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Linear-chain structure of three α clusters in 13 C

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We investigate a linear-chain configuration of three α clusters with a neutron in 13 C. To characterize this configuration, an operator \mathcal{P} is introduced, which is the sum of parity inversion operators for each proton. The states with positive expectation values for this operator are found to form a rotational band structure, and the moment of inertia agrees well with the experimentally suggested value. Allowing a small bending angle stabilizes the linear-chain configuration of three α clusters with a valence neutron, which is a hyper-deformed state.

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The realization of linear-chain configurations has been a long-standing objective of nuclear structure physics. However, it is difficult to stabilize this configuration in nuclear systems, which is contrary to the case in atomic systems. The linearchain structure of three α clusters was suggested nearly half a century ago [1], and the second 0^+ (0_2^+) state of 12 C at $E_x = 7.65$ MeV just above the three α threshold energy is a candidate for having this structure. This state is considered to have an exotic cluster structure that is analogous with the so-called mysterious 0^+ state of 16 O at $E_x = 6.06$ MeV, which has a $^{12}C+\alpha$ cluster structure and is not completely explained by a simple shell-model picture. However, the 0_2^+ state, which plays a crucial role in the synthesis of ¹²C from three ⁴He nuclei in stars [2], has been proven to contain not only the linear-chain configuration but also various three α configurations by many microscopic cluster models [3]. The state is gaslike without a specific geometric shape, and it has been recently reinterpreted as an α -condensed state [4]. The search for linear-chain states of α clusters has been extended to heavier N = Z nuclei [5–8]; however, further investigations are needed to confirm that those states are really linear-chain structures.

The difficulty of the linear-chain configuration is briefly explained in the following way. From the harmonic-oscillator point of view, if three α clusters form a linear configuration on the z axis, four nucleons in the central α cluster occupy the lowest s orbits; however, eight nucleons in the other α clusters are excited to higher orbits such as the p(z) and $sd(z^2)$ orbits due to the antisymmetrization effect. If the system has some bending angle, three α clusters form a two-dimensional configuration in the xz plane, and in this case four nucleons corresponding to the $sd(z^2)$ orbits are deexcited to the p(x) orbits. We may conclude that in light nuclei, where the value of $\hbar\omega$ is about 20 MeV, it is difficult to prevent the mixing of states with different bending angles.

Another difficulty comes from the weak-coupling nature of the nuclear systems. If the state is largely clusterized, i.e., not only the total system of three α clusters, the α - α subsystem (8 Be) tends to have good angular momentum, since the angular momentum projection for the intrinsic wave function of 8 Be to the 0^+ state induces a decrease in the energy by about 10 MeV.

This angular momentum projection of the subsystem implies the rotation of two α clusters with respect to their center of mass. These considerations show that various three α configurations can mix.

This discussion suggests that if the linear-chain configuration of three α clusters exists as a sharp resonance state, there must exist some specific mechanism such that the state corresponds to a local minimum point on the energy surface, because the decrease of energy due to the coupling with the bending motion is large. One of the mechanisms to stabilize the linear-chain configuration is a symmetry created by adding valence neutrons. Even if the linear-chain configurations of only α clusters are difficult to be stabilized in N=Z nuclei, higher stability is possible when neutrons are added.

Recently, the physics of neutron-rich nuclei has been extensively investigated from both the theoretical and experimental sides, and the appearance of cluster structure is one of the most important features. For instance, the presence of rotational bands with the α - α structure in the excited states of ¹⁰Be and ¹²Be and the breaking of the magic number (N = 8) due to the clustering of the core have attracted much attention [9–16]. We have suggested, based on the molecular-orbit model, that these phenomena can be well explained by introducing single-particle orbits around the α - α cluster structure [15]. Such a molecular orbit has been further introduced to survey systems with three α clusters [17–19]. If the neutrons occupy the so-called σ orbit (parallel to the three α axis), a deformed configuration of the core with an elongated shape is favored, because it decreases the excitation energy of the valence neutrons. Eventually, the linear-chain configuration of three α clusters is stabilized, for example, in 16 C dependent on the neutron configuration; however, the excitation energy of such states is high (around the 25 MeV region).

From the experimental side, candidates for the linear-chain configurations of three α clusters in $^{13}\mathrm{C}$ have recently been suggested [20]. It is surprising that such structure can be stabilized by adding only one neutron to the three α system which is placed as a π orbit. In addition, the excitation energies of the bandhead states are 9.898 MeV ($K^{\pi}=3/2^{-}$ band) and 11.080 MeV ($K^{\pi}=3/2^{+}$ band), very small values

(even below the α threshold energy) compared with our previous result for 16 C. Nevertheless, the proposed moment of inertia is compatible with the interpretation as a linear-chain configuration of three α 's with the relative α - α distance of \sim 3 fm (this means the total length of the system is \sim 6 fm), which agrees with the theoretical estimation [19].

In the present study, we introduce a microscopic cluster model to explain this rotational band of 13 C with a linear-chain configuration of three α clusters and a neutron. Here, an orthogonal condition between the cluster states and other low-lying states of 13 C is imposed, which is another mechanism for stabilizing the linear-chain configuration and has not been taken into account in our previous analysis for 16 C. Since shell-model-like configurations are dominant in the lower states of 13 C, the breaking of an α cluster is included.

The total wave function is fully antisymmetrized and is given by a superposition of Slater determinants $\{\Psi_k\}$ with coefficients $\{c_k\}$:

$$\Phi = \sum_{k} c_k P_{MK}^J \Psi_k. \tag{1}$$

Projection onto a good angular momentum (P_{MK}^J) is numerically performed, and the coefficients $\{c_k\}$ are determined by diagonalizing the Hamiltonian matrix after this projection. Each Slater determinant Ψ_k consists of A nucleons,

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

and each nucleon $(\psi_i \chi_i, i=1 \sim A)$ has a local-Gaussian form as in many conventional cluster models. The oscillator parameter $(b=1/\sqrt{2\nu}=1.46~{\rm fm})$ is common for all nucleons to exactly remove the center-of-mass kinetic energy. An α cluster is expressed by assigning a common Gaussian-center parameter for four nucleons (proton spin-up, proton spin-down, neutron spin-up, and neutron spin-down).

As for the Hamiltonian, we use the Volkov No. 2 (V2) effective N-N potential [21] for the central part and the G3RS potential [22] for the spin-orbit part. To reproduce the scattering phase shifts of the $\alpha + n$ and $\alpha + \alpha$ systems, M (Majorana parameter of V2) = 0.6 and V_0 (strength of G3RS) = 2000 MeV should be adopted [23]. Although these parameters give a slight over-binding for the ground states of C isotopes [24], we use these values because we focus on the cluster states around the α threshold energy. Also, values of B = H = 0.125 are introduced for V2 to reproduce the binding energy of the deuteron and to remove the bound state of the neutron-neutron system. By diagonalizing the Hamiltonian, we obtain many states, and it is necessary to analyze which state has the linear-chain configuration.

We introduce a new operator \mathcal{P} as a measure of the "linearity" of the chain configurations,

$$\mathcal{P} = \sum_{i = \text{protons}} P_i, \tag{3}$$

which is the sum of parity-inversion operators for each proton (P_i) . The eigenvalue of P_i is 1 for a proton in a positive-parity orbit and -1 for one in a negative-parity orbit. For example, the expectation value of $\mathcal{P}(\langle \mathcal{P} \rangle)$ for the lowest state of $^{12}\mathrm{C}$ is -2, since two protons occupy the s orbits (eigenvalue of P_i is 1),

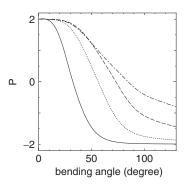


FIG. 1. Expectation value of \mathcal{P} (see text) for the 0^+ states of the three α system (12 C). The horizontal axis is the bending angle of three α . The solid, dotted, dashed, and dash-dotted lines show results with the relative α - α distances of 1, 2, 3, and 4 fm, respectively.

and four protons occupy the p orbits (eigenvalue -1) from the shell-model point of view.

In Fig. 1, the $\langle \mathcal{P} \rangle$ value for the 0⁺ states of the three α system ($^{12}\mathrm{C}$) are presented. Here, the relative distance between the left α cluster and the central one and that between the right α cluster and the central one are taken to be equal (symmetric configuration). The horizontal axis is the bending angle, and 0 and 120 correspond to linear-chain and equilateral triangular configurations of three α clusters, respectively. The solid, dotted, dashed, and dash-dotted lines show the result for the relative α - α distances of 1, 2, 3, and 4 fm, respectively (optimal distance for the linear-chain configuration is 3 fm [19]).

When the system has a linear-chain configuration at 0° , the $\langle \mathcal{P} \rangle$ value is 2 independent of the α - α distance. This is explained in the following way. The single-particle orbits for the protons $\psi(R)$, $\psi(0)$, and $\psi(-R)$ are centered at R, 0, -Ron the z axis, respectively. Because of the antisymmetrization effect, it is possible to rearrange the linear combination of these orbits. The $\psi(0)$ orbit has positive parity, and in addition to this orbit, another positive-parity orbit $[\psi(R) + \psi(-R) +$ $a\psi(0)$, a is a constant value] and a negative-parity orbit $[\psi(R) - \psi(-R)]$, which are orthogonal with each other, can be defined. Thus the $\langle \mathcal{P} \rangle$ value becomes 2 (spin degeneracy) \times (1+1-1)=2 at the bending angle of 0° independent of the α - α distance. With the increase of the bending angle, the $\langle \mathcal{P} \rangle$ values decrease drastically and converge to -2 at large bending angles, since two protons occupy the lowest s orbits and four protons occupy the p(x) and p(z) orbits (2-4=-2). This example illustrates that the value of \mathcal{P} is very useful in characterizing the linear-chain configuration. If the calculated expectation value of P is larger than 1, we can roughly conclude that the bending angle is less than 50° .

In a different viewpoint, the principal quantum number of the harmonic oscillator $[N = \sum_i \vec{a}^\dagger \cdot \vec{a}(\vec{r}_i)]$ for protons is not a good measure of the linear-chain state, as shown in Fig. 2. Although the deexcitation feature of protons with increasing bending angle can be expressed by the $\langle N \rangle$ value (for example, the solid line decreases from 6 to 4 with increasing bending angle), the value has a quadratical dependence on the α - α distance. The wave functions for the localized particles contain higher partial waves if we expand them with respect to the origin. Since this distance dependence is sensitive, the value

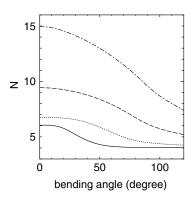


FIG. 2. Expectation value of the principal quantum number of the protons (N) for the 0^+ states of the three α system (12 C). Definitions of the horizontal axis and lines are the same as in Fig. 1.

at 0° for the dashed line (3 fm) is almost the same as that at 90° for the dash-dotted line (4 fm). This situation does not drastically change when we use the quadrupole moment as a measure of the linear-chain state, and it is much more useful to use $\mathcal P$ to characterize the linear-chain configuration.

To characterize the results, we consider the energy convergence of the three 0⁺ states of ¹²C as shown in Fig. 3. The horizontal axis corresponds to the number of the basis states introduced. The basis states of type 1 on the horizontal axis have a $2\alpha + 4N$ configuration, where the breaking effect of one of the α clusters is included using a simplified method to include the spin-orbit interaction (SMSO [25], R = 2 fm, $\Lambda = 0.3$). The states numbered from 2 to 126 have various three α configurations, and we introduce generator coordinates to prepare different configurations. To reduce the number of the basis states, when the inclusion of one Slater determinant decreases the sum of the energies of the three lowest 0^+ states by more than 0.03 MeV, this Slater determinant is adopted in the same way as in the AMD triple-S [26]. The ground 0^+ state is calculated to be at an energy of -92.7 MeV, to be compared with the experimental value of -92.2 MeV. The 0_2^+ state is calculated at 1 MeV above the threshold (three α threshold is shown by the dashed line).

These three 0^+ states are calculated to have the rms radii of 2.33, 3.25, and 3.42 fm, respectively, and the values for

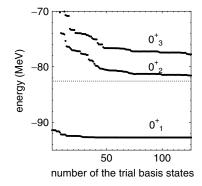


FIG. 3. Energy convergence of three lowest 0^+ states of 12 C. Basis state 1 on the horizontal axis has a $2\alpha + 4N$ configuration (SMSO, R = 2 fm and $\Lambda = 0.3$). Basis states from 2 to 126 have various three α configurations. Dashed line shows the three α threshold energy.

the second and third 0^+ states are large, since they have well-developed cluster structures. The calculated $\langle \mathcal{P} \rangle$ values are -1.70 for the ground state (close to -2 of the shell-model picture) and -0.01 for the second 0^+ state. Since the values are negative, these states are not linear-chain states. On the other hand, the third 0^+ state has a value of 0.75, and this is the candidate for the state with small bending angle. The result is consistent with recent discussions that the third 0^+ state has a banana-like shape of three α clusters [27,28]. However, this state may correspond to the fourth 0^+ state when the resonance condition is properly treated, as discussed in Ref. [29].

Similar calculations have been further performed for the K = 3/2 states of ¹³C, since the lowest orbit around the three α with the linear-chain configuration is a π orbit with $K^{\pi} = 3/2^{-}$. Here, generator coordinates are introduced for the three α configurations, and the positions of the Gaussian center parameter of the valence neutron are randomly generated. We introduce 160 Slater determinants, and the selection of the important basis states is performed in the same way as in 12 C for each J^{π} state independently. Out of the many obtained energy levels, the states with positive expectation values for the operator \mathcal{P} are plotted with respect to the $3\alpha + n$ threshold energy (-82.71 MeV in this model, experimentally $E_x = 12.2$ MeV in ¹³C) as solid circles in Fig. 4. The obtained states almost form a rotational band structure, and the moment of inertia agrees with the experimental one, although the theoretical bandhead energy is higher by several MeV compared with the experimental one. The states at $1.70 (3/2^{-}), 3.13 (5/2^{-}), 5.81 (7/2^{-}), 6.23 (9/2^{-}), and$ $9.25 \text{ MeV} (11/2^{-})$ with respect to the threshold have overlaps with the linear-chain configuration of 0.80, 0.82, 0.69, 0.86, and 0.87, respectively. The values indicated in this figure show the calculated $\langle \mathcal{P} \rangle$ values of individual states. Except for the $7/2^-$ state, the states have similar values around 1.5. Therefore, it can be concluded that by allowing a small bending angle, the linear-chain configuration of three α clusters is stabilized by a valence neutron and appears in the $E_x = 15$ MeV excitation energy region around the α threshold energy. The same analysis has been done for the positive-parity $(K^{\pi} = 3/2^{+})$ band. It is considered that the neutron occupies the ungerade? π orbit. Since the valence neutron has two nodes, this band appears above the negative-parity band by several MeV. The

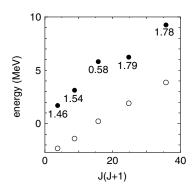


FIG. 4. $K^{\pi}=3/2^-$ rotational band of ¹³C (theoretical results: solid circles; experimental: open circles). Measured from the $3\alpha+n$ threshold energy at $E_x=12.2$ MeV.

bandhead state $(3/2^+)$ at 7.85 MeV from the threshold has the $\langle \mathcal{P} \rangle$ value of 0.73 and an overlap with the linear-chain state of 0.64. The moment of inertia is almost the same as the negative-parity band; however, further investigation (e.g., explicitly imposing the resonance condition) is needed, since the resonance energy is high. Experimentally, these are two parity split bands with K=3/2, corresponding to an intrinsic $^9\mathrm{Be} + \alpha$ structure. The single-particle orbit of neutrons for these doublet bands is discussed in Ref. [20], and such an analysis is in progress based on the present method. The $\langle \mathcal{P} \rangle$ value can be calculated also for the neutron part, and by subtracting the proton part from the neutron part, the single-particle parity of the valence neutron can be extracted, since the information on the three α clusters vanishes.

To conclude, we have investigated a linear-chain configuration of three α clusters stabilized by adding a neutron in 13 C. An operator \mathcal{P} , which is the sum of the parity inversion operators for each proton, has been introduced and found to be very useful in characterizing the linear-chain configuration. The linear-chain structure with a small bending angle appears around the α threshold energy, and the moment of inertia agrees well with the experimentally suggested value. Thus the calculation confirms the experimental result of a hyper-deformed rotational band in 13 C.

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