Consistent description for cluster dynamics and single-particle correlation

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Cluster dynamics and single-particle correlation are simultaneously treated for the description of the ground state of $^{12}\text{C}$. The recent development of the antisymmetrized quasi cluster model (AQCM) makes it possible to generate $jj$-coupling shell-model wave functions from $\alpha$ clusters models. The cluster dynamics and the competition with the $jj$-coupling shell-model structure can be estimated rather easily. In the present study, we further include the effect of single-particle excitation; the mixing of the two-particle-two-hole excited states is considered. The single-particle excitation is not always taken into account in the standard cluster model analyses, and the two-particle-two-hole states are found to strongly contribute to the lowering of the ground state owing to the pairing-like correlations. By extending AQCM, all of the basis states are prepared on the same footing, and they are superposed based on the framework of the generator coordinate method (GCM).

I. INTRODUCTION

The $^4\text{He}$ nuclei have been known to have large binding energy in the light mass region. On the contrary, the relative interaction between $^4\text{He}$ nuclei is weak. Therefore, they can be subsystems called $\alpha$ clusters in some of light nuclei [1, 2]. The search for the candidates for the $\alpha$ cluster structure has been performed for decades, and the most famous example is the second $0^+$ state of $^{12}\text{C}$ called Hoyle state, which has a developed three-$\alpha$ cluster structure [3, 4]. The cluster models have been found to be capable of describing various properties of the Hoyle state [5, 6].

In most of the conventional cluster models, the clusters treated as subsystems have been limited to nuclei corresponding to the closure of the three-dimensional harmonic oscillator, such as $^4\text{He}$, $^{16}\text{O}$ and $^{40}\text{Ca}$. In these cases, the contribution of the non-central interactions (spin-orbit and tensor interactions) vanishes. This is because the closure configurations of the major shells can create only spin zero systems owing to the antisymmetrization effect. This point was the big problem of these traditional cluster models; the non-central interactions work neither inside clusters nor between $\alpha$ clusters. The spin-orbit interaction is known to be quite important in nuclear systems, especially in explaining the observed magic numbers; the subclosure configurations of the $jj$-coupling shell model ($j_{7/2}$, $g_{9/2}$, and $h_{11/2}$) correspond to the observed magic numbers of 28, 50, and 126 [7]. Indeed this spin-orbit interaction is known to work as a driving force to break the traditional clusters corresponding to the closures of the major shells, when the model space is extended and the path to another symmetry is opened [8].

To include the spin-orbit contribution in the theoretical model starting with the traditional cluster model side, we proposed the antisymmetrized quasi cluster model (AQCM) [3, 21]. This method allows us to smoothly transform $\alpha$ cluster model wave functions to $jj$-coupling shell model ones, and we call the clusters that feel the effect of the spin-orbit interaction owing to this model quasi clusters. In AQCM, we have two parameters: $R$ representing the distance between $\alpha$ clusters and $\Lambda$ characterizing the transition of $\alpha$ cluster(s) to quasi cluster(s). The $jj$-coupling shell model states can be obtained starting with the $\alpha$ cluster model by changing $\alpha$ clusters to quasi clusters (giving finite $\Lambda$ values to $\alpha$ clusters) and taking small distance limit of $R$. It has been known that the conventional $\alpha$ cluster models cover the model space of closure of major shells ($N = 2$, $N = 8$, $N = 20$, etc.). In addition, by changing $\alpha$ clusters to quasi clusters, the subclosure configurations of the $jj$-coupling shell model, $p_{3/2}$ ($N = 6$), $d_{5/2}$ ($N = 14$), $f_{7/2}$ ($N = 28$), and $g_{9/2}$ ($N = 50$), which arise from the spin-orbit interaction in the mean-field, can be described by our AQCM [13].

We have previously introduced AQCM to $^{12}\text{C}$ and discussed the competition between the cluster states and $jj$-coupling shell model state [3]. The consistent description of $^{12}\text{C}$ and $^{16}\text{O}$, which has been a long-standing problem of microscopic cluster models, has been achieved. In this paper, we examine again $^{12}\text{C}$, where not only the competition between the cluster states and the lowest shell-model configuration, the effect of single-particle excitation is further included for the description of the ground state. The mixing of the two-particle-two-hole excited states owing to the pairing-like correlations is examined. By extending AQCM, all of the basis states are prepared on the same footing, and they are superposed based on the framework of the generator coordinate method (GCM). Although it has been analytically shown to be feasible to prepare some of the two-particle-two-hole configurations of the $jj$-coupling shell model within the framework of AQCM [17], here we try to use...
much simpler method. The two-particle-two-hole states around the optimal AQCM basis state are generated using numerical technique. Owing to the generation of many states compared with our previous approach, much larger effect for the lowering of the energy due to the mixing of two-particle-two-hole states will be discussed.

The nucleus of $^{12}$C is the typical example which has both characters of cluster and shell aspects. Recently, various kinds of microscopic approaches have shown the importance of the mixing of shell and cluster components. Not only the energy levels, various properties including electromagnetic transition strengths, $\alpha$-decay widths, and scattering phenomena have been discussed. Especially, based on the antisymmetrized molecular dynamics (AMD), the one-particle-one-hole states are discussed in relation with the isoscalar monopole and dipole resonance strengths. In this approach, one-particle-one-hole states are expressed by the small shift of one particle around the optimal AQCM basis state. This cluster is the spin-isospin part of the wave function. For the size parameter $\nu$, here we use $\nu = 0.23$ fm$^{-2}$, which gives the optimal $0^+$ energy of $^{12}$C within a single AQCM basis state. The Slater determinant is constructed from these single-particle wave functions by antisymmetrizing them.

Next we focus on the Gaussian center parameters $\{\zeta_i\}_\alpha$. As in other cluster models, here four single-particle wave functions with different spin and isospin sharing a common $\zeta$ value correspond to an $\alpha$ cluster. This cluster wave function is transformed into $jj$-coupling shell model based on the AQCM. When the original value of the Gaussian center parameter $\zeta_i$ is $R$, which is real and related to the spatial position of this nucleon, it is transformed by adding the imaginary part as

$$\zeta = R + i\Lambda e^{\text{spin}} \times R,$$

where $e^{\text{spin}}$ is a unit vector for the intrinsic-spin orientation of this nucleon. The control parameter $\Lambda$ is associated with the breaking of the cluster, and with a finite value of $\Lambda$, the two nucleons with opposite spin orientations have the $\zeta$ values, which are complex conjugate with each other. This situation corresponds to the time-reversal motion of two nucleons. After this transformation, the $\alpha$ clusters are called quasi clusters.

Here we explain the intuitive meaning of this procedure. The inclusion of the imaginary part allows us to directly connect the single-particle wave function to the spherical harmonics of the $jj$-coupling shell model. Suppose that the Gaussian center parameter $\zeta_i$ has the $x$ component, and the spin direction is defined along the $z$ axis (this is spin-up nucleon). According to Eq. (2), the imaginary part of $\zeta$ is given to its $y$ component. When we expand $-\nu (r - \zeta)^2$ in the exponent of Eq. (1), a factor $\exp [2\nu \zeta \cdot r]$ corresponding to the cross term of this expansion appears. The factor $\exp [2\nu \zeta \cdot r]$ contains all the information of the angular momentum of this single particle. The Taylor expansion allows us to show that the $p$ wave component of $\exp [2\nu \zeta \cdot r]$ is $2\nu \zeta \cdot r$, which is proportional to $(x + i\Lambda y)$. At $\Lambda = 1$, this is proportional to $Y_{11}$ of the spherical harmonics. The nucleon is spin-up, and thus the coupling with the spin part gives the stretched state of the angular momentum, $|3/2 \ 3/2\rangle$ of the $jj$-coupling shell model, where the spin-orbit interaction acts attractively. For the spin-down nucleon, we introduce the complex conjugate $\zeta$ value, which gives $|3/2 \ -3/2\rangle$.

In the case of $^{12}$C, we prepare three quasi clusters. The next two nucleons are generated by rotating the $\zeta$ values and spin-directions of these two nucleons by $2\pi/3$. The last two nucleons are generated by changing the rotation angle to $4\pi/3$. Eventually, all the six nucleons have spin-stretched states, and after the antisymmetrization, the configuration becomes the subclosure configuration of $(s1/2)^2 (p3/2)^4$. This procedure is applied for both proton and neutron parts. The detail is shown in Ref. [14].

### II. FRAMEWORK

#### A. Basic feature of AQCM

AQCM allows the smooth transformation of the cluster model wave functions to the $jj$-coupling shell model ones. In AQCM, each single particle is described by a Gaussian form as in many other cluster models including the Brink model.

$$\phi_{r,s} (r) = \left(\frac{2\nu}{\pi}\right)^{\frac{1}{2}} \exp \left[-\nu (r - \zeta)^2\right] \chi_{r,s},$$

where the Gaussian center parameter $\zeta$ is related to the expectation value of the position of the nucleon, and $\chi_{r,s}$ is the spin-isospin part of the wave function. For the size parameter $\nu$, here we use $\nu = 0.23$ fm$^{-2}$, which gives the optimal $0^+$ energy of $^{12}$C within a single AQCM basis state. The Slater determinant is constructed from these single-particle wave functions by antisymmetrizing them.

Next we focus on the Gaussian center parameters $\{\zeta_i\}_\alpha$. As in other cluster models, here four single-particle wave functions with different spin and isospin sharing a common $\zeta$ value correspond to an $\alpha$ cluster. This cluster wave function is transformed into $jj$-coupling shell model based on the AQCM. When the original value of the Gaussian center parameter $\zeta_i$ is $R$, which is real and related to the spatial position of this nucleon, it is transformed by adding the imaginary part as

$$\zeta = R + i\Lambda e^{\text{spin}} \times R,$$

where $e^{\text{spin}}$ is a unit vector for the intrinsic-spin orientation of this nucleon. The control parameter $\Lambda$ is associated with the breaking of the cluster, and with a finite value of $\Lambda$, the two nucleons with opposite spin orientations have the $\zeta$ values, which are complex conjugate with each other. This situation corresponds to the time-reversal motion of two nucleons. After this transformation, the $\alpha$ clusters are called quasi clusters.

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the Gaussian center parameters of the first quasi cluster are given as
\[
\zeta_{1}^{p, n \uparrow} = R (e_{x} + i \Delta e_{y}) / \sqrt{3}, \tag{3}
\]
for spin-up proton (\(\zeta_{1}^{p \uparrow}\)) and neutron (\(\zeta_{1}^{n \uparrow}\)) and
\[
\zeta_{1}^{p, n \downarrow} = R (e_{x} - i \Delta e_{y}) / \sqrt{3}, \tag{4}
\]
for spin-down proton (\(\zeta_{1}^{p \downarrow}\)) and neutron (\(\zeta_{1}^{n \downarrow}\)). Here \(e_{x}\) and \(e_{y}\) are unit vectors of the \(x\)- and \(y\)-axis, respectively. The spin-isospin part of the wave function are denoted as \(\chi_{1}^{p \uparrow}, \chi_{1}^{p \downarrow}, \chi_{1}^{n \uparrow}\), and \(\chi_{1}^{n \downarrow}\), for spin-up proton, spin-up neutron, spin-down proton, and spin-down neutron in the first quasi cluster. For the second and third quasi clusters, we introduce a rotation operator around the \(y\) axis \(R_{y}(\Omega)\). The Gaussian center parameters of the four nucleons in the second quasi cluster are generated by rotating the those in the first quasi cluster around the \(y\) axis by \(2\pi/3\) radian;
\[
\zeta_{2}^{p, n \uparrow, p \downarrow, n \downarrow} = R_{y} (2\pi/3) \chi_{1}^{p, n \uparrow, p \downarrow, n \downarrow}, \tag{5}
\]
It is important to note that the spin-isospin part (\(\chi_{2}^{p \uparrow}, \chi_{2}^{p \downarrow}, \chi_{2}^{n \uparrow}\), and \(\chi_{2}^{n \downarrow}\)) also needs to be rotated as
\[
\chi_{2}^{p, n \uparrow, p \downarrow, n \downarrow} = R_{y} (2\pi/3) \chi_{1}^{p, n \uparrow, p \downarrow, n \downarrow}, \tag{6}
\]
where the axis of the spin orientation is also tilted around the \(y\) axis by \(2\pi/3\) radian (but the isospin parts do not change). The third quasi cluster is introduced by changing the rotation angle around the \(y\) axis to \(4\pi/3\) radian,
\[
\zeta_{3}^{p, n \uparrow, p \downarrow, n \downarrow} = R_{y} (4\pi/3) \chi_{1}^{p, n \uparrow, p \downarrow, n \downarrow}, \tag{7}
\]
for the Gaussian center parameters (\(\zeta_{3}^{p \uparrow}, \zeta_{3}^{p \downarrow}, \zeta_{3}^{n \uparrow}, \) and \(\zeta_{3}^{n \downarrow}\)) and
\[
\chi_{3}^{p, n \uparrow, p \downarrow, n \downarrow} = R_{y} (4\pi/3) \chi_{1}^{p, n \uparrow, p \downarrow, n \downarrow}, \tag{8}
\]
for the spin-isospin part (\(\chi_{3}^{p \uparrow}, \chi_{3}^{p \downarrow}, \chi_{3}^{n \uparrow}, \) and \(\chi_{3}^{n \downarrow}\)).

For the values of \(R\) and \(\Lambda\), we introduce \(R = 0.5, 1.0, 1.5, 2.0, 2.5, 3.0\) fm and \(\Lambda = 0.0, 0.2, 0.4\) and 100 two-particle-two-hole states introduced in II C (50 are for proton-proton excitation and 50 are for neutron-neutron excitation) are superposed based on GCM. These 18 basis states are superposed based on GCM.

C. Two-particle-two-hole states of \(^{12}\text{C}\)

The innovation of the present study is the inclusion of many two-particle-two-hole states, by which pairing-like correlation can be taken into account. These two-particle-two-hole basis states are generated from the optimal AQCM basis state. It will be shown that the AQCM basis state with \(R = 2.1\) fm and \(\Lambda = 0.2\) gives the lowest energy, and Gaussian center parameters of two nucleons in the first quasi cluster are shifted from this basis state using the random numbers. We consider two sets of the basis states; shifted two particles in the first quasi cluster are either protons (with spin-up and spin-down) or neutrons (with spin-up and spin-down). Both of these two corresponds to the isovector pairing-like excitation of protons and neutrons. In principle, it is possible to consider the isoscalar pairing of proton-neutron excitation, but this effect will be shown to be small, maybe because the proton-neutron correlation is already included in the quasi cluster model. Here, the distance of the shifts are giving using a random numbers \(\{r_{i}\}\), which has the probability distribution \(P (|r_{i}|) \propto \exp [- |r_{i}| / \sigma]\),
\[
P (|r_{i}|) \propto \exp [- |r_{i}| / \sigma]. \tag{9}
\]
The value of \(\sigma\) is chosen to be 1 fm. After generating \(\{r_{i}\}\), we multiply the sign factor to each \(r_{i}\), which allows \(r_{i}\) to be positive and negative with equal probability. The shifts of all three \((x, y, z)\) directions for the two nucleons originally in the first quasi cluster are given using random numbers generated in this way. Importantly, the random numbers used for the proton-proton excitation are identical to those of neutron-neutron excitation. Therefore, the model space still keeps the room to be isoscalar, which is achieved when the amplitude for the wave functions for the proton excitation and neutron excitation are obtained to be identical. The mixing of the isovector component in the wave function is not the numerical artefact but due to the presence of the Coulomb interaction.

It is known that proton-neutron pairing is quite important in \(N = Z\) nuclei \([36–39]\), which can be probed in the same manner. For the basis states corresponding to the proton-neutron pairing, the Gaussian center parameters of spin-up proton and spin-up neutron in one quasi cluster are randomly generated. However, the number of basis states must to be reduced due to the computational time.

D. Superposition of the basis states

The 18 AQCM basis states introduced in II B \((R = 0.5, 1.0, 1.5, 2.0, 2.5, 3.0\) fm and \(\Lambda = 0.0, 0.2, 0.4\) and 100 two-particle-two-hole states introduced in II C (50 are for proton-proton excitation and 50 are for neutron-neutron excitation) are superposed based on GCM. These 118 basis states are abbreviated to \(\{\Phi_{i}\}\) \((i = 1–118)\). They are projected to the eigen states of parity and angular momentum by using the projection operator \(P_{f}^{K}\),
\[
P_{f}^{K} = P^{n} 2J + 1 \over 8\pi^{2} \int d\Omega D_{MK}^{J} \ast R (\Omega). \tag{10}
\]
Here \(D_{MK}^{J}\) is the Wigner \(D\)-function and \(R (\Omega)\) is the rotation operator for the spatial and spin parts of the wave function. This integration over the Euler angle \(\Omega\) is numerically performed. The operator \(P^{n}\) is for the parity projection \((P^{n} = (1 + P^{\pi}) / \sqrt{2}\) for the positive-parity states, where \(P^{\pi}\) is the parity-inversion operator\), which is also performed numerically. This angular momentum projection enables to generate different \(K\) number states as independent basis states from each Slater
determinant. Therefore, the total wave function \( \Psi_{J^\pi} \) after the \( K \)-mixing is denoted as

\[
\Psi_{J^\pi} = \sum_{i,K} c^K_i P^K_{J^\pi} \Phi_i.
\]  

The coefficients \( \{ c^K_i \} \) are obtained together with the energy eigenvalue \( E \) when we diagonalize the norm and Hamiltonian \( (H) \) matrices, namely by solving the Hill-Wheeler equation. Even if the number of the basis states is 118 for the \( 0^+ \) state, which has only \( K = 0 \), the dimension of the matrices for the other \( J^\pi \) states increases through the \( K \)-mixing process.

### E. Hamiltonian

The Hamiltonian consists of the kinetic energy and potential energy terms. For the potential part, the interaction consists of the central (\( V_{\text{central}} \)), spin-orbit (\( V_{\text{spin-orbit}} \)), and Coulomb terms. For the central part, the Tohsaki interaction [40] adopted. This interaction consists of two-body (\( V_{\text{2-body}} \)) and Coulomb terms. For the spin-orbit part, we use the spin-orbit term of the G3RS interaction [41], which is a realistic interaction originally developed to reproduce the nucleon-nucleon scattering phase shifts.

The Tohsaki interaction consists of two-body (\( V^{(2)} \)) and three-body (\( V^{(3)} \)) terms:

\[
V_{\text{central}} = \frac{1}{2} \sum_{i \neq j} V^{(2)}_{ij} + \frac{1}{6} \sum_{i \neq j, j \neq k, i \neq k} V^{(3)}_{ijk},
\]

where \( V^{(2)}_{ij} \) and \( V^{(3)}_{ijk} \) have three ranges,

\[
V^{(2)}_{ij} = \sum_{\alpha=1}^{3} V^{(2)}_{\alpha} \exp \left[ -\frac{(\vec{r}_i - \vec{r}_j)^2}{\mu^2_{\alpha}} \right] \left( W^{(2)}_{\alpha} - M^{(3)}_{\alpha} \right) P^{\sigma} P^{\tau}_{ij},
\]

\[
V^{(3)}_{ijk} = \sum_{\alpha=1}^{3} V^{(3)}_{\alpha} \exp \left[ -\frac{(\vec{r}_i - \vec{r}_j)^2}{\mu^2_{\alpha}} - \frac{(\vec{r}_i - \vec{r}_k)^2}{\mu^2_{\alpha}} \right] \times \left( W^{(3)}_{\alpha} - M^{(3)}_{\alpha} \right) P^{\sigma} P^{\tau}_{ijk},
\]

where \( P^{\sigma} P^{\tau} \) represents the exchange of the spin-isospin part of the wave functions of interacting two nucleons. The physical coordinate for the \( i \)th nucleon is \( \vec{r}_i \). The details of the parameters are shown in Ref. [40], but we use the F1’ parameter set for the Majorana parameter \( M^{(3)}_{\alpha} \) of the three-body part introduced in Ref. [8].

The G3RS interaction [41] is a realistic interaction, and the spin-orbit term has the following form:

\[
V_{\text{spin-orbit}} = \frac{1}{2} \sum_{i \neq j} V^{ls}_{ij},
\]

\[
V^{ls}_{ij} = \left( V^{(2)}_{ij} e^{-d_1(r_i - r_j)^2} - V^{(2)}_{ij} e^{-d_2(r_i - r_j)^2} \right) P^{(3)O} \vec{L} \cdot \vec{S}.
\]

\[
V^{ls}_{ij} = \left( V^{(2)}_{ij} e^{-d_1(r_i - r_j)^2} - V^{(2)}_{ij} e^{-d_2(r_i - r_j)^2} \right) P^{(3)O} \vec{L} \cdot \vec{S}.
\]

IV. RESULTS

### A. AQCM basis states

We start the discussion with the result of AQCM basis states. Figure 1 shows the \( 0^+ \) energy curves of \( ^{12}\text{C} \) calculated with AQCM. The horizontal axis shows the parameter \( R \) representing the distance between the quasi clusters with the equilateral triangular configuration. The dotted, solid, and dashed curves are the cases of \( \Lambda \) equal to 0.0, 0.2, and 0.4.

\[
V^{ls}_{ij} = \left( V^{(2)}_{ij} e^{-d_1(r_i - r_j)^2} - V^{(2)}_{ij} e^{-d_2(r_i - r_j)^2} \right) P^{(3)O} \vec{L} \cdot \vec{S}.
\]

Here, \( \vec{L} \) is the angular momentum for the relative motion between the \( i \)th and \( j \)th nucleons, and \( \vec{S} \) is the sum of the spin operator for these two interacting nucleons. The operator \( P^{(3)O} \) stands for the projection onto the triplet-odd state. The strength of the spin-orbit interactions is set to \( V^{ls}_{ij} = V^{ls}_{2ij} = 1800 \text{MeV} \), which allows consistent description of \( ^{12}\text{C} \) and \( ^{16}\text{O} \).
lowest $0^+$ state at $-88.04$ MeV, lower than the energy of the optimal basis state ($R = 2.1$ fm, $\Lambda = 0.2$) by about 1.4 MeV.

### B. Inclusion of two-particle-two-hole states

Then we mix the two-particle-two-hole states to the AQCM basis states. Figure 2 shows the energy convergence for the $0^+$ state of $^{12}$C when we add 100 two-particle-two-hole basis states to the 18 AQCM basis states. The basis states from 19 to 68 on the horizontal axis are excited states of the two protons, and from 69 to 118 are excited states of the two neutrons. The inclusion of the proton excited states (69–118 on the horizontal axis) has an effect of the lowering of the energy by about 2 MeV, which is quite large. It is not perfect due to the limitation of the model space, but the energy is almost converged within the 50 basis states.

Next, we start superposing the basis states corresponding the two-particle-two-hole excitation of the neutrons from 69 on the horizontal axis. At first, the energy again strongly decreases. This is because the mixing of the excited states of the neutrons has the effect of the restoration of the isospin symmetry. The isospin symmetry is broken when proton excited states are included, and the broken symmetry is restored by the inclusion of the neutron excited states. As mentioned in the framework section, the random numbers to shift of the Gaussian centers of the two nucleons from the quasi cluster are identical in both cases of proton excitation and neutron excitation. Thus the model space still contains the room to form the isoscalar configuration even after two-particle-two-hole effect is considered; indeed the isospin symmetry is broken by the Coulomb interaction. The $0^+$ energy converges to $-91.66$ MeV, and the mixing of the two-particle-two-hole states contributed to the lowering of the ground state energy by more than 3.5 MeV (the experimental energy of $^{12}$C ground state is $-92.2$ MeV).

### C. Level spacing of $0^+$ and $2^+$

It has been known that traditional $\alpha$ cluster models give very small level spacing for the $0^+$ and first $2^+$ state; normally the value is about 2–3 MeV compared with the observed value of 4.6 MeV. It is also known that this defect can be overcome by including the $\alpha$ breaking effect. The ground state corresponds to the subclosure configuration of $p_{3/2}$ in terms of the $jj$-coupling model, and the spin-orbit interaction works attractively especially for the $0^+$ state (on the other hand, the excitation to spin-orbit unfavored orbits mixes in the $2^+$ state).

Our result for the $0^+-2^+$ energy spacing is summarized in Fig. 3. Here, the column "AQCM" shows the result obtained after diagonalizing the Hamiltonian consisting of the 18 AQCM basis states with $K = 0$. The column "p-2p2h" shows the result after adding 50 two-particle-two-hole states for the protons within $K = 0$. In the column "n-2p2h", 50 two-particle-two-hole states for the neutrons are mixed, where $K$ quantum number is still fixed to $K = 0$. The mixing of the two-particle-two-hole states allows the $K$-mixing for the $2^+$ state, and the effect is shown in the column "K-mixing".

![FIG. 2. Energy convergence for the $0^+$ state of $^{12}$C; 100 two-particle-two-hole basis states are coupled to the 18 AQCM basis states. The basis states from 19 to 68 on the horizontal axis are excited states of the two protons, and from 69 to 118 are excited states of the two neutrons.](image1)

![FIG. 3. $0^+–2^+$ energy spacing of $^{12}$C. The column “AQCM” shows the result obtained after diagonalizing the Hamiltonian consisting of the 18 AQCM basis states with $K = 0$. The column “p-2p2h” shows the result after adding 50 two-particle-two-hole states for the protons within $K = 0$. In the column “n-2p2h”, 50 two-particle-two-hole states for the neutrons are mixed, where $K$ quantum number is still fixed to $K = 0$. The mixing of the two-particle-two-hole states allows the $K$-mixing for the $2^+$ state, and the effect is shown in the column “K-mixing”.](image2)
creases the level spacing between $0^+$ and $2^+$. However, the mixing of the two-particle-two-hole states allows the $K$-mixing for the $2^+$ state. The angular momentum projection procedure produces different $K$ states ($K = 1, 2$) as independent basis states from each two-particle-two-hole state, while AQCM basis states ($i = 1–18$) only contains the $K = 0$ component due to the symmetry of the equilateral triangular ($D_{3h}$) symmetry even after breaking $\alpha$ clusters. After taking into account this $K$-mixing effect, as shown in the column “$K$-mixing”, the energy of the $2^+$ state significantly comes down and finally the spacing becomes $4.9$ MeV, quite reasonable value.

D. Isospin mixing in the ground state

The $\alpha$ cluster wave function is isoscalar, and this situation is the same even if we change $\alpha$ clusters to quasi clusters. However, here we included in the model space the two-particle-two-hole excitation of protons and neutrons as independent basis states, thus the isospin symmetry can be broken by the Coulomb interaction (the nuclear part of the interaction is still isoscalar). The mixing of the finite isospin can be estimated by the square of the isospin operator. However, the square of the isospin operator is always constant, thus we consider the square of the isospin operator after running the summation over the particle, As a result, the operator becomes two-body one,

$$\hat{O}^{T^2} = \sum_{i,j} \tau_i \cdot \tau_j,$$

(17)

where $\tau_i$ is the isospin operator for the $i$-th nucleon. The ground state of the present model gives the value of 0.016. The eigen values of this operator are 0, 2, and 6 for the $T = 0$, $T = 1$, and $T = 2$ state, respectively. Thus, the present value of 0.016 means that the isospin is broken at least by the order of $10^{-3}$, which is consistent with other calculations. For instance, the mixing of $T = 1$ component in the order of $10^{-4}$ in $^8\text{Be}$ is discussed based on the Green’s Function Monte Carlo approach [42]; however, the breaking of the isospin symmetry is taken into account in the nuclear interaction level there, contrary to the present work. As mentioned previously, our model space has the room to form the isoscalar configuration, thus the present result of the isospin mixing is not the numerical artefact.

E. Principal quantum number

The physical quantity which reflect the mixing of two-particle-two-hole excitation is required to confirm the effect. As such candidate, the expectation value of the principal quantum number $\hat{N}$ of the harmonic oscillator,

$$\hat{N} = \sum_i a_i^\dagger a_i,$$

(18)

FIG. 4. Energy convergence for the $0^+$ state of $^{12}\text{C}$; 120 two-particle-two-hole basis states are coupled to the 18 AQCM basis states. The basis states from 19 to 58 on the horizontal axis are excited states of the two protons, from 59 to 98 are excited states of the two neutrons, and from 99 to 118 are excited states of a proton and a neutron.

can be easily calculated. Here the summation is over all the nucleons. The lowest value for $^{12}\text{C}$ is 8, corresponding to the state, where four nucleons are in the lowest $s$ shell and eight nucleons are in the $p$ shell. The result obtained with the 18 AQCM basis states give the value of 9.15, and after inclusion of the two-particle-two-hole state, the values slightly changes to 9.13, but almost identical. Thus, unfortunately, this quantity cannot be utilized to discriminate the effect of two-particle-two-hole states.

F. Effect of the proton-neutron pairing

We have examined the effect of two-particle-two-hole of protons and neutrons. However, it is known that proton-neutron pairing is quite important in $N = Z$ nuclei [36–39]. We can partially probe this effect; however, it is necessary to reduce the number of the basis states for each component of the two-particle-two-hole excitation from 50 to 40 because of the calculation time. For the basis states corresponding to the proton-neutron pairing, the Gaussian center parameters of spin-up proton and spin-up neutron in one quasi cluster are randomly generated.

The energy convergence for the $0^+$ state of $^{12}\text{C}$ is shown in Fig. 4. 120 two-particle-two-hole basis states are coupled to the 18 AQCM basis states. The basis states from 19 to 58 on the horizontal axis are excited states of the two protons, from 59 to 98 are excited states of the two neutrons, and from 99 to 118 are excited states of a proton and a neutron. The number of basis states is not enough and the energy convergence is not perfect; nevertheless, we can see the basic trend. Unexpectedly, the contribution of the proton-neutron excitation is rather limited. It is considered that the proton-neutron corre-
lations are already included within the dynamics of the three quasi cluster model.

IV. CONCLUSIONS

It has been shown that the cluster and single-particle correlations are taken into account in the ground state of $^{12}$C. The recent development of the antisymmetrized quasi cluster model (AQCM) allows us to generate $jj$-coupling shell model wave functions from $\alpha$ clusters models. The cluster dynamics and the competition with the $jj$-coupling shell-model structure can be estimated rather easily. In the present study, we further included the effect of single-particle excitation; the mixing of the two-particle-two-hole excited states was considered. The single-particle excitation had not always been taken into account in the standard cluster model analyses.

The two-particle-two-hole states are found to strongly contribute to the lowering of the ground state owing to the pairing-like correlations. By extending AQCM, all of the basis states were prepared on the same footing, and they were superposed based on the framework of GCM. For the preparation of the two-particle-two-hole states, we used random numbers to the shift of the Gaussian centers of the two nucleons from the quasi cluster. It is stressed that identical sets of random numbers were used in generating the basis states of both proton excitation and neutron excitation. Thus, in principle, the model space contains the room to form the isoscalar configuration even after two-particle-two-hole effect is considered.

The two-particle-two-hole states were prepared on the same footing, and after inclusion of $\alpha$ clusters in the present model.

The $0^+$ energy converges to $-91.66$ MeV compared with the experimental value of $-92.2$ MeV, and the mixing of the two-particle-two-hole states contributed to the lowering of the ground state energy by more than $3.5$ MeV.

The isospin symmetry is now broken by the Coulomb interaction, which can be estimated by the square of the isospin operator. The ground state of the present model gives the value of 0.016. The eigenvalues of this operator are 0, 2, and 6 for the $T = 0, T = 1, \text{ and } T = 2$ state, respectively. Thus, the present value of 0.016 means that the isospin is broken at least by the order of $10^{-3}$.

The physical quantity which reflects the mixing of two-particle-two-hole excitation is required to confirm the effect. As such a candidate, the expectation value of the principal quantum number $N$ of the harmonic oscillator was calculated. The result obtained with the 18 AQCM basis states gives the value of 9.15, and after inclusion of the two-particle-two-hole state, the value slightly changes to 9.13, but almost identical. Thus, unfortunately, this quantity cannot be utilized to discriminate the effect of two-particle-two-hole states.

The proton-neutron pairing is known to play an important in $N = Z$ nuclei, and we can prepare proton-neutron two-particle-two-hole states as the basis states, but unexpectedly, the contribution is rather limited. It is considered that the proton-neutron correlations are already included within the dynamics of the three quasi clusters in the present model.

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