Improved version of simplified method for including tensor effect in cluster models

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I. INTRODUCTION

The binding energy per nucleon of \(^4\text{He}\) is quite large in light mass region and \(\alpha\) particles are considered as good building blocks for the nuclear structure. Cluster models, especially the \(\alpha\) cluster models, are based on this idea, and they have been widely used for the description of molecular structure of nuclei \([1, 2]\). One of the well-known examples is the so-called Hoyle state \([3]\); formation of \(^{12}\text{C}\) from three \(^4\text{He}\) nuclei (\(\alpha\) clusters) is a key process of the nucleosynthesis. The second \(0^{+}\) state at \(E_x = 7.6542\) MeV plays a crucial role, which is the second excited state of \(^{12}\text{C}\) and located just above the threshold energy to decay into three \(^4\text{He}\) nuclei. The existence of a state which has the character of three \(\alpha\) clusters just at this energy is really an essential factor in the synthesis of various elements in stars. Such three-\(\alpha\)-state is described by various cluster models, and among them, the Tohsaki-Horiuchi-Schock-Röpke (THSR) wave function is a powerful tool to describe gas-like cluster states with spatial extension \([4]\). Based on the shell-model picture, which is standard in nuclear structure physics, we often need large model space to describe cluster states. Since some of the nucleons are spatially correlated around the nuclear surface, the cluster states are difficult to be described with a framework in which the wave function of each nucleon is expanded around the origin. Therefore the cluster structures are challenge of the shell models, including modern \textit{ab initio} ones \([5, 7]\).

Nuclear systems have characteristic features that non-central interactions play a crucial role; however in most of the cluster models, the spin-orbit and tensor interactions do not contribute inside \(\alpha\) clusters and also between \(\alpha\) clusters because of the antisymmetrization effect and spatial symmetry of \(\alpha\) cluster. In cluster models, each \(\alpha\) cluster is often defined as a simple \((0s)^4\) configuration at some spatial point, and \(\alpha\) cluster is a spin singlet system, which is free from the non-central interactions. Concerning the spin-orbit interaction, this is known to be quite important in explaining the observed magic numbers. The \(jj\)-coupling shell model, which is the standard model for the nuclear structure, is based on this picture.

Our goal is to pave the way to generally describe the nuclear structure, including shell and cluster structures simultaneously. Here, contrary to the standard approaches, we start with the cluster model side and try to include shell correlations. This is because our approach requires much less computational efforts compared with the case starting with the shell model side. To include the spin-orbit contribution starting with the cluster model, we proposed the antisymmetrized quasi-cluster model (AQCM) \([8–10]\), which allows smooth transition of \(\alpha\) cluster model wave function to \(jj\)-coupling shell model one. In AQCM, this transition can be controlled by only two parameters: \(R\) representing the distance between \(\alpha\) clusters and \(\Lambda\), which characterizes the transition of \(\alpha\) cluster(s) to \(jj\)-coupling shell model wave functions and quantifies the role of the spin-orbit interaction. We call the transformed \(\alpha\) clusters in this way quasi-clusters. As it is well known, the conventional \(\alpha\) cluster models cover the model space of closure of major shells \((N = 2, N = 8, N = 20, etc.)\) and in addition, the subclosure configurations of the \(jj\)-coupling shell model, \(p_{3/2} (N = 6), d_{5/2} (N = 14), j_{7/2} (N = 28)\), and \(g_{9/2} (N = 50)\) can be described by our AQCM. In this way the cluster and \(jj\)-coupling shell model wave functions can be described on the same footing, and the spin-orbit interaction, which is the rank one non-central interaction, can be successfully taken into account in the cluster model.

However the rank two non-central interaction, the tensor interaction, is more complicated to be treated in the cluster model. The tensor interaction has two features,
the first order type and the second order type. The first order one is rather weak and characterized by the attractive effect for a proton (neutron) with the j-upper orbit of the jj-coupling shell model and a neutron (proton) with j-lower orbit, or repulsive effect for the j-upper (j-lower) two protons or two neutrons. This effect can be included just by switching on the tensor interaction in the Hamiltonian, after transforming cluster wave function to jj-coupling shell model one using AQCM mentioned above. The second order effect of the tensor is much stronger. According to the ab initio calculations, the (negative) contribution of the tensor interaction in \(^4\)He is quite large, more than \(-65\) MeV, and this is even more important than the central interaction. Here, it is found that the two particle two hole (2p2h) excitation to higher shells, especially to the p shell, is quite important. According to the tensor optimized shell model (TOSM) calculations, the p orbits of this 2p2h states must have very shrunk shape compared with the normal shell model orbits, and this means that mixing of very high momentum components is quite important.

This second order effect of the tensor interaction is more difficult to be treated in the cluster model, and we need an additional framework; we have proposed a simplified model to directly take into account the contribution of the tensor interaction (SMT) \([24]\). The tensor contribution was estimated in \(^4\)He, \(^8\)Be, and \(^{12}\)C, and the relation to the clustering was quantitatively discussed. However the contribution of the tensor interaction was rather limited, about \(-10\) MeV in the \(\alpha\) cluster, and improvement of the model was needed. In our previous SMT, we started with an \(\alpha\) cluster with a \((0s)^4\) configuration and expressed deuteron-like excitation of a proton and neutron to higher shells by shifting the values of the Gaussian center parameters of these two particles. However, shifting the positions of Gaussian center parameters may not be enough for the purpose of mixing higher momentum components of 2p2h configurations, and this could be the reason. In the present article, we introduce improved version of SMT, which is iSMT. Here, imaginary part of Gaussian center parameters is shifted in stead of the real part. The imaginary part of Gaussian center parameter corresponds to the expectation value of momentum for the nucleon. The tensor interaction has the character which is suited to be described in the momentum space, and this method is considered to be more efficient in directly mixing the higher momentum components of 2p2h configurations.

The purpose of the present work is to incorporate the 2p2h nature of the tensor contribution in the cluster model in a simplified and more efficient way compared with the previous SMT. We improve SMT and newly propose iSMT. Firstly we apply it to \(^4\)He and next discuss that the clustering of four \(\alpha\)'s is closely related to the tensor effect in \(^{16}\)O. There have been fundamental discussion for the appearance of cluster structure in the 1960s; one-pion exchange potential (OPEP) vanishes in the direct terms when each \(\alpha\) cluster is described as a \((0s)^4\) configuration, and this is the reason why inter-cluster interaction is weak. However, it is important to show that clustering is still important, even if the model space is extended and the tensor contributions in each \(\alpha\) cluster is taken into account. We discuss that the clustering is enhanced because of the tensor interaction in \(^{16}\)O.

Recently, many other attempts of directly taking into account the tensor part of the interaction in microscopic cluster models have begun. For instance, by combining unitary correlation method (UCOM) and Fermionic molecular dynamics (FMD) \([25, 27]\), or using antisymmetrized molecular dynamics (AMD) \([28]\), cluster structure has been extensively studied. In UCOM, the tensor contribution can be taken into account by unitary transforming the Hamiltonian, where two-body correlator is introduced in the exponent of the unitary operator. If we expand this power based on the cluster expansion method, in principle, the Hamiltonian contains many-body operators up to \(A\) (mass number) body, thus the truncation of the model space is required. Our strategy is slightly different. Although the framework is phenomenological, we do not perform the unitary transformation of the Hamiltonian, and we introduce an effective model wave function to directly take into account the tensor effect.

For the central part of the interaction, we use the Tohsaki interaction, which has finite range three-body terms. This interaction is a phenomenological one and designed to reproduce the \(\alpha\)-\(\alpha\) scattering phase shift. Also it gives reasonable size and binding energy of the \(\alpha\) cluster, which is rather difficult in the case of the zero-range three-body interaction, and the binding energy is less sensitive to the choice of size parameter of Gaussian-type single particle wave function. Furthermore, the saturation property is reproduced rather satisfactory.

II. THE MODEL

A. Hamiltonian

The Hamiltonian \((\hat{H})\) consists of kinetic energy \((\hat{T})\) and potential energy \((\hat{V})\) terms,

\[\hat{H} = \hat{T} + \hat{V}, \tag{1}\]

and the kinetic energy term is described as one-body operator,

\[\hat{T} = \sum_i \hat{t}_i - T_{cm}, \tag{2}\]

and the center of mass kinetic energy \((T_{cm})\), which is constant, is subtracted. The potential energy has central \((V_{central})\), spin-orbit \((V_{spin-orbit})\), tensor \((V_{tensor})\), and the Coulomb parts.

For the central part of the potential energy \((V_{central})\), the Tohsaki interaction is adopted, which consists of two-
for nucleon-nucleon scattering phase shift, is adopted;

\[ V_{ij}^{(2)} = \sum_{\alpha=1}^{3} V_{ij}^{(2) \alpha} \exp\left[-(\vec{r}_i - \vec{r}_j)^2/\mu_\alpha^2\right](W^{(2)}_\alpha + M^{(2)\alpha}P^r)_{ij}, \]

(3)

where \( V_{ij}^{(2)} \) and \( V_{ij}^{(3)} \) consist of three terms with different range parameters,

\[ V_{ij}^{(2)} = \sum_{\alpha=1}^{3} V_{ij}^{(2)\alpha} \exp\left[-(\vec{r}_i - \vec{r}_j)^2/\mu_\alpha^2\right](W^{(2)}_\alpha + M^{(2)\alpha} P^r)_{ij}, \]

(4)

\[ V_{ijk}^{(3)} = \sum_{\alpha=1}^{3} V_{ijk}^{(3)\alpha} \exp\left[-(\vec{r}_i - \vec{r}_j)^2/\mu_\alpha^2 - (\vec{r}_i - \vec{r}_k)^2/\mu_\alpha^2\right] \times (W^{(3)}_\alpha + M^{(3)\alpha} P^r)_{ij}(W^{(3)}_\alpha + M^{(3)\alpha} P^r)_{jk}. \]

(5)

Here, \( P^r \) represents the exchange of spatial part of the wave functions of interacting two nucleons. In this article, we use F1’ parameter set \[12\], which was designed to avoid small overbinding of \(^{16}\)O when the original F1 parameter set is adopted. The difference of F1 and F1’ is only for the three-body Majorana exchange parameter for the shortest range.

For the spin-orbit part, G3RS \[30\], which is a realistic interaction originally determined to reproduce the nucleon-nucleon scattering phase shift, is adopted;

\[ V_{\text{spin-orbit}}^{(3)} = \frac{1}{2} \sum_{i \neq j} V_{ij}^{(3)\alpha}, \]

(6)

\[ V_{ij}^{(3)\alpha} = V_{ij}^{(3)\alpha}(e^{-d_1(\vec{r}_i - \vec{r}_j)^2} - e^{-d_2(\vec{r}_i - \vec{r}_j)^2})P(3O)\vec{L} \cdot \vec{S}. \]

(7)

For the strength, \( V_{ij} = 1800 \text{ MeV} \) has been suggested to reproduce the various properties of \(^{12}\)C \[15\], and we use this value.

Up to this point, the interaction is the same as in Ref. \[15\], and the main purpose of the present article is to switch on the tensor interaction. For the tensor part, we use Furutani interaction \[31\]. This interaction nicely reproduces the tail region of one pion exchange potential, and the comparison is shown as Fig. 1 in Ref. \[24\].

### B. Wave function

The single particle wave function has a Gaussian shape \[\Pi\],

\[ \phi_i = \left(\frac{2\nu}{\pi}\right)^{3/4} \exp\left[-\nu(\vec{r}_i - \vec{R}_i)^2\right] \eta_i, \]

(8)

where \( \eta_i \) represents the spin-isospin part of the wave function, and \( \vec{R}_i \) is a parameter representing the center of a Gaussian wave function for the \( i \)-th particle. The size parameter \( \nu \) is chosen to be 0.25 fm\(^{-2}\) for \(^{4}\)He (0.20 fm\(^{-2}\) for \(^{16}\)O). In Brink-Bloch wave function, four nucleons in one \( \alpha \) cluster share a common and real value for the Gaussian center parameter. Hence, the contribution of the spin-orbit and tensor interactions vanishes.

The wave function of the total system \( \Psi \) is antisymmetrized product of these single particle wave functions;

\[ \Psi = A\{\psi_1\psi_2\psi_3 \cdots \psi_A\}, \]

(9)

where \( A \) is a mass number. The projections onto parity and angular momentum eigenstates can be performed by introducing the projection operators \( P^M K \) and \( P^\pi \), and these are performed numerically in the actual calculation.

Based on generator coordinate method (GCM), the superposition of different Slater determinants can be done,

\[ \Phi = \sum_i c_i P^M K P^\pi \Psi_i. \]

(10)

Here, \( \{\Psi_i\} \) is a set of Slater determinants, and the coefficients for the linear combination, \( \{c_i\} \), are obtained by solving the Hill-Wheeler equation \[\Pi\].

### C. SMT and sSMT

Here we explain how we can incorporate the tensor effect starting with the \( \alpha \) cluster model. Previously, we have introduced SMT \[24\]. In SMT, we started with an \( \alpha \) cluster with a \((0s)^4\) configuration and changed it for the purpose of including the tensor contribution. For the \((0s)^4\) configuration, the Gaussian center parameter (\( \vec{R} \) in Eq. \[8\]) for the spin-up proton (\( \vec{R}_{p\uparrow} \)), spin-down proton (\( \vec{R}_{p\downarrow} \)), spin-up neutron (\( \vec{R}_{n\uparrow} \)), and spin-down neutron (\( \vec{R}_{n\downarrow} \)) were all set to zero. In SMT, we mimicked deuterons, where a proton and a neutron have aligned spin orientation and spatially displaced in this spin orientation. For \(^4\)He, we transformed it to two deuterons with spin up and down; we shifted the Gaussian center of the spin-up proton to the \( z \) direction, which forms a deuteron together with the spin-up neutron at the origin, and we also shifted the spin-down neutron to the \(-z\) direction, which forms a deuteron with the spin-down proton at the origin. The Gaussian center parameters were introduced in the following way;

\[ \vec{R}_{p\uparrow} = d\vec{e}_z, \]

(11)

\[ \vec{R}_{n\uparrow} = 0, \]

(12)

\[ \vec{R}_{p\downarrow} = 0, \]

(13)

\[ \vec{R}_{n\downarrow} = -d\vec{e}_z, \]

(14)
about −10 MeV in the α cluster. Shifting the positions of Gaussian center parameters may not be enough for the purpose of mixing higher momentum components of 2p2h configurations, and this could be the reason why the effect of the tensor interaction was rather limited. According to TOSM, the higher-nodal orbits of the 2p2h states must be introduced to have very shrunk shape compared with the normal shell model orbits. In Fig. 1 Fourier transformation of one dimensional $p$ orbits are shown. The $p$ orbit on the $x$ axis before the Fourier transformation is proportional to $x \exp[-\nu x^2]$, and $\nu = 1/2b^2$. The horizontal axis is the wave number $k$ (fm$^{-1}$). The dotted line is for the normal $p$ orbit after the Fourier transformation with the standard size parameter ($b = 1.4$ fm), and the solid line is the one used in TOSM with a shrunk size parameter ($b = 0.6 \times 1.4$ fm).

In iSMT, the Gaussian center parameters are introduced in the following way:

$$\vec{R}_p^\uparrow = d \vec{c}z,$$
$$\vec{R}_n^\uparrow = 0,$$
$$\vec{R}_p^\downarrow = 0,$$
$$\vec{R}_n^\downarrow = -d \vec{c}z,$$  (17)

and $d$ values are 0, 1, 2, ⋅⋅⋅ 10 fm (11 Slater determinants). In addition, we prepare the basis states, where neutron spin-up is shifted in stead of neutron spin-down:

$$\vec{R}_p^\uparrow = d \vec{c}z,$$
$$\vec{R}_n^\uparrow = -d \vec{c}z,$$
$$\vec{R}_p^\downarrow = 0,$$
$$\vec{R}_n^\downarrow = 0,$$  (18)

and $d$ values are 1, 2, ⋅⋅⋅ 10 fm (10 Slater determinants). Eventually, we superpose these 21 Slater determinants in total based on GCM. According to Eq. (18) the expectation value of the momentum for $d = 10$ fm is 5 fm$^{-1}$.

III. RESULTS

A. $^4$He

First we start with $^4$He. The energy convergence for the ground state of $^4$He described based on iSMT is shown in Fig. 2 as a function of number of basis states. Here iSMT is a linear combination of 21 GCM basis states; the basis state “1” is (0s)$^4$ configuration, and in 2-11 (12-21), the imaginary part of the Gaussian center parameters for the spin-up proton and spin-down (spin-up) neutron are shifted as in Eq. (17) (Eq. (18)), where $d$ values are 1, 2, 3, ⋅⋅⋅ 10 fm. At “1” on the horizontal axis, the tensor interaction does not contribute, and the energy gets lower by more than 20 MeV with increasing the number of the GCM basis states.

In Table I we compare the energies of $^4$He calculated using the (0s)$^4$ configuration, conventional SMT, and newly introduced iSMT. Here total, $T$, $V^2$, $V^3$, $V^{ls}$, $V^4$, and $V^{Coul}$ mean the expectation value of the total energy, kinetic energy, two-body interaction, three-body interaction, spin-orbit interaction, tensor interaction, and Coulomb interaction, respectively. The tensor contribution of iSMT is −41.56 MeV, which is more than four times compared with the previous version. The kinetic energy of iSMT increases from the value for the (0s)$^4$ configuration by about 25 MeV in the positive direction, and this is because of the mixing of higher momentum components. Here we can see that the contribution of the two-body interaction increases by about 9 MeV in the negative direction. Compared with the so called ab initio calculations, the tensor contribution is still small, but we can include the effect to the level of −40 MeV.
TABLE I: Energies of $^4$He calculated using the $(0s)^4$ configuration, conventional SMT, and newly introduced $i$SMT. Here total, $T$, $V^2$, $V^3$, $V^{ls}$, $V^t$, and $V^{Coul}$ mean the expectation value of the total energy, kinetic energy, two-body interaction, three-body interaction, spin-orbit interaction, tensor interaction, and Coulomb interaction, respectively. All units are in MeV.

| Energy ($\text{MeV}$) | $(0s)^4$ | SMT | iSMT |
|----------------------|---------|-----|------|
| total                | $-27.50$ | $-32.85$ | $-50.64$ |
| $T$                  | $46.65$  | $53.14$  | $71.96$  |
| $V^2$                | $-79.38$ | $-83.75$ | $-88.65$ |
| $V^3$                | $4.41$   | $6.22$   | $6.18$   |
| $V^{ls}$             | $0.0$    | $0.11$   | $0.57$   |
| $V^t$                | $0.0$    | $-9.40$  | $-41.56$ |
| $V^{Coul}$           | $0.81$   | $0.84$   | $0.87$   |

(our central part of the interaction is phenomenological one without short range core, thus precise comparison with \textit{ab initio} calculations is rather difficult).

The amplitude for the linear combination of the basis states ($c_i$ in Eq. [10]) for $^4$He described based on $i$SMT is shown in Fig. 2. In principle the amplitudes can be complex numbers; however here we obtained real numbers after diagonalizing the Hamiltonian. The basis state “1” on the horizontal axis corresponds to the $(0s)^4$ configuration. In the basis states 2-11 (12-21), the imaginary part of the Gaussian center parameters for the spin-up proton and spin-down (spin-up) neutron are shifted as in Eq. [17] (Eq. [18]). The amplitude for the basis state “2” is obtained as a negative value, and this is to create a node for the wave function, which means particle-hole excitation (however we shift the Gaussian center parameters of two particles simultaneously, thus direct correspondence to the $p$ orbits is rather difficult to be seen). The amplitude for the basis state “3” returns back to positive value, which means excitation to even higher shells, and absolute value of the amplitude gets smaller with increasing $d$ value. From “12”, spin-up neutron is shifted in stead of spin-down neutron. Although the absolute value of the amplitude is smaller, the basis tendency is the same as the spin-down neutron case.

B. $^{16}$O

The same procedure can be applied to $^{16}$O and we can discuss the relation between the tensor contribution and the clustering effect. Here, $^{16}$O is introduced as a tetrahedral configuration of four-$\alpha$ clusters, and one of the clusters is deformed using $i$SMT to include the tensor contribution. The $0^+$ state energy of $^{16}$O with a tetrahedral configuration of four-$\alpha$ clusters as a function of distance between $\alpha$-$\alpha$ is shown in Fig. 3. The solid and dotted lines show the results with and without the tensor interaction. We can confirm that with the tensor interaction, the clustering is even enhanced. The decrease of the energy after switching on the tensor interaction is only 5.7 MeV at the $\alpha$-$\alpha$ distance of 0.1 fm. Here the contribution of the tensor interaction in the Hamiltonian is only $-10.2$ MeV. The tensor contribution is suppressed at small relative distances (the wave function corresponds to the closed shell configuration of the $p$ shell at the zero-distance limit). This is because, the $2p2h$ excitation from the lowest $s$ shell to the $p$ shell is forbidden, even though the excitation from the $p$ shell to $sd$ shell is allowed. With increasing the $\alpha$-$\alpha$ distance, the decrease of the energy due to the tensor interaction is enhanced. The decrease is about 20 MeV around the lowest energy point, and the matrix element of the tensor interaction is $-32.7$ MeV at the $\alpha$-$\alpha$ distance of 2 fm. Therefore, it can be concluded that the tensor interaction has a certain effect for the stability of clusterized configurations. In Refs. [32, 33], it has been suggested that tensor contribution is suppressed in $^{16}$O, since $2p2h$ excitation from...
turned out to be large in model limit. This is true; however tensor contribution of the lowest α between dural configuration of four-α clusters as a function of distance without the tensor interaction.

In the present case, this 2p2h tensor effect is already renormalized in the central part of the effective interaction as in many conventional models, and the result gives very large overbinding. In the next step, the modification of the central part of the two-body and three-body interactions to reproduce the binding energies of many nuclei including this kind of tensor effect will be carried out.

IV. SUMMARY

It has been shown that the tensor contribution can be incorporated in the cluster model in a simplified way. In conventional α cluster models, the contribution of the non-central interactions cancels because of the antisymmetrization effect and spatial symmetry of each α cluster, and the mixing of the breaking components of α clusters to take into account the spin-orbit and tensor effects is needed. Previously we proposed a simplified method to include the spin-orbit effect, and also for the tensor part, a simplified method to take into account the tensor contribution in the cluster model (SMT) was introduced. Here we improved SMT, which is called iSMT, where the imaginary part of Gaussian center parameters of nucleons in one α cluster was shifted in stead of the real part. The imaginary part of Gaussian center parameter corresponds to the expectation value of momentum for the nucleon. The tensor interaction has the character which is suited to be described in the momentum space, and this method is considered to be more efficient in directly mixing the higher momentum components of 2p2h configurations.

Using newly proposed iSMT, the contribution of the tensor interaction in 4He is more than −40 MeV, four times larger than the previous version. The method was applied to four-α-cluster structure of 16O. In 16O, the tensor contribution is suppressed at the limit of small relative distance corresponding to the closed shell configuration of the p shell. With increasing the α-α distance, the decrease of the energy due to the tensor interaction is enhanced; about 20 MeV around the lowest energy point. Therefore, it can be concluded that the tensor interaction has a certain effect for the stability of clusterized configurations.

In the present case, this 2p2h tensor effect is already renormalized in the central part of the effective interaction as in many conventional models, and the result gives very large overbinding. As a future work, we modify the central part of the two-body and three-body interactions to reproduce the binding energies of many nuclei including this kind of tensor effect.

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