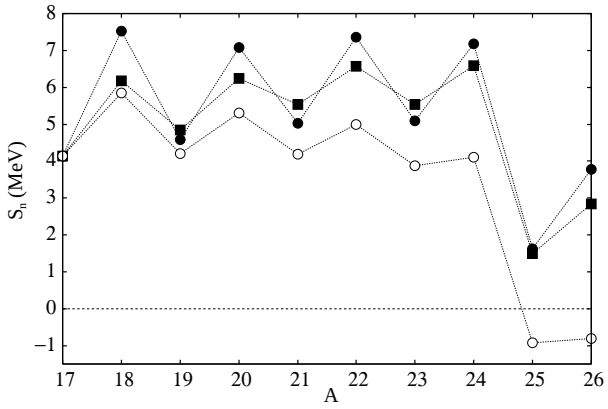

Fig. 1: Calculated one neutron separation energies for oxygen isotopes. Solid circles, solid squares and open circles are obtained by VN2, MN and VN2', respectively. See text.

Therefore, we modify the potential parameter so as to reproduce the drip-line of the oxygen isotopes at ^{24}O. In order to make a weaker potential than VN2, we use the parameters $M = 0.58$ and $H = B = 0.25$ in Volkov No.2 potential (VN2'). This potential parameter gives reasonable unbound nature for ^{25}O and ^{26}O. However, due to the weakness of the attraction, the even-odd staggering in the change of mass number becomes smaller than those obtained by the original Volkov potential, VN2.

Using the potentials, VN2, MN and VN2', we calculate the r.m.s.radii. Fig. 2 shows the calculated results and the experimental values for r.m.s.radii of oxygen isotopes. For the original potential strength cases, i.e. VN2 and MN, r.m.s.radii are not enhanced at ^{23}O. The small change occurring at ^{23}O is caused by the presence of the s-wave component in the valence nucleons. For the VN2' case, on the other hand, the calculated r.m.s.radii are the same until ^{22}O, but show an enhancement at ^{23}O compared with the results of the VN2 and MN cases.

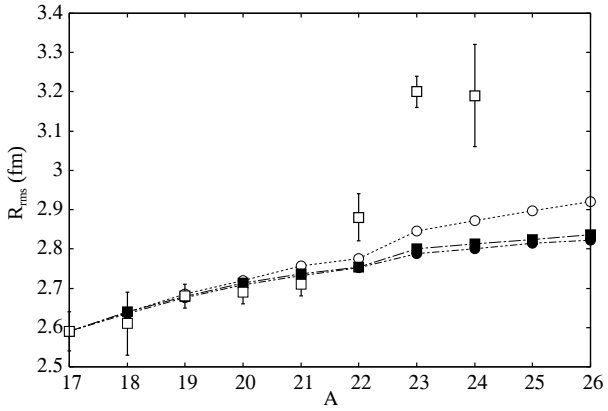

Fig. 2: Calculated and experimental r.m.s.radii for oxygen isotopes. Solid circles, solid squares and open circles are obtained by VN2, MN and VN2', respectively. Open squares with error bars are experimental value [1].

We consider that one of the reason of this enhancement is the weakness of the nucleon-nucleon interaction, which reproduce the drip-line at ^{24}O. And other reason is the presence of the s-wave component in ^{23}O and heavier isotopes.

In order to confirm the mechanism of the enhancement at ^{23}O, we investigate the components of the partial waves in the isotopes. Results are shown in Table 1. The difference between the VN2 and

Table 1: Calculated components of partial waves in the oxygen isotopes. For the definition of VN2 and VN2', see text.

	Components	**VN2 (%)**	**VN2' (%)**
^{22}O	$(d_{5/2})^6$	78.7	95.0
	$(s_{1/2})^2(d_{5/2})^4$	15.9	3.1
	$(d_{5/2})^4(d_{3/2})^2$	4.2	1.7
^{23}O	$(s_{1/2})(d_{5/2})^6$	91.2	97.0
	$(s_{1/2})(d_{5/2})^4(d_{3/2})^2$	2.1	0.1
	$(s_{1/2})(d_{5/2})^5(d_{3/2})$	5.6	2.1
^{24}O	$(s_{1/2})^2(d_{5/2})^6$	94.6	98.5
	$(s_{1/2})^2(d_{5/2})^4(d_{3/2})^2$	4.3	1.2
	$(d_{5/2})^6(d_{3/2})^2$	0.6	0.1

VN2' cases is the Heisenberg and Bartret exchange parameters, H and B. For ^{22}O, in which the lowest configuration for neutron is $(0d_{5/2})^6$ of the shell model picture, the d-wave component increases in the VN2' case. Therefore, even if the binding energy of the VN2' case is smaller than that of VN2, the r.m.s.radius does not become so large. On the other hand, in ^{23}O and ^{24}O, the $0d_{5/2}$-orbit is almost occupied. Hence, the change of the exchange parameters, H and B, affects mainly to the $1s_{1/2}$-orbit. As shown in Table 1, the dominance of the sum of the s-wave states for the VN2' case is stronger than that of the VN2 case. This makes the enhancement of the radius at ^{23}O. However, the effect is still too small to reproduce the experimental value.

Even if the small binding energies of ^{23}O and ^{24}O and the drip-line of the oxygen isotopes are reproduced by using VN2', the abrupt increase of r.m.s.radii of ^{23}O and ^{24}O are still smaller than that of the experiments [1] as shown in Fig. 2. This result suggests that other mechanisms are necessary to be introduced in order to make a consistent understanding for the binding energies and r.m.s.radii, simultaneously.

4 Summary and Discussions

We proposed an m-scheme approach of the cluster-orbital shell model (COSM). In our formalism, the interaction between the core nucleus and a valence nucleon is constructed in the semi-microscopic way. Hence, the structure of the core is considered in the calculation. Parameters are determined so as to reproduce the ^{17}O and ^{18}O, in the VN2 case. However, both of the VN2 and MN cases do not describe the correct neutron drip-line, in other words, the attraction of the interaction is too strong in the drip-line region. Therefore, we modify the exchange parameters in Volkov potential (VN2') in order to reproduce the drip-line.

Even though we use a weaker potential, VN2', the r.m.s.radii of ^{23}O and ^{24}O do not become so large. We consider the abrupt increase of the r.m.s.radius of ^{23}O and ^{24}O can not be explained by a simple picture such that one or two neutron(s) are loosely bound around the core such as ^{11}Be, ^{6}He, ^{11}Li. Of course, the s-wave component would play an important role in the weakly bound systems. Furthermore, not only the loosely bound picture, but also other mechanisms, such as a core-excitation or modification due to the presence of many valence neutrons would be necessary to explain the very large r.m.s.radii of ^{23}O and ^{24}O. Also, in order to reproduce the binding energies, the drip-line and r.m.s.radii simultaneously, it might be necessary to introduce the potential which is based on the realistic nucleon-nucleon force, and three-body interaction.

Acknowledgements

We would like to thank the members of the nuclear theory group at Hokkaido university for the fruitful discussion. This work was supported by the Grant-in-Aid for Scientific Research (No. 21740154) from the Japan Society for the Promotion of Science.

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