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Cluster-shell competition in light nuclei
---- inclusion of non-central interactions in $\alpha$-cluster model

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Abstract. The competition between the cluster and shell structure of light nuclei is discussed. First, we demonstrate in $^{12}\text{C}$ by superimposing many Slater determinants that the cluster structure dissolves when the shell-model-like model space is introduced. The decrease of the energy from the $3\alpha$ configuration by about 6 MeV is a clue to resolve a long-standing problem of the binding energies of $^{12}\text{C}$ and $^{16}\text{O}$. As a next step, we propose a simple model to include the spin-orbit interaction (SMSO). By introducing only one parameter ($\Lambda$) to the wave function, describing an asymptotic transition of $^{12}\text{C}$ from a $3\alpha$ configuration to a $2\alpha + 4N$ configuration is represented, and we show a strong contribution of the spin-orbit interaction in the ground state. Furthermore, we propose a simplified model to directly take into account the contribution of the tensor interaction (SMT) for light nuclei by extending $\alpha$-cluster model. The coupling effect of SMSO and SMT is shown to be important in $^{12}\text{C}$, contrary to $^{9}\text{Be}$.

1. Introduction
Nuclei are quantum many-body systems consisting of protons and neutrons, and these nucleons have been known to construct some self-consistent mean field and to perform independent-particle motions. The nuclear shell-model, which is one of the most standard models for the nuclear structure, is based on this picture, and strong spin-orbit interaction in the mean field has been known to be a key mechanism to fully explain the observed magic numbers.

On the other hand, the $\alpha$-particle, which corresponds to the doubly closed-shell of the lowest s-shell in the shell-model, is strongly bound, and since relative $\alpha - \alpha$ interaction is weak, strongly interacting four nucleons ($\alpha$ particle) become a subunit of the nuclear structure in some light nuclei, contrary to the mean-field picture. This molecular viewpoint has been introduced even before the shell-model, and such `cluster' feature of light nuclei has been extensively studied for more than four decades. In the so-called Ikeda diagram, the threshold rule has been proposed as a guiding principle to explain the appearance of the cluster structure in stable 4N nuclei: cluster structure appears around the corresponding threshold energy. Recently, theoretical and experimental investigations have further proceeded to systems beyond the 4N nuclei, and cluster structure with valence neutrons has become one of the main subjects concerning the structure of unstable nuclei. If a $\alpha$-cluster is expressed as the lowest ($s_{1/2}$) configuration, it is a spin-zero system, and non-central interactions do not contribute for it. However, the dissolution of the $\alpha$-cluster should be taken into account in systems, where the spin-orbit interaction, which is a characteristic interaction in the mean-field picture, strongly acts. Therefore,
it is intriguing to study the cluster-shell competition for the unified understanding of the nuclear structure.

2. Cluster-shell competition
To see the effect of cluster-shell competition, at first, we superimpose many Slater determinants[1]. The energy convergence of $^{12}\text{C}$ is shown in Fig. 1. The basis states from 1 to 100 have various configurations of $3\alpha$, and those from 101 to 600 have $\alpha+\alpha+2p+2n$ model space (relative $\alpha-\alpha$ distances of 2, 3, and 4 fm). Here, the decrease of energy from $3\alpha$-model is 5.2 MeV due to strong spin-orbit interaction. Furthermore, the shell-model like wave functions of the $\alpha+4p+4n$ model space are added (from 601 to 800), where two of $\alpha$-clusters are broken. However, the decrease of the energy by adding these basis states is only about 1 MeV, and it is considered that the contribution of the spin-orbit interaction is almost taken into account when one of $\alpha$-clusters is broken. The squared overlaps between the ground state of the final solution and the lowest, the second, and the third $0^+$ states of the $3\alpha$-cluster configuration (1-100 basis states) are 0.56, 0.06, and 0.01, respectively. Therefore, although the ground state has the $3\alpha$ component of about 60%, large amount of $\alpha$-breaking component mixes.

![Fig. 1 The energy convergence of $^{12}\text{C}$ ($0^+$).](image1)

![Fig. 2 The nuclear chart of the cluster-shell competition.](image2)

On the other hand, the calculated second $0^+$ state (observed at Ex = 7.65 MeV) mainly has the $3\alpha$-component. The sum of the squared overlaps between the second $0^+$ state and the lowest three $0^+$ states of $3\alpha$-cluster configuration exceeds 0.8. This state is a typical cluster state, and the shell-model study by Cohen and Kurath gives very high excitation energy (13-14 MeV) for the state, suggesting that it is out of the model space. In stellar nucleosynthesis, the second $0^+$ state just above the $3\alpha$ threshold plays a crucial role in forming $^{12}\text{C}$. It is formed as triple-$\alpha$ resonance state and decays first to the $2^+$ state and next to the ground $0^+$ state by emitting $\gamma$-rays. The B(E2, $0^+ \rightarrow 2^+$) value (experimentally $13 \pm 4 \text{ e}^2\text{fm}^4$) strongly affects the abundance of $^{12}\text{C}$, however, it has been about half ($5.6 \text{ e}^2\text{fm}^4$) in the traditional $3\alpha$ model based on the Resonating Group Method (RGM). In the present case, the mixing of $3\alpha$ and $\alpha$-breaking components affects the B(E2) value ($14.1 \text{ e}^2\text{fm}^4$) and it becomes consistent with the experimental value.
The coupling effects between the cluster states and shell-model states are summarized as nuclear chart of the cluster-shell competition in Fig. 2. Here, $\Delta$ represents the increase of the binding-energy when the breaking of one of $\alpha$-clusters is taken into account. The nuclei $^8\text{Be}$, $^{16}\text{Be}$, and $^{10}\text{B}$ have the $\Delta$ values of about 2 MeV, and essentially $\alpha+\alpha$ structure is dominant configuration of the ground states. However, the $\Delta$ values are very large in $^{12}\text{C}$ (5.2 MeV). For $^{12}\text{C}$, $\Delta(2)$ is also shown, which is the increase of the binding energy when the breaking of two of $\alpha$-clusters is taken into account (6.2 MeV).

The present result gives a clue to resolve a long standing problem of the binding energy between $^{12}\text{C}$ and $^{16}\text{O}$. It has been known that in microscopic cluster model, when we use the effective interaction which reproduces the binding energy of the $3\alpha$ system, the $4\alpha$-system becomes over-binding by about 20 MeV. On the contrary, if the binding energy of $4\alpha$ is reproduced, $3\alpha$-system becomes under-binding by about 10 MeV. We have previously discussed that the experimental binding energy difference between $^{12}\text{C}$ and $^{16}\text{O}$ cannot be fully reproduced, even if we utilize a finite-range and density-dependent interaction, when the model space is restricted to $\alpha$-clusters[2]. Now it is shown that by incorporating the $\alpha$-breaking component, the binding energy of $^{12}\text{C}$ becomes deeper by several MeV due to the spin-orbit interaction. Since this effect is considered to be less important for $^{16}\text{O}$ with doubly closed configuration of the p-shell, the spin-orbit interaction would be one of the important keys to resolve this long-standing problem.

3. Simplified method to include the spin-orbit contribution (SMSO)

As we have shown, currently, microscopically calculating the cluster-shell competition is possible. However, the next question we must ask is how we can simplify the model and establish a new picture as a general concept of the nuclear structure? For example, how the effect of the spin-orbit interaction, which is the key quantity for this transition, can be implanted in the wave function, and what is the order parameter for the transition from the cluster state to the shell state? In this section, therefore, we propose a simple model to describe cluster-shell competition[3]. It will be shown that by introducing only one parameter ($\Lambda$), it is possible to describe a transition for example in $^{12}\text{C}$, and the strong contribution of the spin-orbit interaction in the ground state can be described.

The total wave function is fully antisymmetrized as

$$\Phi = P^\uparrow \mathcal{P}_{MK} \Psi,$$

$$\Psi = A((\phi_1 \chi_1)(\phi_2 \chi_2) \cdots),$$

and projection onto a good parity ($P^\uparrow$) and angular momentum ($P_{MK}$) is numerically performed. Each nucleon ($\phi_i \chi_i$, $i = 1 \sim A$) has a local Gaussian form with the Gaussian-center parameter $R_i$ the same as many conventional cluster models. When we assume the presence of an $\alpha$-cluster(s), it is expressed by assuming a common $R_i$ value for four nucleons (proton spin-up, proton spin-down, neutron spin-up, and neutron spin-down).

If $\{R_i\}$ are real numbers, the wave function corresponds to the Brink-Bloch wave function, and the spin-orbit interaction vanishes for the $N\alpha$-systems. However, in the present case, they are allowed to be complex parameters. The real and imaginary parts of $R_i$ represent the expectation values of the position and momentum of the single particle as in AMD[4]:

$$<r> = \text{Re}[R_i],$$

$$<p> = 2\sqrt{\hbar} \text{Im}[R_i].$$

We introduce a "general rule" to take into account the spin-orbit interaction, where the dissociation of one of (Brink-Bloch) clusters to a "quasi cluster" is expressed by introducing a parameter $\Lambda$. Suppose that a nucleus consists of a quasi-cluster $C_1'$ and $\alpha$-clusters $\{C_2, C_3, \ldots, C_m\}$. The Gaussian-center
parameters for nucleons in $\alpha$-clusters are real numbers. However, for the nucleons in the quasi-cluster, in addition to the real part of $\text{Re}[R_i] = S_i (i \in C')$, imaginary part is introduced, which expresses the momentum components of the nucleons. The direction of the imaginary part of the Gaussian-center parameter is introduced for each nucleon as

$$ R_i = S_i + i \Lambda e_i(\text{spin}) \times S_i, $$

where $e_i(\text{spin})$ is the unit vector for the intrinsic-spin orientation, and $\Lambda$ is an order parameter of the dissolution of the cluster. The contribution of the spin-orbit interaction vanishes at $\Lambda = 0$, and it acts attractively or repulsively, if $\Lambda$ is positive or negative, respectively. This can be understood in the following way: the spin-orbit interaction is intuitively interpreted as $(r \times p) \cdot s$ and this is equal to $(s \times r) \cdot p$, where $r$, $p$, and $s$ represent the position, momentum, and spin of the nucleon, respectively. Therefore, if the nucleons in the quasi-cluster have the momentum components parallel to $s \times r$, the spin-orbit interaction acts attractively, and if they have momentum components anti-parallel to $s \times r$, it acts repulsively, although the spin-orbit interaction is a two-body operator in the actual calculation.

![Fig. 3](image1.png)  Schematic figure of SMSO for $^{12}$C.  

![Fig. 4](image2.png)  The energy curves for $^{12}$C.

Three $\alpha$-clusters are introduced to have an equilateral triangular configuration on the $xz$-plane as shown in Fig. 3, which is known to be the dominant configuration for the ground state when the spin-orbit interaction does not work. In Fig. 3, $R_1$ represents the distance between two $\alpha$-clusters on the $z$-axis and the remaining $\alpha$-cluster is placed on the $x$-axis. We introduce $\Lambda$ for one $\alpha$-cluster on the $x$-axis. Due to the Pauli principle, these nucleons are automatically excited to the $p$-shell. This parameterization and setup of the coordinate space could be called a "general rule" for preparing cluster-breaking wave functions. First, we put the cluster to be broken on the $x$-axis. Next, we change the Gaussian centers of nucleons in this cluster from $R e_x$ to $R (e_x + i \Lambda e_y)$ for the spin-up nucleons, and to $R (e_x - i \Lambda e_y)$ for the spin-down nucleons, where $R$ is some distance and $\Lambda$ is an "order parameter" of cluster-shell competition, and $e_x$ and $e_y$ are unit vectors of $x$ and $y$ axes. Since the directions of the spins are defined along the $z$-axis, the spin and orbital parts of the angular momenta become parallel, and the spin-orbit interaction acts attractively with an increasing $\Lambda$. In other words, by introducing these imaginary parts, we can mimic the spherical harmonics. Namely, when $\Lambda$ is equal to 1, the wave function for the spin-up neutron corresponds exactly to the shell-model one of
\((x+iy)\exp[-y r^2] \sim r Y _{11} \exp[-y r^2] \) and the wave function for the spin-down neutrons corresponds to \((x-iy)\exp[-y r^2] \sim r Y _{11} \exp[-y r^2] \), respectively, at the limit of \(R_1 = 0\).

The energy curve of the 0\(^+\) state of \(^{12}\)C as a function of parameter \( \Lambda \) is shown in Fig. 4, where the solid, dotted, and dashed lines represent the cases of \(R_1 = 2.0, 2.5, \) and \(3.0 \) fm, respectively. The interaction adopted here is Volkov No.2 with \(M=0.6\) for the central part and G3RS with the strength parameter of 2000 MeV for the spin-orbit part, determined by \(\alpha - \alpha\) and \(\alpha - n\) scattering phase-shift analysis. When the \(\Lambda\) value is zero, the total spin of the system is also zero; the spin-orbit interaction does not work, and the dotted line \((R_1 = 2.5 \) fm\) gives the lowest energy. However, when \(\Lambda\) becomes a finite value, one \(\alpha\)-cluster on the x-axis is changed to a "quasi \(\alpha\)". and four nucleons start to perform independent motions around the remaining two \(\alpha\) clusters located on the z axis, such that the picture is close to molecular-orbital motion around the \(\alpha - \alpha\) core[5,6]. In this case, the solid line \((R_1 = 2.0 \) fm\) gives the lowest energy, and the decrease of this energy in comparison with \(\Lambda = 0\) is more than 5 MeV.

4. Simplified method to include the tensor contribution (SMT)

Finally, we introduce simplified model to take into account the tensor contribution (SMT)[7]. In cluster models, nucleon-nucleon interactions adopted have been effective interactions instead of bare ones, constructed by renormalizing the short-range core and tensor parts in the central part so as to be used in model spaces of the cluster models, where each nucleon is usually described as Gaussian-type wave functions. Recently, several attempts of directly taking into account the tensor part of the interaction in microscopic cluster models have been started, and strong contribution has been discussed, for example in the \(^4\)He nucleus. The purpose of the present study is to establish a simplified method to take into account the tensor contribution and show the applicability for \(^4\)He, \(^8\)Be and \(^{12}\)C.

When the \(\alpha\)-cluster is described as the simplest \((0s)^4\) configuration, it is a spin-zero system, and non-central interactions of either spin-orbit or tensor type do not contribute. Furthermore, the tensor interaction does not act attractively even if we break the \(\alpha\)-cluster with the \((0s)^4\) configuration to two cluster system of p+t or n+\(^3\)He. Suppose that the position of the spin-up proton is shifted from other three nucleons forming a triton (t) cluster. The tensor interaction acts between this spin-up proton and spin-up neutron in the t cluster, since they have deuteron-like \(S = 1, T = 0\) component. However, in the triton cluster, a spin-down neutron occupies the same spatial orbit as the spin-up neutron. Thus, the tensor contribution between the spin-up proton and spin-up neutron is canceled by the presence of this spin-down neutron, which has the same spatial wave function as the spin-up neutron but with the opposite spin-direction.

This discussion suggests that we must break the \(\alpha\)-cluster not to two clusters as p+t or n+\(^3\)He but at least to three clusters such as p+n+\(^2\)H. As for the coordinate system, the energy surface of the deuteron system[8] suggests that the tensor interaction acts attractively when a spin-up proton and spin-up neutron stay along the spin-direction. Therefore, we remove the spin-down neutron from the spin-up proton-neutron pair along their spin-direction (z axis). The Gaussian center parameters of the four nucleons \((R_i)\) are defined as:

\[ R_{p \uparrow} = d e_z, \quad R_{p \downarrow} = 0, \quad R_{n \uparrow} = 0, \quad R_{n \downarrow} = -d e_z. \]

The spin-up proton-neutron pair have the component of \(S = 1, T = 0\), similarly, the spin-down proton and neutron have an \(S = 1, T = 0\) component. Here, the spin-down neutron (spin-up proton) does not stay inside the spin-up proton-neutron pair (spin-down proton-neutron pair), so the tensor correlation is not disturbed. Hereafter, this transformation is called as the simplified method to include the tensor contribution (SMT). Here, \(^4\)He is described as the linear combination of eleven Slater determinants \((d = 0\sim 7 \) fm\). We adopted Furutani interaction as an effective tensor interaction, and the calculated 0\(^+\)
energy (E) is -33.27 MeV. The 0\(^+\) energy is lower by 5.7 MeV by the inclusion of the tensor terms, which is a little smaller than other more sophisticated calculations but reasonable.

The simplified method to include the tensor contribution (SMT) is further applied to \(^{12}\text{C}\). Three \(^{\alpha}\)-clusters have an equilateral-triangular configuration, and here, only two of them are transformed to take into account the tensor contribution for simplicity (transforming three \(^{\alpha}\)-clusters is possible but the result does not change drastically). The energy of the 0\(^+\) ground state of \(^{12}\text{C}\) is calculated as -92.80 MeV by using SMT when we superpose the states with the \(^{4}\text{He}\)-\(^{4}\text{He}\) distances of 2, 2.5 and 3 fm. This is lower than that of the \((0s)^4\) model space by 6.1 MeV, and here, the matrix element of the tensor interaction is -7.18 MeV. However, the spin-orbit interaction, which plays an important role in \(^{12}\text{C}\) give a small contribution for this model space (0.07 MeV).

Therefore, we couple two model spaces of SMT and SMSO. The energy becomes -96.29 MeV, which is lower than the energy for the \((0s)^4\) configuration for each \(^{\alpha}\)-cluster by about 9.6 MeV. Here, the spin-orbit and tensor interactions contribute by -8.77 MeV and -5.00 MeV, respectively. Here, the tensor contribution in SMT is weakened when SMSO model space is coupled, since the tensor interaction acts repulsively between the protons in j-upper orbits and the neutrons in j-upper orbits[9]. Since spin-orbit interaction acts attractively for these orbits, this means that the competition between the tensor and spin-orbit contributions occurs in \(^{12}\text{C}\).

From these analyses, two roles of tensor contributions have been clarified. One role is to bind the \(^{4}\text{He}\) cluster. The tensor interaction strongly acts inside each \(^{4}\text{He}\) nucleus; however it is not strong for the relative motion between \(^{4}\text{He}\) nuclei. The tensor interaction contributes to increase the binding energy of each \(^{4}\text{He}\), however the cluster structure persists. This can be expressed by using SMT. The other role of the tensor interaction is to give a correct spin-dependence for the motion of the single particles rotating around the core nucleus. This tensor contribution is relatively weak compared to the first one, and it acts repulsively for the j-upper proton and neutron (attractive for the j-upper proton and j-lower neutron), which is expressed by the SMSO model. To take into account these two natures of the tensor interaction, the coupling of the two model spaces of SMT and SMSO is necessary.

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