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}C. The recent development of the antisymmetrized quasicluster model (AQCM) makes it possible to generate jj-coupling shell-model wave functions from α cluster 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).

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I. INTRODUCTION

In the light mass region, the ^{4}He nucleus, due to its spin and isospin saturated nature, has a large binding energy. On the other hand, the interaction between ^{4}He nuclei is rather weak. Therefore, they form subsystems called α clusters in some light nuclei [1,2]. The search for candidates with a cluster structure has been ongoing for decades, and the most famous example is the second 0^+ state of ^{12}C called the Hoyle state, which has a developed three-α 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}He, ^{16}O, and ^{40}Ca. In these cases, the contribution of the noncentral 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 noncentral interactions work neither inside clusters nor between α 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 ($f_{7/2}$, $g_{9/2}$, $h_{11/2}$, and $i_{13/2}$) correspond to the observed magic numbers of 28, 50, 82, 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, we proposed the antisymmetrized quasicluster model (AQCM) [9–21]. This method allows us to smoothly transform α 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 quasiclusters. In AQCM, we have two parameters: R representing the distance between α clusters and Λ characterizing the transition of α cluster(s) to quasicluster(s). The jj-coupling shell-model states can be obtained starting with the α cluster model by changing α clusters to quasiclusters (giving finite Λ values to α clusters) and taking the small-distance limit of R. It has been known that the conventional α cluster models cover the model space of closure of major shells ($N = 2$, $N = 8$, $N = 20$, etc.). In addition, by changing α clusters to quasiclusters, 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 [15].

We previously introduced AQCM to ^{12}C and discussed the competition between the cluster states and the jj-coupling shell-model state [9]. The consistent description of ^{12}C and ^{16}O, which has been a longstanding problem of microscopic cluster models, has been achieved. In this paper, we examine again ^{12}C, where not only the competition between the cluster states and the lowest shell-model configuration, but also 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 a much simpler method. The two-particle–two-hole states around the optimal AQCM basis state are generated using a numerical technique. Owing to the generation of many states compared with our previous approach, a 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 characters of both 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, but various properties including electromagnetic transition strengths, α-decay widths, and scattering phenomena have been discussed [22–35]. 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 [26]. In this approach, one-particle–one-hole states are expressed by the small shift of one particle around the optimal AMD solution. Here in our study, we focus on the two-particle–two-hole excitation, which covers the model space of one-particle–one-hole excitation, and the lowering of the energy owing to the effect of BCS-like paring can be clarified. Some of the preceding works are based on modern *ab initio* approaches, where the tensor and short-range correlations are included. Compared with these, our approach is rather phenomenological, but here we examine the natural extension of the AQCM framework and include both cluster dynamics and the single-particle excitation.

This paper is organized as follows. The framework is described in Sec. II. The results are shown in Sec. III. The conclusions are presented in Sec. IV.

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 [1]:

$$\phi^{\tau,\sigma}(\boldsymbol{r}) = \left(\frac{2\nu}{\pi}\right)^{\frac{3}{4}} \exp[-\nu(\boldsymbol{r}-\boldsymbol{\zeta})^2]\chi^{\tau,\sigma}, \tag{1}$$

where the Gaussian center parameter $\boldsymbol{\zeta}$ is related to the expectation value of the position of the nucleon, and $\chi^{\tau,\sigma}$ is the spin-isospin part of the wave function. For the size parameter ν, 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 $\{\boldsymbol{\zeta}_i\}$. As in other cluster models, here four single-particle wave functions with different spin and isospin sharing a common $\boldsymbol{\zeta}$ value correspond to an α cluster. This cluster wave function is transformed into the jj-coupling shell model based on AQCM. When the original value of the Gaussian center parameter $\boldsymbol{\zeta}$ is $\boldsymbol{R}$, which is real and related to the spatial position of this nucleon, it is transformed by adding the imaginary part as

$$\boldsymbol{\zeta} = \boldsymbol{R} + i\Lambda \boldsymbol{e}^{\rm spin} \times \boldsymbol{R}, \tag{2}$$

where $\boldsymbol{e}^{\rm spin}$ is a unit vector for the intrinsic-spin orientation of this nucleon. The control parameter Λ is associated with the breaking of the cluster, and with a finite value of Λ the two nucleons with opposite spin orientations have the $\boldsymbol{\zeta}$ values. For example, two nucleons with opposite spin orientation have $\boldsymbol{\zeta}$ values that are complex conjugates to each other. This situation corresponds to the time-reversal motion of two nucleons. After this transformation, the α clusters are called quasiclusters.

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 real part of the Gaussian center parameter $\boldsymbol{\zeta}$ 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 $\boldsymbol{\zeta}$ is given to its y component. When we expand $-\nu(\boldsymbol{r}-\boldsymbol{\zeta})^2$ in the exponent of Eq. (1), a factor $\exp[2\nu\boldsymbol{\zeta}\cdot\boldsymbol{r}]$ corresponding to the cross term of this expansion appears. The factor $\exp[2\nu\boldsymbol{\zeta}\cdot\boldsymbol{r}]$ 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 $\exp[2\nu\boldsymbol{\zeta}\cdot\boldsymbol{r}]$ is $2\nu\boldsymbol{\zeta}\cdot\boldsymbol{r}$, 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 mean-field spin-orbit interaction acts attractively. To create a spin-down nucleon, we introduce the complex conjugate $\boldsymbol{\zeta}$ value, which gives $|3/2\ -3/2\rangle$.

In the case of ^{12}C, we prepare three quasiclusters. The next two single-particle states are generated by rotating the $\boldsymbol{\zeta}$ vectors and the spin directions by $2\pi/3$ around the y axis and by $4\pi/3$ for the fifth and sixth single-particle states. Thus, one can put six nucleons in pair-wise stretched states with quantization axes pointing in three different directions. These states are not orthogonal but after antisymmetrization represent the subclosure configuration of $(s_{1/2})^2\,(p_{3/2})^4$. This procedure is applied for both proton and neutron parts. The details are given in Ref. [14].

B. Standard AQCM for ^{12}C

AQCM has been already applied to ^{12}C and the essential part is recaptured here. It has been well studied that the ground state is described by three quasiclusters with equilateral triangular symmetry. The parameter R represents the distance between α clusters with an equilateral triangular configuration, and thus the distance from the origin for each α cluster is $R/\sqrt{3}$. Following Eq. (2), the Gaussian center parameters of the first quasicluster are given as

$$\boldsymbol{\zeta}_1^{p\uparrow,n\uparrow} = R(\boldsymbol{e}_x + i\Lambda\boldsymbol{e}_y)/\sqrt{3}, \tag{3}$$

for spin-up proton ($\boldsymbol{\zeta}_1^{p\uparrow}$) and neutron ($\boldsymbol{\zeta}_1^{n\uparrow}$), and

$$\boldsymbol{\zeta}_1^{p\downarrow,n\downarrow} = R(\boldsymbol{e}_x - i\Lambda \boldsymbol{e}_y)/\sqrt{3}, \tag{4}$$

for spin-down proton ($\boldsymbol{\zeta}_1^{p\downarrow}$) and neutron ($\boldsymbol{\zeta}_1^{n\downarrow}$). Here $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ are unit vectors of the x and y axis, respectively. The spin-isospin part of the wave function is denoted as $\chi_1^{p\uparrow}$, $\chi_1^{n\uparrow}$, $\chi_1^{p\downarrow}$, and $\chi_1^{n\downarrow}$, for spin-up proton, spin-up neutron, spin-down proton, and spin-down neutron in the first quasicluster. For the second and third quasiclusters, we introduce a rotation operator around the y axis $\hat{R}_y(\Omega)$. The Gaussian center parameters of the four nucleons in the second quasicluster are generated by rotating the those in the first quasicluster around the y axis by $2\pi/3$ radian:

$$\boldsymbol{\zeta}_2^{p\uparrow,n\uparrow,p\downarrow,n\downarrow} = \hat{R}_y(2\pi/3)\boldsymbol{\zeta}_1^{p\uparrow,n\uparrow,p\downarrow,n\downarrow}. \tag{5}$$

It is important to note that the spin-isospin part ($\chi_2^{p\uparrow}$, $\chi_2^{n\uparrow}$, $\chi_2^{p\downarrow}$, and $\chi_2^{n\downarrow}$) also needs to be rotated as

$$\chi_2^{p\uparrow,n\uparrow,p\downarrow,n\downarrow} = \hat{R}_y(2\pi/3)\chi_1^{p\uparrow,n\uparrow,p\downarrow,n\downarrow}, \tag{6}$$

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 quasicluster is introduced by changing the rotation angle around the y axis to $4\pi/3$ radian,

$$\boldsymbol{\zeta}_3^{p\uparrow,n\uparrow,p\downarrow,n\downarrow} = \hat{R}_y(4\pi/3)\boldsymbol{\zeta}_1^{p\uparrow,n\uparrow,p\downarrow,n\downarrow}, \tag{7}$$

for the Gaussian center parameters ($\boldsymbol{\zeta}_3^{p\uparrow}$, $\boldsymbol{\zeta}_3^{n\uparrow}$, $\boldsymbol{\zeta}_3^{p\downarrow}$, and $\boldsymbol{\zeta}_3^{n\downarrow}$), and

$$\chi_3^{p\uparrow,n\uparrow,p\downarrow,n\downarrow} = \hat{R}_y(4\pi/3)\chi_1^{p\uparrow,n\uparrow,p\downarrow,n\downarrow}, \tag{8}$$

for the spin-isospin part ($\chi_3^{p\uparrow}$, $\chi_3^{n\uparrow}$, $\chi_3^{p\downarrow}$, and $\chi_3^{n\downarrow}$).

For the values of R and Λ, we introduce $R = 0.5$, 1.0, 1.5, 2.0, 2.5, 3.0 fm and $\Lambda = 0.0$, 0.2, 0.4. These 18 many-body basis states span a 12-body Hilbert space later treated by projection on total angular momentum within GCM.

C. Two-particle–two-hole states of ^{12}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 quasicluster are shifted from this basis state using the random numbers. We consider two sets of the basis states: two shifted particles in the first quasicluster are either protons (with spin up and spin down) or neutrons (with spin up and spin down). Both of these two correspond 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 quasicluster model. Here, the distance of the shifts are giving using random numbers $\{r_i\}$, which have the probability distribution $P(|r_i|)$ proportional to $\exp[-|r_i|/\sigma]$,

$$P(|r_i|) \propto \exp[-|r_i|/\sigma]. \tag{9}$$

The value of σ 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 quasicluster 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. In principle, the two-particle–two-hole states mix nonisoscalar states. However, if the amplitude for each basis state for proton excitation and that for the neutron excitation are identical, the isospin symmetry is restored. Therefore, the model space still keeps the room to be isoscalar, which guarantees that the mixing of nonisoscalar components is a physical effect owing to the Coulomb effect and not a numerical artifact.

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 the spin-up proton and spin-up neutron in one quasicluster 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 Sec. 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 Sec. 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 eigenstates of parity and angular momentum by using the projection operator $P^K_{J^\pi}$,

$$P^K_{J^\pi} = P^\pi \frac{2J+1}{8\pi^2} \int d\Omega\, {D^J_{MK}}^* R(\Omega). \tag{10}$$

Here D^J_{MK} 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 Ω is numerically performed. The operator P^π is for the parity projection ($P^\pi = (1 + P^r)/\sqrt{2}$ for the positive-parity states, where P^r 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 Ψ_{J^π} after the K mixing is denoted as

$$\Psi_{J^\pi} = \sum_{i,K} c_i^K P^K_{J^\pi} \Phi_i. \tag{11}$$

The coefficients $\{c_i^K\}$ 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^π 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 central ($\hat{V}_{\rm central}$), spin-orbit ($\hat{V}_{\rm spin\text{-}orbit}$), and Coulomb terms. For the central part, the Tohsaki interaction [40] is adopted. This interaction has finite range three-body terms in addition to two-body terms, which is designed to reproduce both saturation properties and scattering phase shifts of two α clusters. 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,

$$\hat{V}_{\rm central} = \frac{1}{2}\sum_{i\neq j} V_{ij}^{(2)} + \frac{1}{6}\sum_{i\neq j, j\neq k, i\neq k} V_{ijk}^{(3)}, \tag{12}$$

where $V_{ij}^{(2)}$ and $V_{ijk}^{(3)}$ have three ranges,

$$V_{ij}^{(2)} = \sum_{\alpha=1}^{3} V_\alpha^{(2)} \exp\left[-\frac{(\boldsymbol{r}_i-\boldsymbol{r}_j)^2}{\mu_\alpha^2}\right]\left(W_\alpha^{(2)} - M_\alpha^{(2)} P^\sigma P^\tau\right)_{ij}, \tag{13}$$

$$V_{ijk}^{(3)} = \sum_{\alpha=1}^{3} V_\alpha^{(3)} \exp\left[-\frac{(\boldsymbol{r}_i-\boldsymbol{r}_j)^2}{\mu_\alpha^2} - \frac{(\boldsymbol{r}_i-\boldsymbol{r}_k)^2}{\mu_\alpha^2}\right] \times \left(W_\alpha^{(3)} - M_\alpha^{(3)} P^\sigma P^\tau\right)_{ij}\left(W_\alpha^{(3)} - M_\alpha^{(3)} P^\sigma P^\tau\right)_{ik}. \tag{14}$$

Here, $P^\sigma P^\tau$ represents the exchange of the spin-isospin parts of the wave functions of two interacting nucleons. The physical coordinate for the ith nucleon is $\boldsymbol{r}_i$. The details of the parameters are shown in Ref. [40], but we use the F1′ parameter set for the Majorana parameter ($M_\alpha^{(3)}$) of the three-body part introduced in Ref. [9].

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

$$\hat{V}_{\rm spin\text{-}orbit} = \frac{1}{2}\sum_{i\neq j} V_{ij}^{ls}, \tag{15}$$

where

$$V_{ij}^{ls} = \left(V_{ls}^1 e^{-d_1(\boldsymbol{r}_i-\boldsymbol{r}_j)^2} - V_{ls}^2 e^{-d_2(\boldsymbol{r}_i-\boldsymbol{r}_j)^2}\right) P(^3O)\boldsymbol{L}\cdot\boldsymbol{S}. \tag{16}$$

Here, $\boldsymbol{L}$ is the angular momentum for the relative motion between the ith and jth nucleons, and $\boldsymbol{S}$ is the sum of the spin operator for these two interacting nucleons. The operator $P(^3O)$ stands for the projection onto the triplet-odd state. The strength of the spin-orbit interactions is set to $V_{ls}^1 = V_{ls}^2 = 1800$ MeV, which allows consistent description of ^{12}C and ^{16}O [9].

III. RESULTS

A. AQCM basis states

We start the discussion with the result of AQCM basis states. Figure 1 shows for ^{12}C the expectation value of the Hamiltonian calculated within the 0^+ AQCM basis state as a functions of R representing the distance between the quasiclusters with the equilateral triangular configuration. The dotted, solid, and dashed curves are the cases of Λ equal to 0.0, 0.2, and 0.4. The dotted line ($\Lambda = 0.0$) represents the three-α cluster model, where the α breaking effect and spin-orbit contribution are absent. The spin-orbit effect shows up by setting Λ to finite values. The α cluster model gives the lowest energy at a large R value of about 3 fm. The spin-orbit interaction strongly lowers the energy of the AQCM states with finite Λ, giving minima at smaller R values. However, the finite Λ values cause the increase of the kinetic energy, and the optimal state is obtained as a balance of these two factors. The optimal energy of -86.68 MeV is obtained around $R = 2.1$ fm with $\Lambda = 0.2$.

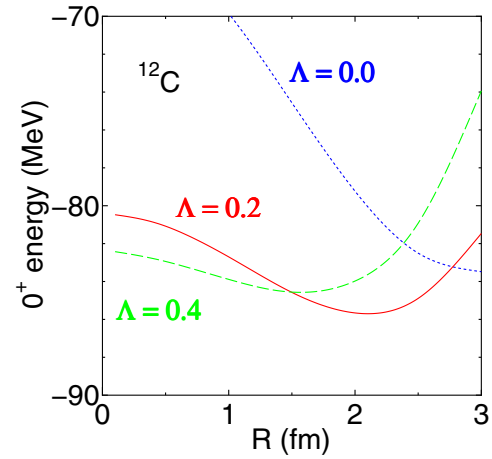

FIG. 1. 0^+ energy curves of ^{12}C calculated with AQCM. The horizontal axis shows the parameter R representing the distance between the quasiclusters with the equilateral triangular configuration. The dotted, solid, and dashed curves are the cases of Λ equal to 0.0, 0.2, and 0.4.

After solving the eigenvalue problem (Hill-Wheeler equations) in the 12-body space spanned by the 18 AQCM basis states ($R = 0.5$, 1.0, 1.5, 2.0, 2.5, 3.0 fm and $\Lambda = 0.0$, 0.2, 0.4), we obtain the 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 add successively to the 18 AQCM basis states 50 proton and 50 neutron two-particle–two-hole states. Figure 2 shows the energy convergence of the ^{12}C ground state as a function of increasing Hilbert space dimension. The inclusion of the basis states from 19 to 68 on the horizontal axis is for the two-particle–two-hole excited states of the two protons and has an effect of lowering the energy by about 2 MeV, which is quite large.

Next we add basis states corresponding to the two-particle–two-hole excitation of the two neutrons (number 69 to 118 on the horizontal axis of Fig. 2). 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.

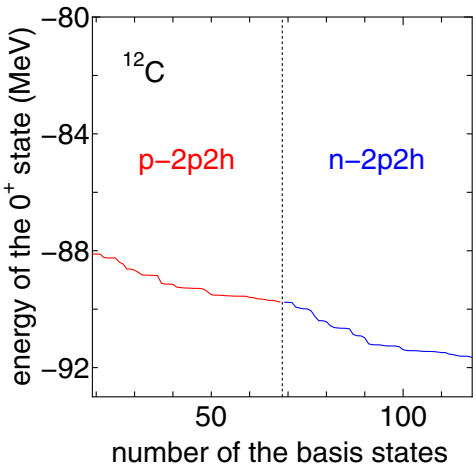

FIG. 2. Energy convergence for the lowest 0^+ state of ^{12}C as a function of Hilbert space dimension. On top of 18 AQCM basis states, 50 proton two-particle–two-hole states (numbers 19 to 68) and 50 neutron two-particle–two-hole states (numbers 69 to 118) are added successively.

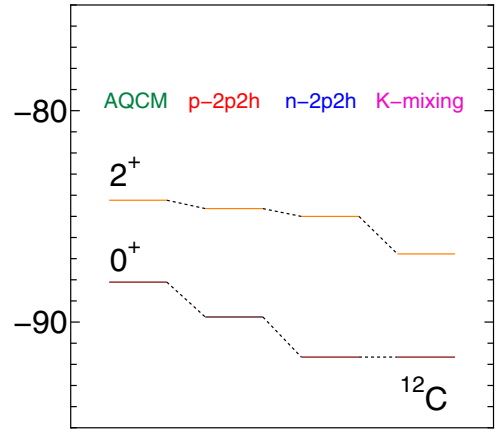

FIG. 3. 0^+-2^+ energy spacing of ^{12}C. The column "AQCM" shows the result obtained after diagonalizing the Hamiltonian consisting of the 18 AQCM basis states with $K = 0$. The column "p-2p2h" shows the result after adding 50 two-particle–two-hole states for the protons within $K = 0$. In the column "n-2p2h", 50 two-particle–two-hole states for the neutrons are mixed, where K quantum number is still fixed to $K = 0$. The last column "K-mixing" shows the energy of the 2^+ state when K mixing is invoked.

As mentioned in the framework section, the random numbers used to shift the Gaussian centers of the two nucleons from the quasicluster are identical in cases of both proton excitation and neutron excitation. The two-particle–two-hole states allows the mixing of nonisoscalar components, but if the amplitude for each basis state for proton excitation and that for the neutron excitation are identical, the isospin symmetry is restored. This guarantees that the isospin breaking calculated here is not a numerical artifact but a physical effect; indeed it 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 α cluster models give very small level spacing for the ground 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 α 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. The 0^+-2^+ energy spacing is obtained as 3.9 MeV, slightly smaller than the experiment. The AQCM model space only contains the $K = 0$ component. The column "p-2p2h" shows the result after adding 50 two-particle–two-hole states for the protons, where K quantum number is still fixed to $K = 0$. The mixing of 50 two-particle–two-hole states strongly contributes to the lowering of the ground state, and the 0^+-2^+ energy spacing increases to 5.1 MeV, larger than the experiment. In the column "n-2p2h" the two-particle–two-hole states for the neutrons are mixed, where K quantum number is still fixed to $K = 0$. The 0^+-2^+ energy spacing further increases to 6.7 MeV, quite larger than the experiment. The result shows that the BCS-like pairing effect is quite important for the 0^+ state and increases 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 contain a $K = 0$ component due to the symmetry of the equilateral triangular (D_{3h}) symmetry even after breaking α 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, a quite reasonable value.

D. Isospin mixing in the ground state

The α cluster wave function is isoscalar, and this situation is the same even if we change α clusters to quasiclusters. However, here we included in the model space the two-particle–two-hole excitation of protons and neutrons as independent basis states, and 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 total isospin operator. As a result, the operator becomes a two-body one,

$$\hat{O}^{T^2} = \sum_{i,j} \boldsymbol{t}_i \cdot \boldsymbol{t}_j, \tag{17}$$

where $\boldsymbol{t} = \boldsymbol{\tau}_i/2$ is the isospin operator for the ith nucleon. 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 $T = 0$, $T = 1$, and $T = 2$ states, 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}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 (many-body $T = 0$) configuration even after the inclusion of the two-particle–two-hole states, and thus the present result of the isospin mixing is a physical effect attributed to the Coulomb interaction and not a numerical artifact.

E. Other physical quantities

A 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 $\hat{N}$ of the harmonic oscillator,

$$\hat{N} = \sum_i \boldsymbol{a}_i^\dagger \cdot \boldsymbol{a}_i, \tag{18}$$

can be easily calculated. Here the summation is over all the nucleons. The lowest value for ^{12}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 gives the value of 9.15, and, after inclusion of the two-particle–two-hole state, the values slightly changes to 9.13, but is almost identical. Thus, unfortunately, this quantity cannot be utilized to discriminate the effect of two-particle–two-hole states. Note that AQCM with $\Lambda = 0$ (equilateral triangular configurations of three-α clusters without breaking) gives a slightly larger value of 10.45, to which the spin-orbit interaction does not contribute. Thus, the attractive effect of the spin-orbit, which is incorporated by introducing finite Λ values, shrinks the relative distances among the quasiclusters.

This shrinkage of the system after transforming α clusters to quasiclusters and incorporating the spin-orbit effect is reflected in the electromagnetic transition probability. The $B(E2)$ value from the first excited state (2^+ state) to the ground state is calculated as 10.19 e^2 fm^4 for the AQCM basis states with $\Lambda = 0$, and the value drops to 6.56 e^2 fm^4 after including the AQCM basis states with finite Λ values, where the experimental value is 7.8 ± 0.4 e^2 fm^4. After taking into account the two-particle–two-hole states, the value again increases to 9.83 e^2 fm^4 (K mixing is performed for the 2^+ state). This value is rather sensitive to the mixing of the two-particle–two-hole states.

The effect of α cluster breaking can be seen in the expectation value of the one-body spin-orbit operator,

$$\hat{O^{LS}} = \sum_i \boldsymbol{l}_i \cdot \boldsymbol{s}_i, \tag{19}$$

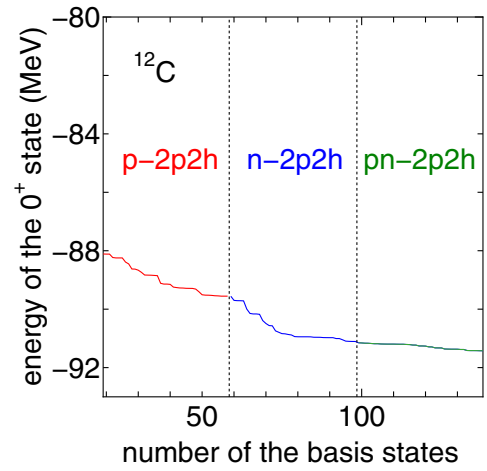

FIG. 4. Energy convergence for the 0^+ state of ^{12}C; 120 two-particle–two-hole basis states are coupled to the 18 AQCM basis states. The basis states from 19 to 58 on the horizontal axis are excited states of the two protons, from 59 to 98 are excited states of the two neutrons, and from 99 to 138 are excited states of a proton and a neutron.

where $\boldsymbol{l}_i$ and $\boldsymbol{s}_i$ are orbital angular momentum and spin operators for the ith nucleon, respectively. The expectation value is zero for the α cluster states and 4 for the $(s_{1/2})^4 (p_{3/2})^8$ configuration of the jj-coupling shell model (0.5 for each nucleon in $p_{3/2}$). The value is 1.88 for the state obtained with 18 AQCM basis states, which is just an intermediate state between the shell and cluster limits. After the inclusion of the two-particle–two-hole states, the value sightly increases to 2.03.

We can also calculate the expectation value of the two-body spin-orbit operator. Here, its functional form is identical to the spin-orbit term in the Hamiltonian [Eq. (16)], and we just show the expectation value of the spin-orbit term, which is -15.38 MeV. Not only the relative angular momenta between nucleons in different clusters, but those in the same cluster are also nonzero after transforming α clusters to quasiclusters, hence this matrix element is huge. However, the inclusion of the spin-orbit effect also induces the kinetic energy, and eventually the net effect becomes smaller.

F. Effects of proton-neutron pairing

We have examined the effect of two-particle–two-hole excitations 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 the spin-up proton and spin-up neutron in one quasicluster are randomly generated.

The energy convergence for the 0^+ state of ^{12}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 138 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. Apparently, the proton-neutron correlations are already included within the dynamics of the three-quasicluster model.

IV. CONCLUSIONS

It has been shown that the cluster and single-particle correlations can be taken into account in the ground state of ^{12}C. The recent development of the antisymmetrized quasicluster model (AQCM) allows us to generate jj-coupling shell-model wave functions from α cluster 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 shift the Gaussian centers of the two nucleons from the quasicluster. It is stressed that identical sets of random numbers were used in generating the basis states of both proton excitation and neutron excitation. Although the two-particle–two-hole states allow the mixing of nonisoscalar components, if the amplitude for each basis state for proton excitation and that for the neutron excitation are identical, the isospin symmetry is restored. Thus, in principle, the model space contains the room to form the isoscalar (many-body $T = 0$) configuration even after two-particle–two-hole effect is considered. This procedure ensures that the isospin breaking here is a physical effect. 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 $T = 0$, $T = 1$, and $T = 2$ states, respectively. Thus, the present value of 0.016 means that the isospin is broken at least by the order of 10^{-3}.

A 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 $\hat{N}$ 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 is 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 role 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 quasiclusters in the present model.

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[1] D. M. Brink, Many-body description of nuclear structure and reactions, in *Proceedings of the International School of Physics "Enrico Fermi,"* Course XXXVI, Varenna, 1965, edited by C. L. Bloch (Academic, New York, 1966), p. 247.
[2] M. Freer, H. Horiuchi, Y. Kanada-En'yo, D. Lee, and U.-G. Meißner, Rev. Mod. Phys. **90**, 035004 (2018).
[3] F. Hoyle, Astrophys. J. Suppl. **1**, 121 (1954).
[4] M. Freer and H. Fynbo, Prog. Part. Nucl. Phys. **78**, 1 (2014).
[5] Y. Fujiwara, H. Horiuchi, K. Ikeda, M. Kamimura, K. Katō, Y. Suzuki, and E. Uegaki, Prog. Theor. Phys. Suppl. **68**, 29 (1980).
[6] A. Tohsaki, H. Horiuchi, P. Schuck, and G. Röpke, Phys. Rev. Lett. **87**, 192501 (2001).
[7] M. G. Mayer and H. G. Jensen, *Elementary Theory of Nuclear Shell Structure* (John Wiley & Sons, New York, 1955).
[8] N. Itagaki, S. Aoyama, S. Okabe, and K. Ikeda, Phys. Rev. C **70**, 054307 (2004).
[9] N. Itagaki, Phys. Rev. C **94**, 064324 (2016).
[10] N. Itagaki, H. Masui, M. Ito, S. Aoyama, and K. Ikeda, Phys. Rev. C **73**, 034310 (2006).
[11] H. Masui and N. Itagaki, Phys. Rev. C **75**, 054309 (2007).
[12] T. Yoshida, N. Itagaki, and T. Otsuka, Phys. Rev. C **79**, 034308 (2009).
[13] N. Itagaki, J. Cseh, and M. Płoszajczak, Phys. Rev. C **83**, 014302 (2011).
[14] T. Suhara, N. Itagaki, J. Cseh, and M. Płoszajczak, Phys. Rev. C **87**, 054334 (2013).
[15] N. Itagaki, H. Matsuno, and T. Suhara, Prog. Theor. Exp. Phys. **2016**, 093D01 (2016).
[16] H. Matsuno, N. Itagaki, T. Ichikawa, Y. Yoshida, and Y. Kanada-En'yo, Prog. Theor. Exp. Phys. **2017**, 063D01 (2017).
[17] H. Matsuno and N. Itagaki, Prog. Theor. Exp. Phys. **2017**, 123D05 (2017).
[18] N. Itagaki and A. Tohsaki, Phys. Rev. C **97**, 014307 (2018).
[19] N. Itagaki, H. Matsuno, and A. Tohsaki, Phys. Rev. C **98**, 044306 (2018).
[20] N. Itagaki, A. V. Afanasjev, and D. Ray, Phys. Rev. C **101**, 034304 (2020).
[21] N. Itagaki, T. Fukui, J. Tanaka, and Y. Kikuchi, Phys. Rev. C **102**, 024332 (2020).
[22] Y. Kanada-En'yo, Prog. Theor. Phys. **117**, 655 (2007).

[23] E. Epelbaum, H. Krebs, D. Lee, and U.-G. Meißner, Phys. Rev. Lett. **106**, 192501 (2011).
[24] E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee, and U.-G. Meißner, Phys. Rev. Lett. **109**, 252501 (2012).
[25] T. Suhara and Y. Kanada-En'yo, Phys. Rev. C **91**, 024315 (2015).
[26] Y. Kanada-En'yo, Phys. Rev. C **93**, 054307 (2016).
[27] M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, and A. Richter, Phys. Rev. Lett. **98**, 032501 (2007).
[28] M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, and A. Richter, Phys. Rev. Lett. **105**, 022501 (2010).
[29] P. Descouvemont and D. Baye, Phys. Rev. C **36**, 54 (1987).
[30] P. Descouvemont, Nucl. Phys. A **709**, 275 (2002).
[31] A. C. Dreyfuss, K. D. Launey, T. Dytrych, J. P. Draayer, and C. Bahri, Phys. Lett. B **727**, 511 (2013).
[32] D. J. Marín-Lámbarri, R. Bijker, M. Freer, M. Gai, T. Kokalova, D. J. Parker, and C. Wheldon, Phys. Rev. Lett. **113**, 012502 (2014).
[33] A. Lovato, S. Gandolfi, R. Butler, J. Carlson, E. Lusk, S. C. Pieper, and R. Schiavilla, Phys. Rev. Lett. **111**, 092501 (2013).
[34] E. Gebrerufael, K. Vobig, H. Hergert, and R. Roth, Phys. Rev. Lett. **118**, 152503 (2017).
[35] K. D. Launey, A. Mercenne, G. H. Sargsyan, H. Shows, R. B. Baker, M. E. Miora, T. Dytrych, and J. P. Draayer, in *Proceedings of the 4th International Workshop on "State of the Art in Nuclear Cluster Physics"* (SOTANCP4), 13–18 May 2018, Texas, edited by M. Barbui, C. M. Folden, III, V. Z. Goldberg, and G. V. Rogachev, AIP Conf. Proc. No. 2038 (AIP, New York, 2018), p. 020004.
[36] W. Satuła and R. Wyss, Phys. Lett. B **393**, 1 (1997).
[37] P. Van Isacker and D. D. Warner, Phys. Rev. Lett. **78**, 3266 (1997).
[38] H. Sagawa, Y. Tanimura, and K. Hagino, Phys. Rev. C **87**, 034310 (2013).
[39] H. Sagawa, C. L. Bai, and G. Colò, Phys. Scr. **91**, 083011 (2016).
[40] A. Tohsaki, Phys. Rev. C **49**, 1814 (1994).
[41] R. Tamagaki, Prog. Theor. Phys. **39**, 91 (1968).
[42] R. B. Wiringa, S. Pastore, S. C. Pieper, and G. A. Miller, Phys. Rev. C **88**, 044333 (2013).