Simplified modeling of cluster-shell competition

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We propose a simple model to describe cluster-shell competition. Introducing only one parameter (Λ) to the wave function makes it possible to describe the asymptotic transition of two valence neutrons in ^{10}Be ($\alpha + \alpha + n + n$) from a di-neutron to independent particles when the contribution of the spin-orbit interaction is taken into account. Similarly in ^{12}C, a transition from a 3α configuration to a $2\alpha + 4N$ configuration is represented, and we show a strong contribution of the spin-orbit interaction in the ground state. We investigate further this transition from the cluster state ($\alpha + ^{16}$O) to the shell-model state (^{16}O + four nucleons) in ^{20}Ne. In these examples, the wave functions for cluster-breaking states are prepared in the same general way.

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I. INTRODUCTION

Nuclear systems consisting of protons and neutrons have been known to show various aspects of quantum many-body systems. One of the standard pictures for the nuclear structure is the shell-model point of view, where nucleons construct self-consistent mean fields and perform independent-particle motions. Here, a strong spin-orbit interaction contrary to the atomic systems has been known to be a key mechanism in fully explaining the observed magic numbers [1,2].

One of the other important aspects of nuclear structure is the cluster structure. The α particle, which corresponds to the doubly closed shell of the lowest s shell in the shell model, is strongly bound. Since relative α-α interaction is weak, α particles can be subunits of the nuclear structure in certain light nuclei. This molecular viewpoint was introduced even before the shell model [3], and cluster structure has been extensively studied for more than four decades [4–6]. Recently, theoretical and experimental investigations have proceeded further to study neutron-rich nuclei, and the cluster structure with valence neutrons has become one of the main subjects concerning the structure of exotic nuclei [7,8].

If each α cluster is expressed as the lowest $(s_{1/2})^4$ configuration, then each α cluster is a spin-zero system, and noncentral interactions do not contribute to the system. However, the dissolution of the α cluster occurs when noncentral interactions act strongly. Therefore, studying cluster-shell competition for a unified understanding of the nuclear structure is intriguing. Recently, we demonstrated this kind of cluster-shell competition in light nuclei by asking how the cluster structure dissolves when the shell-model-like model space is introduced in addition to the cluster model space [9]. By using an extended version of antisymmetrized molecular dynamics (AMD) [10], namely, AMD superposition of selected snapshots (AMD triple-S) [11], it is now feasible to prepare cluster states and α-breaking (shell-model-like) states in the same way and to calculate such mixing of these states by using a common effective interaction. The binding energies of ^{8}Be, ^{10}Be, and ^{10}B become larger by adding shell-model-like basis states, but the amount of the increase is only about 2 MeV, and the $\alpha + \alpha$ structure is essentially a dominant configuration in the ground state. However, an increase in the binding energy from the 3α-cluster state due to the spin-orbit interaction is very large in ^{12}C (about 6 MeV).

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 can the effect of the spin-orbit interaction, which is the key quantity for this transition, 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 paper, therefore, we propose a simple model to describe cluster-shell competition. By introducing only one parameter Λ, it is possible to describe a transition in ^{12}C, for example, and to study the strong contribution of the spin-orbit interaction in the ground state. We begin our discussion of the results with a transition of the two valence neutrons in ^{10}Be ($\alpha + \alpha + n + n$) from a di-neutron to independent particles, with the contribution of the spin-orbit interaction.

This paper is organized as follows: in Sec. II, formulation is summarized; and in Sec. III, numerical results for light

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nuclei, cluster-shell competition are presented. The conclusion is given in Sec. IV.

II. FRAMEWORK

The total wave function is fully antisymmetrized as

$$\Phi = P^{\pi} P^{J}_{MK} \Psi, \tag{1}$$

$$\Psi = \mathcal{A}[(\psi_1\chi_1)(\psi_2\chi_2)\cdots], \tag{2}$$

and projection onto a good parity P^{π} and angular momentum P^{J}_{MK} is numerically performed. The Slater determinant Ψ consists of A nucleons, and each nucleon $\psi_i\chi_i$ ($i = 1$–A) has a Gaussian form the same as many conventional cluster models,

$$\psi_i = \left(\frac{2\nu}{\pi}\right)^{\frac{3}{4}} \exp\left[-\nu(\vec{r} - \vec{z}_i/\sqrt{\nu})^2 + \vec{z}_i^{\,2}/2\right], \tag{3}$$

and the oscillator parameter $b = 1/\sqrt{2\nu}$ is common to all nucleons to exactly remove the center-of-mass kinetic energy. Here, $\{\chi_i\}$ represent the spin-isospin eigenfunctions, and the spin direction is defined parallel to the z axis. When we assume the presence of an α cluster(s), it is expressed by assuming a common $\vec{z}_i$ value for four nucleons (proton spin up, proton spin down, neutron spin up, and neutron spin down).

If $\{\vec{z}_i\}$ are real numbers, the wave function corresponds to the Brink-Bloch wave function [4], 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 $\vec{z}_i$ represent the expectation values of the position and momentum of the single particle, that is, $\langle\vec{r}\rangle = \mathrm{Re}\,[\vec{z}_i]/\sqrt{\nu}$ and $\langle\vec{p}\rangle = 2\sqrt{\nu}\hbar\,\mathrm{Im}\,[\vec{z}_i]$. We introduce a "general rule" to take into account the spin-orbit interaction, which will be applied to ^{10}Be, ^{12}C, and ^{20}Ne, where the dissociation of one (Brink-Bloch) cluster to a "quasicluster" is expressed by introducing a parameter Λ. Suppose that a nucleus consists of a quasicluster C_1' and α clusters $\{C_2, C_3, \ldots, C_m\}$. The Gaussian-center parameters $\vec{z}_i/\sqrt{\nu}$ for nucleons in α clusters are real numbers. However, for the nucleons in the quasicluster, in addition to the real part of $\mathrm{Re}\,[\vec{z}_i/\sqrt{\nu}] = \vec{S}_1$ ($i \in C_1'$), the 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

$$\vec{z}_i/\sqrt{\nu} = \vec{S}_1 + i\,\Lambda\left(\vec{e}^{\,i}_{\mathrm{spin}}\right) \times \vec{S}_1, \tag{4}$$

where $\vec{e}^{\,i}_{\mathrm{spin}}$ is the unit vector for the intrinsic-spin orientation, and Λ 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 Λ is positive or negative, respectively. This can be understood in the following way: the spin-orbit interaction is intuitively interpreted as $(\vec{r} \times \vec{p}) \cdot \vec{s}$ and this is equal to $(\vec{s} \times \vec{r}) \cdot \vec{p}$, where $\vec{r}$, $\vec{p}$, and $\vec{s}$ represent the position, momentum, and spin of the nucleon, respectively. Therefore, if the nucleons in the quasicluster have the momentum components parallel to $\vec{s} \times \vec{r}$, the spin-orbit interaction acts attractively; and if they have momentum components antiparallel to $\vec{s} \times \vec{r}$, it acts repulsively, although the spin-orbit interaction is a two-body operator in the actual calculation.

The Hamiltonian operator $\hat{H}$ has the form

$$\hat{H} = \sum_{i=1}^{A} \hat{t}_i - \hat{T}_{\mathrm{c.m.}} + \sum_{i>j}^{A} \hat{v}_{ij}, \tag{5}$$

where a two-body interaction $\hat{v}_{ij}$ includes the central part, the spin-orbit part, and the Coulomb part. For the central part, we use the following Volkov No. 2 effective N-N potential [12]:

$$V(r) = (W - MP^{\sigma}P^{\tau} + BP^{\sigma} - HP^{\tau}) \times \left[V_1 \exp\left(-r^2/c_1^2\right) + V_2 \exp\left(-r^2/c_2^2\right)\right], \tag{6}$$

where $W = 1 - M$, $M = 0.60$, and $B = H = 0.125$. For the spin-orbit term, we introduce the G3RS potential [13] as

$$V_{ls} = V_0\left(e^{-d_1 r^2} - e^{-d_2 r^2}\right) P(^3O)\vec{L} \cdot \vec{S}, \tag{7}$$

where $d_1 = 5.0\,\mathrm{fm}^{-2}$, $d_2 = 2.778\,\mathrm{fm}^{-2}$, $V_0 = 2000$ MeV, and $P(^3O)$ is a projection operator onto a triplet odd state. The operator $\vec{L}$ stands for the relative angular momentum and $\vec{S}$ is the spin ($\vec{S}_1 + \vec{S}_2$). All of the parameters of this interaction were determined from the $\alpha + n$ and $\alpha + \alpha$ scattering phase shifts and the binding energy of the deuteron [14]. The original Volkov No. 2 potential gives the bound state for the n-n system, but it is eliminated by introducing B and H parameters.

III. RESULTS

A. π orbit versus di-neutron correlation in ^{10}Be

We begin this section by discussing a simplified model to describe the cluster-shell competition with ^{10}Be ($\alpha + \alpha + n + n$). The ground state of ^{10}Be has a large β deformation due to the α-α clustering of the core. We have shown that all of the low-lying states are well described by introducing molecular orbits with $|K|^{\pi} = 3/2^-$, $1/2^-$, and $1/2^+$ around two α's along the z axis [15,16].

Next, we have further discussed a triaxial deformation of the yrast states [17]. If the valence neutrons perform single-particle motions as eigenstates of the K quantum number, the system is axial symmetric; however, the distortion of the single-particle motion occurs when the spin-orbit interaction between the core and the valence neutrons decreases, as in weakly bound systems. When the wave functions of the valence neutrons deviate from the jj-coupling-like orbits and approach the SU(3) limit, a di-neutron configuration with spin zero becomes more important, and the system becomes a three-body-like ($\alpha + \alpha +$ di-neutron) triaxial shape. In this case, the K value of each valence neutron is no longer a good quantum number, and the ratio $B(E2; 2_2^+ \to 2_1^+)/B(E2; 2_1^+ \to 0_1^+)$ calculated with the Davydov-Filippov model [18] and our model coincide at around $\gamma = 19^{\circ}$, suggesting a mixing of the triaxial component in ^{10}Be. The drastic increase of this interband transition probability occurs if the spin-orbit interaction is artificially weakened. Therefore, the spin-orbit interaction is considered the driving force for the valence neutrons to restore single-particle motion, and the neutron is rotated around the core.

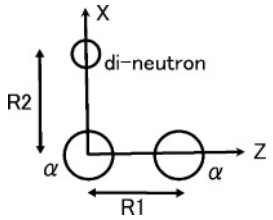

FIG. 1. Coordinate system for ^{10}Be. R_1 and R_2 represent the distance between α clusters and between an α cluster and a di-neutron cluster, which are taken along the z and x axes, respectively.

In this paper, we show that introducing only one parameter Λ makes it possible to describe the situation, namely, the asymptotic transition of the two valence neutrons from the di-neutron configuration ($\alpha + \alpha +$ di-neutron cluster) to independent particles in ^{10}Be. The coordinate system for ^{10}Be is defined as shown in Fig. 1. In Fig. 1, R_1 and R_2 represent the distance between the α clusters and between the α cluster and the di-neutron cluster, which are shown along the z and x axes, respectively. Each α cluster is described by assigning common values for the Gaussian-center parameters $\{z_i\}$ of the four nucleons (spin-up proton, spin-down proton, spin-up neutron, and spin-down neutron). The di-neutron is similarly described by assigning common values for Gaussian-center parameters of the spin-up and spin-down neutrons, which are placed on the x axis. The oscillator parameter $b = 1/\sqrt{2\nu}$ is set equal to 1.46 fm.

Importantly, the valence neutrons with spin up and spin down that make up the di-neutron cluster are pushed up to the p shell due to the Pauli principle between the neutrons and the α clusters, when the value of R_2 is small enough. In the present case, since the neutrons are placed on the x axis, they occupy p_x orbits ($x \exp[-\nu r^2]$) around the origin. This situation can be explained as it was in Ref. [4]: the spin-up neutron in the α cluster and the valence neutron with the spin up placed on the x direction are described as $\exp[-\nu r^2]$ and $\exp[-\nu(\vec{r} - \vec{X})^2]$ ($\vec{X}$ has only the x component), and rearranging the linear combinations of these orbits is possible, when the wave function is antisymmetrized. Then, at the limit of $|\vec{X}| \to 0$, one orbit $\exp[-\nu r^2] + \exp[-\nu(\vec{r} - \vec{X})^2]$ corresponds to $\exp[-\nu r^2]$, and the other $\{\exp[-\nu r^2] - \exp[-\nu(\vec{r} - \vec{X})^2]\}/|\vec{X}|$ to $x \exp[-\nu r^2]$.

When the values of the Gaussian centers of the spin-up and spin-down valence neutrons are in common, the neutrons construct a spin-zero system, and the spin-orbit interaction between the core and the di-neutron vanishes. However, even if the spatial positions of these two neutrons are in common, one can describe the single-particle motion (rotation by the α-α axis) of the valence neutrons by introducing imaginary parts of the Gaussian centers. This orbit is similar to the π orbit in terms of the molecular-orbit model [14,19], where the spin-orbit interaction contributes strongly. The parameters of Gaussian centers for the valence neutrons are given as

$$\vec{z}/\sqrt{\nu} = R_2(\vec{e}_x + i\Lambda\vec{e}_y) \tag{8}$$

for the spin-up neutron, and

$$\vec{z}/\sqrt{\nu} = R_2(\vec{e}_x - i\Lambda\vec{e}_y) \tag{9}$$

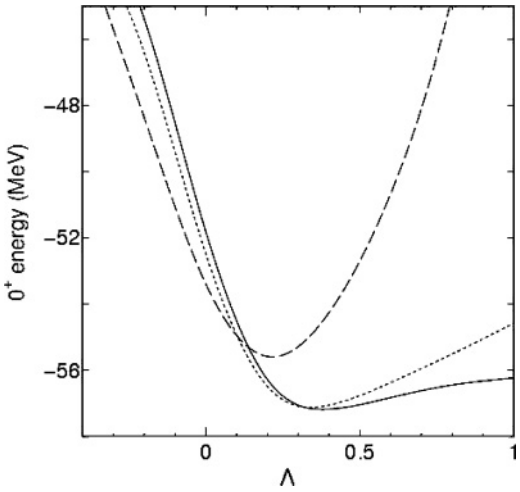

FIG. 2. Energy of the 0^+ state of ^{10}Be as a function of parameter Λ. The α-α distance R_1 is 3 fm, and the solid, dotted, and dashed lines correspond to the cases of $R_2 = 0.5$, 1, and 2 fm, respectively.

for the spin-down neutron. Here, $R_2\vec{e}_x$ is the spatial position of the Gaussian center, the imaginary parts ($R_2\Lambda\vec{e}_y$ and $-R_2\Lambda\vec{e}_y$) express the momenta of the neutrons, and $\vec{e}_x$ and $\vec{e}_y$ are unit vectors of the x and y axes. Since the directions of the spin and real part of $\vec{z}$ are introduced along the z- and x-axis, respectively, the imaginary part of $\vec{z}$ is introduced along the y axis to take into account the spin-orbit interaction, which has the form of $\vec{s} \cdot (\vec{r} \times \vec{p})$. In other words, by introducing these imaginary parts, we can mimic the spherical harmonics. Namely, when Λ is equal to 1, the wave function for the spin-up neutron $\{\exp[-\nu r^2] - \exp[-\nu(\vec{r} - \vec{z}/\sqrt{\nu})^2]\}/|\vec{z}|$ corresponds exactly to the shell-model wave function of $(x + iy)\exp[-\nu r^2] \sim rY_{11}\exp[-\nu r^2]$, and the wave function for the spin-down neutrons corresponds to $(x - iy)\exp[-\nu r^2] \sim rY_{1-1}\exp[-\nu r^2]$, at the limit of $R_2 \to 0$. In this case, the directions of the spin and orbital parts of the angular momentum become parallel, and the spin-orbit interaction acts attractively. When the spin-orbit interaction works, the di-neutron is no longer a cluster with $S = 0$, and two neutrons occupy orbits in time reversal with each other, although the spatial positions still somehow overlap. In this case, the di-neutron is a "quasi" cluster, and Λ is a parameter used to describe the cluster-shell competition. When the value of Λ is equal to 1, the wave function of the neutron corresponds exactly to the jj-coupling orbit around the left α cluster if the rotation radius R_2 is small enough, and Λ equal to zero is the di-neutron limit.

The energy of the 0^+ ground state of ^{10}Be as a function of parameter Λ is shown in Fig. 2. In this figure, the α-α distance R_1 is 3 fm, optimal for the ground state [15,16], and the solid, dotted, and dashed lines correspond to the cases of $R_2 = 0.5$, 1, and 2 fm, respectively. When the position of the di-neutron is close to the α cluster, the value of R_2 is small, and the motion of each valence neutron is as a single-particle motion around the α-α core. The minimal Λ values for the solid and dotted lines are 0.3–0.4. The optimal energy of about -57.2 MeV is consistent with our previous result based on the molecular-orbit approach [15]. However,

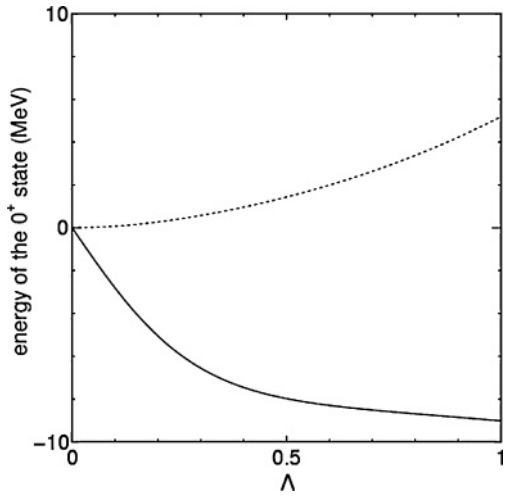

FIG. 3. Spin-orbit (solid line) and kinetic (dotted line) energies for the 0^+ state of ^{10}Be as a function of parameter Λ. R_1 and R_2 are 3.0 and 1.0 fm, respectively. The kinetic energy is shifted to zero at $\Lambda = 0$.

the exchange effect of one neutron between α clusters (mixing of the $^5\mathrm{He} + {}^5\mathrm{He}$ configuration) is missing in the present case; this effect is known to decrease the kinetic energy with respect to the z axis by about 1 MeV. On the contrary, when the case valence neutrons are located far from the core, the spin-orbit interaction does not work strongly, and the di-neutron system does not receive the driving force for the single-particle motion. As shown in the dashed line, the optimal value of Λ decreases to about 0.2, and the di-neutron becomes the dominant component.

In Fig. 3, the spin-orbit (solid line) and the kinetic (dashed line) energies for the 0^+ state of ^{10}Be are shown as a function of parameter Λ. Here, R_1 and R_2 are 3.0 and 1.0 fm, respectively. The kinetic energy is shifted to zero at $\Lambda = 0$. The spin-orbit interaction contributes strongly with increasing Λ. However, not only does the absolute value of the spin-orbit interaction increase, but the kinetic energy also increases with the increasing Λ value. The contribution of the spin-orbit interaction, which is attractive, is almost saturated around $\Lambda = 0.5$, and the decrease of the energy is monotonic; however, the increase in the kinetic energy becomes quadratic. The optimal Λ value is therefore obtained as a cancellation of these two components, and the sum of these becomes minimum around $\Lambda \sim 0.4$, close to the optimal value for the total energy.

In the present model, Λ can be taken as a negative value, and we can describe states where the spin-orbit interaction acts repulsively. In Refs. [15,16], such a state appears as a highly excited state, where the dominant configuration of the valence neutrons is $(|K^\pi| = 1/2^-)^2$; however, the state has not been observed yet. In Fig. 2, the energy of the 0^+ state with negative Λ is also shown, and the energy increases as an increase of $|\Lambda|$.

B. π orbit versus α correlation in ^{12}C

Many successful calculations for ^{12}C have been made by assuming the 3α configuration [20–22], and the second 0^+ state just above the 3α threshold has been well described

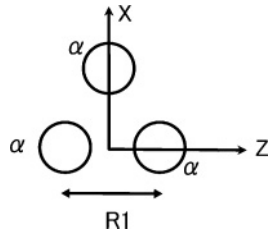

FIG. 4. Coordinate system for ^{12}C. Three α clusters have an equilateral triangular configuration on the xz plane. R_1 represents the distance between two α clusters on the z axis and, the remaining α cluster is placed on the x axis.

by the cluster models. However, the breaking effect of the α cluster is also known to be important, especially for the ground state [9,23,24] in explaining the observed electromagnetic properties. If one of the α clusters is broken, the configuration is $\alpha + \alpha + 4N$, and picture is close to "the molecular-orbit for four nucleons around the $\alpha + \alpha$ core" [25]. If the spin-orbit interaction is very strong and two α clusters are broken, the configuration is $\alpha + 8N$ and the picture approaches the jj-coupling shell model. In Ref. [9], we have shown that by incorporating the breaking effect of only one of the α clusters, the effect of the spin-orbit interaction can be incorporated to some extent. Therefore, in this paper, we investigate this cluster-shell mixing using the current model, where one α cluster is changed to a quasicluster due to the spin-orbit interaction.

Three α clusters are introduced as having an equilateral triangular configuration on the xz plane as shown in Fig. 4; this is known to be the dominant configuration for the ground state when the spin-orbit interaction does not work. In Fig. 4, R_1 represents the distance between two α clusters on the z axis and the remaining α cluster is placed on the x axis. We introduce Λ for the α cluster on the x axis. Similar to Eqs. (8) and (9), the $\vec{z}$ parameters of the spin-up proton and spin-up neutron are changed so that the imaginary parts have a positive value

$$\vec{z}/\sqrt{\nu} = (\sqrt{3}R_1/2)(\vec{e}_x + i\Lambda\vec{e}_y), \tag{10}$$

and those for the spin-down proton and spin-down neutron are changed to have the imaginary parts with a negative value

$$\vec{z}/\sqrt{\nu} = (\sqrt{3}R_1/2)(\vec{e}_x - i\Lambda\vec{e}_y). \tag{11}$$

Due to the Pauli principle, these nucleons are automatically excited to the p shell. This parametrization 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 $R\vec{e}_x$ to $R(\vec{e}_x + i\Lambda\vec{e}_y)$ for the spin-up nucleons, and to $R(\vec{e}_x - i\Lambda\vec{e}_y)$ for the spin-down nucleons, where R is some radius and Λ is an "order parameter" of cluster-shell competition. 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 Λ. The oscillator parameter ($b = 1/\sqrt{2\nu}$) is set equal to 1.46 fm.

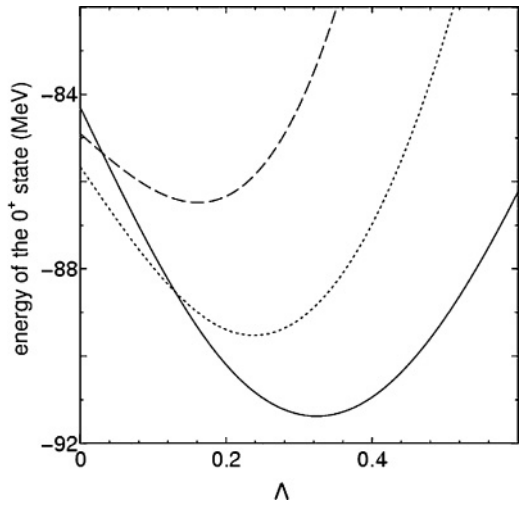

FIG. 5. Energy of the 0^+ state of ^{12}C as a function of parameter Λ. Solid, dotted, and dashed lines correspond to the cases of $R_1 =$ 2.0, 2.5, and 3.0 fm (respectively), and Λ is introduced for one α cluster on the x axis.

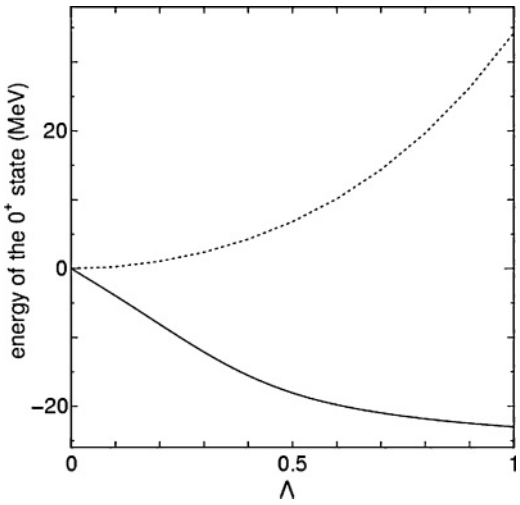

FIG. 6. Spin-orbit (solid line) and kinetic (dotted line) energies for the 0^+ state of ^{12}C as a function of parameter Λ. R_1 is 1.0 fm, and the kinetic energy is shifted to zero at $\Lambda = 0$.

The energy curve of the 0^+ state of ^{12}C as a function of parameter Λ is shown in Fig. 5, where the solid, dotted, and dashed lines represent the cases of $R_1 = 2.0$, 2.5, and 3.0 fm, respectively. When the Λ 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 Λ becomes a finite value, one α cluster on the x axis is changed to a "quasi α", and four nucleons start to perform independent motions around the remaining two α clusters located on the z axis, such that the picture is close to molecular-orbital motion around the α-α core. 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.

In Fig. 6, the spin-orbit (solid line) and the kinetic (dashed line) energies for the 0^+ state of ^{12}C are shown as a function of parameter Λ. Here, R_1 is 1.0 fm, and the kinetic energy is shifted to zero at $\Lambda = 0$. The same as in ^{10}Be, the spin-orbit interaction strongly contributes with increasing Λ; however, the kinetic energy also increases rapidly with an increasing Λ value. Therefore, the optimal Λ value is obtained as a cancellation of these two components, and the sum of these becomes minimum around $\Lambda \sim 0.4$, close to the optimal value for the total energy.

To obtain the optimal Λ value, solving the frictional cooling method in AMD [10] only for the y components of the imaginary parts of the four valence nucleons rotating around α-α is also a convenient way:

$$\frac{d(\vec{z}_k)_y}{d\tau} = -\mathrm{Im}\left(\frac{\partial\langle H\rangle}{\partial(\vec{z}_k^*)_y}\right) i \qquad (k = 1 \sim 4). \tag{12}$$

The energy decreases as the imaginary time τ increases, and an optimal Λ value is obtained. The form of Eq. (12) is similar to the equation in AMD triple-S [11]; however, in this case, the equation is reinterpreted as the equation for cluster-shell competition.

In the present analysis, breaking only one α cluster has been taken into account, and the relation between the present model and the *jj*-coupling shell model is explained as follows: when we take the limit of $R_1 = 0$ and $\Lambda = 1$, one α cluster occupies the $(s)^4$ configuration and the other α-cluster occupies the $(p_z)^4$ configuration, and four nucleons in a quasi-α cluster occupy the $p3/2$ orbits, in terms of the shell model. Therefore, the difference between the present model and the lowest configuration of the *jj*-coupling shell model is the treatment of the one α cluster which occupies the $(p_z)^4$ configuration. If we properly dissolve this α cluster into four independent nucleons, the wave function becomes identical to that of the *jj*-coupling shell model. However, to do this, we need to introduce two quasi-α clusters, and this will be a next step to be performed in near future.

C. Case of σ orbit

We have discussed how the nucleons rotate by the α-α axis. Although it is not directly related to cluster-shell competition, we next introduce a simplified model for the valence neutrons located on the symmetry axis. If a neutron is placed on the α-α axis, a so-called σ orbit in terms of molecular-orbit [14,19] occurs. Since two α clusters already exit on this axis, the neutrons are pushed up to the *sd* shell. In this case, the two valence neutrons reduce the kinetic energy by enhancing the α-α distance (up to around 4 fm) [15,16,26]. This intruder state $[(1/2^+)^2$ for the two neutrons] is the dominant configuration of the second 0^+ state of ^{10}Be [15].

If the two valence neutrons are staying along the α-α axis, the spatial parts of the wave functions are the same and the system becomes spin zero, thus the spin-orbit interaction vanishes. Actually, even in the case where only one valence neutron occupies the α-α axis ($K^\pi = 1/2^+$), the spin-orbit interaction vanishes. This is because the rotation radius of the neutron around the $\alpha + \alpha$ core becomes zero, even though the neutron participates in the rotation of the whole system.

Mathematically, this means that the orbital part of the wave function of the neutron along the α-α axis has only the real part and therefore an eigenstate of time-reversal operator, thus the matrix element of the spin-orbit operator whose spatial part $\vec{L}$ is time odd becomes zero. If the distribution of a neutron deviates from the α-α axis as in the π orbit, the wave function acquires a component of the imaginary part during the projection process of the K quantum number, and the spin-orbit interaction can be taken into account (if it is not di-neutron with spin zero). This has been the situation in traditional molecular-orbital models [14,27], where $1/2^+$ orbit is estimated to be too high in energy, and the models are unable to explain the well-recognized level inversion in the ground state of ^{11}Be [28].

We introduce a simplified model to describe the deviation of the σ orbit due to the spin-orbit interaction. We consider the $1/2^+$ state of ^{9}Be in the following discussion, where there is only one valence neutron around two α clusters. The coordinate space is the same as in Fig. 1; however, R_2 is defined along the negative direction of the z axis. One valence neutron with spin up which occupies the original σ orbit is simplified by giving the Gaussian center as

$$\vec{z}/\sqrt{\nu} = -R_2\vec{e}_z. \tag{13}$$

The oscillator parameter $b = 1/\sqrt{2\nu}$ is set equal to 1.46 fm. The neutron stays on the z axis, and since two α clusters are already staying on this axis, because of the Pauli principle, the neutron is pushed up to the *sd* shell. Next, we prepare a wave function with the deviation from the z axis. When the wave function deviates, a rotational motion by the z axis is possible, and the orbital angular momentum around the α-α axis (K) becomes finite. Therefore, the spin must be flipped down to have $K^\pi = 1/2^+$ totally. Unfortunately, this deviation cannot be described as an asymptotic transition of a single Gaussian wave packet, and linear combination of two Gaussians is necessary, contrary to the case of the π orbit. Therefore the single-particle orbit ϕ of the neutron can be expressed by introducing mixing angle Λ as

$$\phi = \cos(\Lambda\pi/2)\psi(-R_2\vec{e}_z)|\uparrow\rangle - \sin(\Lambda\pi/2)\psi(R_2\vec{e}_x)|\downarrow\rangle, \tag{14}$$

where, $\psi(-R_2\vec{e}_z)$ expresses the Gaussian wave packet whose center $\vec{z}/\sqrt{\nu}$ is equal to $-R_2\vec{e}_z$, and $|\uparrow\rangle$ and $|\downarrow\rangle$ are spin parts. At the limit of $R_1, R_2 \to 0$, the first term corresponds exactly to the shell-model wave function of $r^2Y_{20}\exp[-\nu r^2]|\uparrow\rangle \sim z^2\exp[-\nu r^2]|\uparrow\rangle$, and the second term corresponds to $r^2Y_{21}\exp[-\nu r^2]|\downarrow\rangle \sim (x+iy)z\exp[-\nu r^2]|\downarrow\rangle$ after the K and parity projections (the parity projection for the ^{9}Be system generates one node along the z axis for the valence neutron, since the α-α-core part mainly has the positive-parity component).

The energy of the $1/2^+$ state of ^{9}Be as a function of the mixing angle of these two wave functions Λ is shown in Fig. 7, where the R_1 and R_2 values are 3 fm and 1.5 fm, respectively. The solid and dotted lines are calculated with and without the spin-orbit interaction, respectively. When the spin-orbit interaction is switched on, the solid line shows that the energy is minimum around $\Lambda \sim 0.2$, and the decrease in energy due to the spin-orbit interaction is more than 2 MeV; the decrease does not happen in the case of the dotted line without the spin-orbit interaction. If the wave function becomes pure $(x+iy)z\exp[-\nu r^2]|\downarrow\rangle$, because the directions of the spin and orbital parts of angular momentum become antiparallel, and the spin-orbit interaction acts repulsively, then the energy of the solid line in Fig. 7 is higher than that of the dotted line around $\Lambda = 0.8$–1.0.

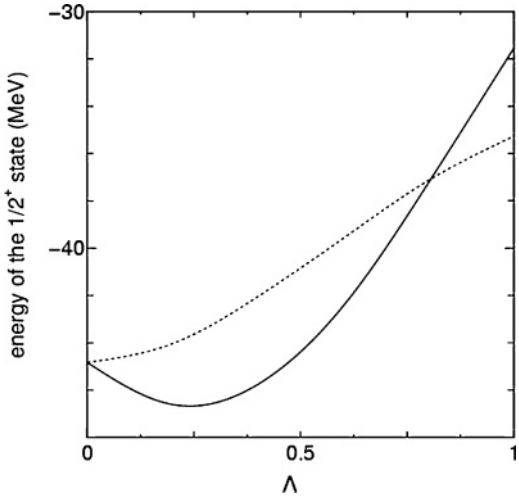

FIG. 7. Energy of the $1/2^+$ state of ^{9}Be as a function of parameter Λ. The solid and dotted lines represent the case with and without the spin-orbit interaction. The coordinate space is the same as Fig. 1, however, R_2 is defined along the negative direction of the z axis. R_1 and R_2 are 3 fm and 1.5 fm, respectively.

It is shown that the neutron-orbit surely deviates from the pure σ orbit. This deviation is also proved by the energy surface for the $1/2^+$ state of ^{9}Be in Ref. [14]. Actually, calculation based on the molecular-orbit model [26] shows that the contribution of the spin-orbit interaction due to the deviation of the σ orbit is stronger if two valence neutrons are present. It is essential in accounting for the disappearance of the $N = 8$ magic number in the ground state of ^{12}Be, where the lowering of the $(1/2^+)^2$ state due to the spin-orbit interaction is about 4.5 MeV.

D. $d5/2$ orbits versus α correlation in ^{20}Ne

We have developed a model to describe the deviation of the orbit from the cluster structure due to the spin-orbit interaction, and this model can be applied to heavier systems. For example, although numerous calculations exist within the model space of $^{16}\mathrm{O} + \alpha$ or $^{12}\mathrm{C} + \alpha + \alpha$ for ^{20}Ne [29–31], from the shell-model point of view, four nucleons are located in the $d5/2$ orbits and the spin-orbit interaction acts strongly [32,33]. This effect cannot be taken into account with the cluster model space. Later, hybrid models [34,35] and AMD [36,37] were applied to express both cluster structure and single-particle motions of nucleons around the ^{16}O core. Therefore, applying the present model to describe single-particle motion as a deviation of the orbits from an α cluster and establishing a simple picture of cluster-shell competition is intriguing.

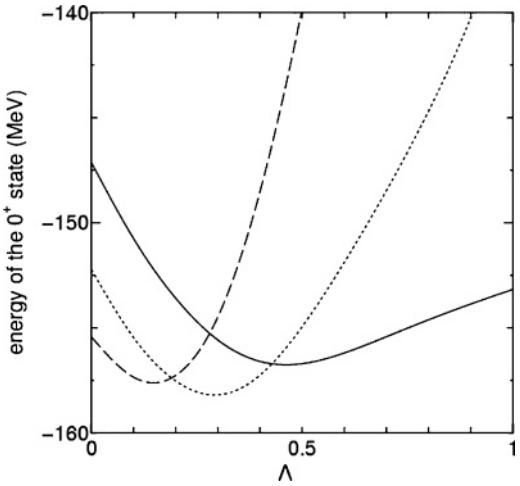

FIG. 8. Energy of the 0^+ state of ^{20}Ne as a function of parameter Λ. R_1 is 1 fm, and the solid, dotted, and dashed lines correspond to the cases of $R_2 = 1$, 2, and 3 fm, respectively.

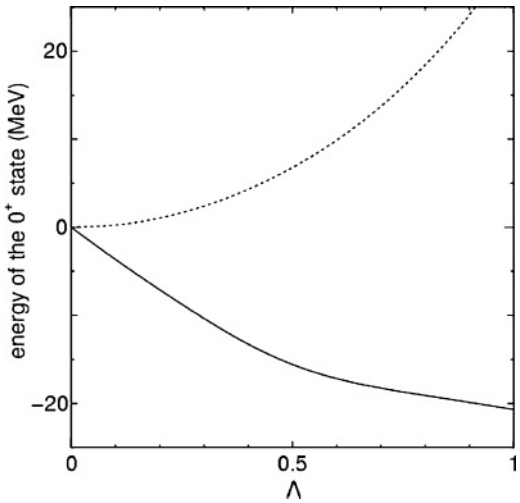

FIG. 9. Spin-orbit (solid line) and kinetic (dotted line) energies for the 0^+ state of ^{20}Ne as a function of parameter Λ. R_1 and R_2 are 1.0 and 2.0 fm, respectively. The kinetic energy is shifted to zero at $\Lambda = 0$.

In our model, four of the α clusters form a tetrahedron configuration, which corresponds exactly to the doubly closed shell of the p shell at the limit of relative distance R_1 equal to zero. One remaining α cluster is located on the x axis. The α-α distance of the 4α-tetrahedron is parametrized as R_1, and the distance between the last α cluster on the x axis and center of mass of the 4α tetrahedron is R_2. Now we introduce our "general rule" for preparing a cluster-breaking wave functions for ^{20}Ne. Since we take into account the breaking effect of the last α cluster, we place the α cluster on the x axis, and we change the Gaussian centers of the nucleons in this cluster from $R\vec{e}_x$ to $R(\vec{e}_x + i\Lambda\vec{e}_y)$ for the spin-up nucleons and to $R(\vec{e}_x - i\Lambda\vec{e}_y)$ for the spin-down nucleons, so as to make the directions of the spin and orbital parts of the angular momentum parallel, in the same manner as ^{12}C, that is,

$$\vec{z}/\sqrt{\nu} = R_2(\vec{e}_x + i\Lambda\vec{e}_y) \tag{15}$$

for the spin-up proton and neutron and

$$\vec{z}/\sqrt{\nu} = R_2(\vec{e}_x - i\Lambda\vec{e}_y) \tag{16}$$

for the spin-down proton and neutron. Because of the Pauli principle, these nucleons are automatically excited to the *sd* shell. When Λ is zero, the orbits of nucleons in this α cluster become a wave function of $x^2\exp[-\nu r^2]$ at the limit of $R_1, R_2 \to 0$; and with increasing Λ value, the orbits approach $(x+iy)^2\exp[-\nu r^2] \sim r^2 Y_{22}\exp[-\nu r^2]$ for the spin-up proton and neutron, and $(x-iy)^2\exp[-\nu r^2] \sim r^2 Y_{2-2}\exp[-\nu r^2]$ for the spin-down proton and neutron, and the spin-orbit interaction acts attractively.

In this subsection, Majorana exchange parameter M and oscillator parameter of the Gaussian wave packet $b = 1/\sqrt{2\nu}$ are changed to 0.62 and 1.6 fm, respectively. The energy curves of the 0^+ state of ^{20}Ne are shown in Fig. 8, where R_1 is fixed to 1 fm and the solid, dotted, and dashed lines correspond to $R_2 = 1$, 2, and 3 fm, respectively. When the R_2 value is 3 fm, the dashed line shows the minimal point around $\Lambda = 0.1$, and the 5α cluster is essentially the dominant configuration. However, with a decreasing R_2 value, the optimal Λ value gradually increases; and in the case of $R_2 = 1$ fm, the solid line shows the minimal point around $\Lambda = 0.5$, and the energy curves become rather flat. Since the energies of these three minimal points are close to each other, the real ground state lies somehow in between the cluster and shell-model states. When we diagonalize the Hamiltonian consisting of the three states, which are the lowest points of each line [$\Lambda = 0.5$ (solid), $\Lambda = 0.3$ (dotted), and $\Lambda = 0.1$ (dashed)], the calculated energy (-159.2 MeV) is lower than the energy calculated using the cluster states ($R_2 = 1, 2, 3, 4, 5$ fm, $\Lambda = 0$) by 2.4 MeV and lower than the energy of the shell-model limit ($R_2 = 1$ fm, $\Lambda = 1.0$) by 6.1 MeV.

In Fig. 9, the spin-orbit (solid line) and the kinetic (dashed line) energies for the 0^+ state of ^{20}Ne are shown as a function of parameter Λ. R_1 and R_2 are 1.0 and 2.0 fm, respectively, and the kinetic energy is shifted to zero at $\Lambda = 0$. The same as in ^{10}Be and ^{12}C, the spin-orbit interaction contributes strongly with increasing Λ; however, the kinetic energy also increases rapidly with an increasing Λ value. Therefore, the optimal Λ value is obtained as a cancellation of these two components, and the sum of these energies becomes minimum around $\Lambda \sim 0.4$, close to the optimal value for the total energy.

IV. CONCLUSION AND FURTHER OUTLOOK

Microscopically calculating the cluster-shell competition recently became possible, and in this paper, we further introduced a model to describe the competition in a simple way as a general concept of the nuclear structure. The spin-orbit interaction is the key quantity for transition from cluster states to shell states; and the effect is now implanted in the wave function by introducing the parameter Λ. The parametrization of the wave function and the setup of the coordinate space we introduced could be called a "general rule" for preparing cluster-breaking wave functions.

We have shown that describing the asymptotic transition of the two valence neutrons in ^{10}Be ($\alpha + \alpha + n + n$) from a di-neutron configuration to independent-particle motions is possible, by which the contribution of the spin-orbit interaction is taken into account. Similarly, in ^{12}C and ^{20}Ne, transitions from an α-cluster configuration to the molecular-orbit picture or the shell-model picture are represented by introducing one parameter, and a strong contribution of the spin-orbit interaction in the ground states has been taken into account. The present analysis takes into account the breaking of only one α cluster. To prepare the *jj*-coupling configuration of ^{12}C, for example, dissolving one more α cluster into four independent nucleons is necessary, and introducing two quasi-α clusters will be a next step of the framework.

As a remaining problem, it is necessary to introduce some extensions of cluster breaking into the traditional cluster models for the expression of the tensor interaction. In the 1960s, a microscopic α-α potential was derived based on the meson theory [38,39], and appearance of the cluster structure was explained by saying that the contribution of one pion exchange potential vanishes from the direct terms when each α cluster is described as a $(0s)^4$ configuration. This idea has been generalized as a threshold rule and proposed as a mechanism for explaining the appearance of various cluster structure [40]. However, recently, many microscopic calculations to directly take into account the tensor term have been started [41–44], and a strong contribution in ^{4}He is discussed there. Therefore, now it is necessary to show that the interaction between two ^{4}He nuclei is still weak, even if the model space is extended and tensor contribution can be incorporated. Although the tensor interaction strongly contributes to each ^{4}He nucleus and ^{4}He nuclei are no longer simple α clusters with the $(0s)^4$ configuration, the tensor interaction may not act strongly enough to change the relative motion between two ^{4}He nuclei and the cluster structure may survive. Projecting out the relative coordinates of the two ^{4}He nuclei to estimate the tensor contribution for the relative motion is a difficult task, thus, establishing a simple picture to describe "broken α clusters" is desirable.

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