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# Alpha clustering near nuclear surface and harmonic-oscillator excitations

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**Abstract.** We quantify how it is difficult to describe an alpha($\alpha$)-cluster state with single-particle harmonic-oscillator (HO) bases in the low-lying $^{16}$O states by counting the number of HO quanta of $^{12}$C+$n$+$n$+$p$+$p$ five-body wave functions. We also discuss how many HO quanta are needed for describing a localized $\alpha$ cluster near the nuclear surface towards understanding of the shell and cluster coexistence in heavier nuclei.

## 1. Introduction

One of the characteristic features of an atomic nuclear system is coexistence and competition of the shell and cluster structure. Especially, describing a localized $\alpha$ clustering near the nuclear surface is essential to understand excitations of light nuclei as well as $\alpha$-decay phenomena in heavy nuclei. Since these two different aspects are often studied with the different models, a unified description is desired for deep understanding of the nuclear clustering phenomena.

A simultaneous description of the ground and the first excited $0^+$ states in $^{16}$O is one of the most famous and long-standing problems in nuclear theory. Calculations based on nuclear shell model have still been difficult to describe them even in present-day large-scale calculations [1, 2]. Among many efforts for resolving the problem, Ref. [3, 4] showed that both the ground and first excited $0^+$ states could be understood naturally if $^{12}$C+$\alpha$ cluster structure was considered.

Recently we showed that both the $0^+$ states were described very well with a $^{12}$C+$n$+$n$+$p$+$p$ five-body model [5]. Five-body dynamics with Pauli constraint from the $^{12}$C core was fully taken into account by using explicitly correlated Gaussian bases with use of stochastic sampling for huge number of variational parameters. We concluded that, without an assumption of the $\alpha$ cluster, the first excited state had well-developed $^{12}$C+$\alpha$ cluster structure.

In this contribution, we quantitatively discuss how it is difficult to describe the nuclear $\alpha$-clustering near nuclear surface by means of the HO excitations. In the next section, we briefly explain the explicitly correlated Gaussian method. The results of the $^{12}$C+$n$+$n$+$p$+$p$ five-body model calculations are reviewed in Sec. 3. With counting the number of HO quanta, we quantify the difficulty of representing the cluster state with the shell-model basis. In Sec. 3, we discuss how many HO quanta are needed to have an $\alpha$-cluster near the nuclear surface by using a simple $\alpha$-cluster model wave function. Conclusions and future perspectives are given in Sec. 4.

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## 2. Correlated Gaussian method

In order to study the nuclear clustering and shell structure in a unified manner, here we take a powerful and a flexible few-body approach, that is, correlated Gaussian (CG) method [6, 7, 8]. Many examples have confirmed that the method can describe complex few-body dynamics, e.g., describing different types of structure and correlated motion of the particles, and accurately describing the tail of the wave function in the asymptotic region. The method has been applied not only to nuclear physics but also other quantum mechanical fields (See recent review [9]). Our strategy to understand the coexistence of the cluster and shell structure is the following: First, we choose degrees of freedom of interest and determine the Hamiltonian. Two-body interactions are chosen consistently with properties of the two-body system, e.g., energy, phase-shift. Once the Hamiltonian is determined, the many-body Schrödinger equation is accurately solved without recourse to any many-body approximation. Appearance and distortion of clusters are naturally taken into account within the degrees of freedom chosen in the calculation.

A nuclear system is specified by the angular momentum $J$, its $z$ component $M_J$, parity $\pi$, and isospin quantum numbers $T$, $M_T$. The total wave function is expressed by a combination of various components of orbital and spin angular momenta. Here the basis function we use takes a general form in the $LS$ coupling scheme

$$\Phi^{\pi}_{(LS)JM_J,TM_T} = \mathcal{A}\left\{[\phi^{\pi}_L \times \chi_S]_{JM_J}\,\eta_{TM_T}\right\}, \tag{1}$$

where $\mathcal{A}$ is the antisymmetrizer for nucleons, and the symbol $[\phi^{\pi}_L \times \chi_S]_{JM_J}$ stands for angular momentum coupling. The total spin (isospin) function $\chi_S$ ($\eta_T$) is constructed by a successive coupling of all spin (isospin) functions of a nucleon.

For the spatial part of the basis function, $\phi^{\pi}_L$, we use the CG. Let $\boldsymbol{x}$=($\boldsymbol{x}_i$) denote a set of the Jacobi coordinates excluding the center-of-mass coordinate. We express $\phi^{\pi}_L$ as a combination of CG [6, 7] and the two global vectors [8]

$$\phi^{\pi}_{(L_1L_2)LM_L}(A,u_1,u_2) = \exp(-\tilde{\boldsymbol{x}}A\boldsymbol{x})[\mathcal{Y}_{L_1}(\tilde{u}_1\boldsymbol{x}) \times \mathcal{Y}_{L_2}(\tilde{u}_2\boldsymbol{x})]_{LM_L} \tag{2}$$

with a solid harmonic $\mathcal{Y}_\ell(\boldsymbol{r}) = r^\ell Y_\ell(\hat{\boldsymbol{r}})$. Here $\tilde{\boldsymbol{x}}A\boldsymbol{x} = \sum_{i,j} A_{ij}\boldsymbol{x}_i\cdot\boldsymbol{x}_j$ and $\tilde{u}_i\boldsymbol{x} = \sum_k (u_i)_k\boldsymbol{x}_k$, where the positive-definite symmetric matrix $A$, the vectors of $u_1$ and $u_2$ are variational parameters. It is noted that all coordinates are explicitly correlated through them. Both $u_1$ and $u_2$ define the global vectors, $\tilde{u}_1\boldsymbol{x}$ and $\tilde{u}_2\boldsymbol{x}$, that are responsible for the rotational motion of the system. With the two global vectors, any $L^\pi$ states except for $0^-$ can be constructed with a suitable choice of $L_1$ and $L_2$. An advantage of the CG is that it keeps its functional form under a linear transformation of the coordinates [6, 7], which is a key for describing both the cluster and shell structure in a unified manner.

## 3. $\alpha$ clustering near the nuclear surface

### *3.1. The low-lying $0^+$ states of $^{16}O$*

A $^{12}$C+$n+n+p+p$ five-body model successfully describes the ground and first excited $0^+$ states of $^{16}$O [5]. Here we review Ref. [5] and discuss how the cluster state is represented by the HO excitations. The five-body system is characterized by the Hamiltonian which consists of an $NN$ potential for valence nucleons and a $^{12}$C-nucleon ($CN$) potential. A central Minnesota (MN) potential [10] is employed as the $NN$ potential. To fine tune the binding energy of the $\alpha$ particle, the potential strengths are multiplied by 0.9814. Symmetrized Woods-Saxon and its derivative forms are assumed for the central and spin-orbit $CN$ potential, respectively. Their parameters are determined so as to reproduce the low-lying spectrum of $^{13}$C with $1/2^-$, $1/2^+$, and $5/2^+$. Our $CN$ potential is deep enough to accommodate some redundant or Pauli-forbidden states. To eliminate such states we impose the orthogonality constraint for the relative

motion of the valence nucleons, which is practically achieved by adding a pseudo potential to the Hamiltonian [11]. Here we assume the HO wave functions of $0s_{1/2}$ and $0p_{3/2}$ as the occupied orbits of $^{12}$C. The HO frequency is set to be 16.0 MeV, which reproduces the size of the $^{12}$C ground state. The core excitation of $^{12}$C may be included, for example, based on a collective model [12]. However, for the sake of simplicity, the core excitation is ignored in this calculation.

We express the wave function in terms of a linear combination of many basis states of Eq. (1). Each basis element contains so many variational parameters that discretizing them on grids leads to an enormous dimension of at least $10^{10}$. The stochastic variational method [6, 7] provides us with an efficient way to obtain an accurate solution with reducing the number of bases. We test a number of candidate bases with stochastic sampling and select the best one among them, and increase the basis dimension one by one until the convergence is reached.

Energy convergence is very slow and more than 9000 basis states were required [5]. This number is very large compared to a four-nucleon system with the same MN interaction that requires only few tens of basis states [6]. The present problem belongs to a class of quantum few-body problem with orthogonality constraints, which often appears in atomic and subatomic physics when the system contains composite particles [7]. Solving such a problem is quite challenging. In the present case, the most basis states are used for eliminating the forbidden states. Since the valence nucleons are strongly correlated, the basis states may have a large overlap with the forbidden states, and thus many basis states are needed to get a converged solution. After the convergence two $0^+$ states appear below the $^{12}$C+$\alpha$ threshold and their energies are both remarkably close to experiment [5].

For quantitative discussion of the clustering degree, we calculate the $^{12}$C+$\alpha$ spectroscopic amplitude of $^{16}$O (See Fig. 3 of Ref. [5]). For the $0^+_1$ state, the highest peak is located below the touching distance of $^{12}$C+$\alpha$ ($\sim$ 5.9 fm). In such a case, the $\alpha$ particle is strongly distorted by the core nucleus. In fact, a spectroscopic factor (SF), is small (0.105), whereas the $^{12}$C+$\alpha$-cluster-model calculation gives 0.300 [3]. In this study, we do not assume the $\alpha$ cluster, and thus the distortion of the $\alpha$ cluster shows up naturally. In the $0^+_2$ state, the amplitude is much larger than that of the $0^+_1$ state and peaked at the touching distance of $^{12}$C+$\alpha$, showing very long tail which suggests the well developed $\alpha$-cluster structure. The SF is 0.680 which is in agreement with the value of the $^{12}$C+$\alpha$ calculation, 0.679. The phase space of the first excited state of $^{16}$O is exhausted by the $^{12}$C+$\alpha$ cluster component.

Why is it so difficult to describe the $0^+_2$ state with the ordinary shell model truncation? To answer this, it is useful to calculate the probability distribution of the total HO quanta $Q$ in our wave functions (See Fig. 4 of Ref. [5]). The oscillator frequency is set to be the same as the forbidden states in the $^{12}$C core. For the ground state, the distribution starts with $Q = 4$, which may correspond to the configuration of $(0p_{1/2})^2_\nu(0p_{1/2})^2_\pi$. The distribution converges rapidly with increasing $Q$. Since a few major shell configurations, $Q \leq 8$, are required to cover more than 90% of the model spaces, the state may be described with the shell model picture.

As predicted by the cluster model [3, 4], the distribution of the first excited state of $^{16}$O is quite different from the ground state. Since the ground state exhausts the $Q = 4$ component, the component for the excited state becomes small approximately 10%. The HO quanta are again peaked at $Q = 12$ and widely distributed showing still undiminished probability even at $Q = 30$. One needs at least $Q = 26$ to cover more than 90% of our model space. Therefore, it is practically difficult to describe such a state by the HO basis with the usual major shell truncation.

The $\alpha$-cluster structure is a key to understand $N = Z$ and doubly closed nuclei. Interestingly, $^4$He itself also exhibits the coexistence of shell and cluster structure in its spectrum [13]. The first excited state is $0^+$ as like $^{16}$O and parity inverted partners are actually observed. Similarly to the $^{16}$O case, if one considers the cluster excitation of $3N + N$ ($^3$He+$n$ and $^3$H+$p$), the first excited state can be regarded as the excitation of the relative motion function between $3N$ and

$N$. Differently from the case of $^{16}$O, the two cluster have the spin and isospin degrees of freedom, and thus seven negative parity states are possible having $3N+N$ with the $P$-wave relative motion, excluding the center-of-mass excitation with $T = 0$ state. In fact, the occupation probability of the HO quanta for those states show extended distributions indicating the $(3N + N)$-cluster structure [14]. For the $0^+_2$ state, the high $Q$ component is used for describing the $S$-wave relative motion wave function between $3N$ and $N$. Inversion doublet partners also need high $Q$ components in order to describe the asymptotic behavior of the $P$-wave relative motion wave function.

*3.2. HO components of $\alpha$-cluster wave function near nuclear surface*

Let us consider more about the role of the HO components to describe such cluster states with a simple $\alpha$-cluster wave function. Detailed discussions are given in the recent review book [15]. We assume that a $(0s)^4$-$\alpha$ cluster located at position $\boldsymbol{s}$ is represented by the product of the Gaussian-wave packet with width parameter $\nu^{-1/2}$

$$\phi^{\nu}_{\boldsymbol{s}}(\boldsymbol{r}) = \left(\frac{2\nu}{\pi}\right)^{3/4} \exp(-\nu(\boldsymbol{r}-\boldsymbol{s})^2). \tag{3}$$

The spin- and isospin-wave functions are totally antisymmetrized. Therefore, the spacial part of the wave function is totally symmetric. The probability that $\phi^{\nu}_{\boldsymbol{s}}$ contains shell model orbits with the orbital angular momentum $l$ is calculated by

$$P_{\eta}(l) = \sum_{m=-l}^{l} \frac{1}{4\pi} \int d\hat{\boldsymbol{s}} \int_0^{\infty} dr r^2 |\, \langle Y_{lm}(\hat{\boldsymbol{r}}) | \phi^{\nu}_{\boldsymbol{s}}(\boldsymbol{r}) \rangle \,|^2 = (2l+1) i_l(\eta) e^{-\eta}, \tag{4}$$

where $i_l(z)$ is the modified spherical Bessel function, and $\eta = \nu s^2$ is a dimensionless quantity which can be a measure of spatial localization of the cluster. In case that the cluster size is the free-$\alpha$ particle ($\nu = 0.26$ fm$^{-2}$), $\eta$ quickly increases, while if $\nu$ is taken to be the standard value, $\nu = 0.48A^{-1/3}$ fm$^{-2}$, $\eta$ gradually increases. Now we put the free-$\alpha$ particle around the nuclear surface at $|\boldsymbol{s}| = 1.1A^{1/3}$ fm. In cases of $^{16}$O ($\eta = 2.0$) and $^{212}$Po ($\eta = 11$), cumulative sum $\sum_{l=0}^{l_{\max}} P_{\eta}(l)$ exceeds 80% at $l_{\max}$ =3 and 6 for $\eta = 2.0$ and 11, respectively.

Applying this analysis to the $(0s)^4$-$\alpha$-cluster wave function, we can discuss partial-wave components of the wave function [15]. For $^{16}$O case, $l_{\max} = 2$ is required for satisfying about 90% of the probability following the distribution in Eq. (4). The most of HO quanta are used to describe the spatial extent of the $^{12}$C+$\alpha$ $S$-wave relative motion wave function rather than increasing the partial angular momentum. This information will be a guide to a theoretical description of the $\alpha$ clustering. In case of $^{212}$Po, a famous $\alpha$ emitter, higher partial wave ($l_{\max} = 7$) is required to describe the surface clustering around the $^{208}$Pb core.

## 4. Summary and future perspectives

Applying the $^{12}$C+$n$+$n$+$p$+$p$ five-body model to the low-lying spectrum of $^{16}$O, we succeeds in describing both the shell-model and cluster configurations in a unified scheme. By counting the number of the harmonic-oscillator (HO) quanta of the realistic five-body wave functions as well as the simple $\alpha$-cluster ones, we quantify how it is difficult to describe the cluster configurations with the HO shell-model basis.

It is interesting to study the $\alpha$ clustering in the other spin-parity states of $^{16}$O as important inputs for astrophysical reactions. A description of the $\alpha$ decay of $^{212}$Po has of particular interest as a typical phenomena of $\alpha$-clustering near the nuclear surface. Those projects are underway and will be reported, hopefully, in the next Cluster conference.

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