

## Five-body calculation with Pauli constraint for shell- and cluster-structure in $^{16}\text{O}$

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**Abstract.** A  $^{12}\text{C}$ +four-nucleon ( $4N$ ) five-body model is applied for the ground and first excited states of  $^{16}\text{O}$ . The  $4N$  configurations are selected in a wide Hilbert space under the fulfillment of the Pauli principle excluding the occupied orbits in  $^{12}\text{C}$ . The energies of both the states are obtained in excellent agreement with experiment. Analysis of the wave functions indicates a spatially localized alpha-particle-like cluster structure for the excited state and a shell-model-like delocalized structure for the ground state. The difficulty of describing the cluster structure by a standard shell model approach is discussed by calculating components of the harmonic-oscillator quanta in the wave functions.

### 1 Introduction

A simultaneous description of the ground and first excited  $0^+$  states of  $^{16}\text{O}$  is one of the outstanding and challenging problems in nuclear theory. Since a fully microscopic calculation is not practical at present, it is interesting to perform the  $^{12}\text{C}+4N$  five-body calculation without assuming an alpha ( $\alpha$ ) cluster [1]. The five-body dynamics is solved with the stochastic variational method on the correlated Gaussian (CG) reinforced with global vectors [2–4]. No restriction is imposed on the  $4N$  configurations except for the Pauli principle excluding the occupied orbits in  $^{12}\text{C}$ . This problem belongs to a class of quantum few-body problems with orthogonally constraints and often appears in atomic and subatomic physics when the system contains composite particles. Solving such a problem is quite challenging if the system has more than four particles. In this paper, we present our recent application of the CG method to  $^{16}\text{O}$ , as well as  $^{16}\text{C}$  with a  $^{12}\text{C}+4N$  five-body model with Pauli constraint.

### 2 Hamiltonian and correlated Gaussian method

A five-body system we consider here is characterized by the Hamiltonian which consists of an  $NN$  potential for valence nucleons and a  $^{12}\text{C}$ -nucleon ( $CN$ ) potential. The interactions between the constituent particles are chosen consistently with the energies of bound subsystems, especially  $^{12}\text{C}-N$  and  $\alpha$  particle [1]. The  $CN$  potential is determined so as to reproduce the low-lying spectrum of  $^{13}\text{C}$  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 [5]. Here we assume the harmonic-oscillator (HO) wave functions of  $0s_{1/2}$  and  $0p_{3/2}$  as the occupied orbits of  $^{12}\text{C}$ .

We express the five-body wave function with total angular momentum  $J$  in terms of a linear combination of many CG basis states of the following form

$$\Psi_{JM} = \mathcal{A} \left\{ \exp[-\tilde{\mathbf{x}}A\mathbf{x}] \left[ \left[ \mathcal{Y}_{L_1}(\tilde{u}_1\mathbf{x})\mathcal{Y}_{L_2}(\tilde{u}_2\mathbf{x}) \right]_L \chi_S \right]_{\mathcal{J}} \phi_I(^{12}\text{C}) \right\}_{\mathcal{J}M_{\mathcal{J}}} \eta_{TM_T}, \quad (1)$$

where  $\mathcal{A}$  is an antisymmetrizer,  $\mathcal{Y}_L(\mathbf{r})$  is a solid spherical harmonic. The  $\chi_{SM_S}(\eta_{TM_T})$  is the spin (isospin) function of the valence nucleons. The  $\phi_I(^{12}\text{C})$  is the wave function of the core nucleus. In this calculation, the core excitation is ignored, and  $I$  is set to be 0. The  $\mathbf{x}$  denotes the 4-dimensional vector whose element is the 3-dimensional Jacobi coordinate excluding the center-of-mass coordinate of the  $A = 16$  system. The  $4 \times 4$  matrix  $A$  and 4-dimensional vectors  $u_1$  and  $u_2$  are variational parameters to be optimized and a tilde denotes a transpose of a matrix. It is noted that all coordinates are explicitly correlated. An advantage of this method is that its functional form does not change under any coordinate transformation, and thus both cluster- and shell-model like configurations can be expressed in a single scheme. Because of this flexibility the method have been applied to many quantum mechanical systems (See recent review [6]).

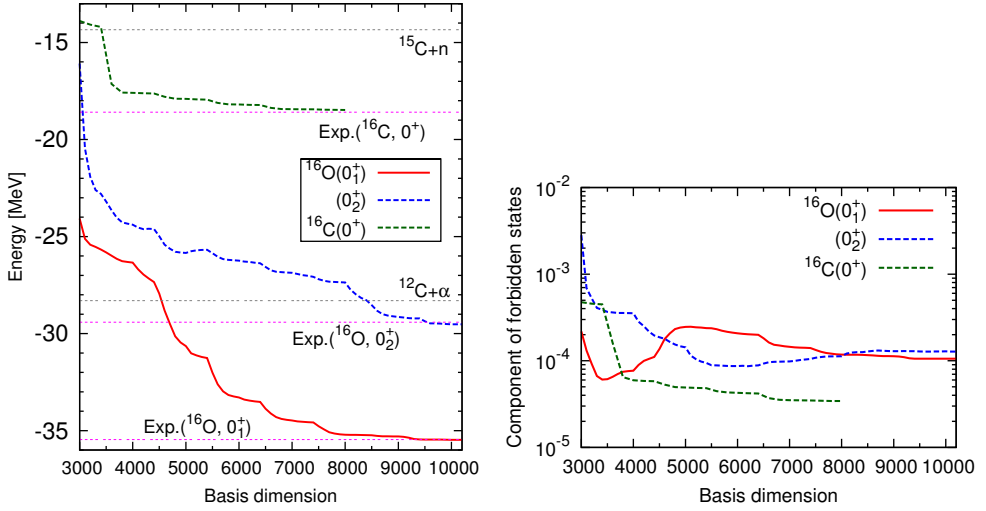
We expand the wave function in terms of a linear combination of many CG states of Eq. (1). Each basis element contains so many variational parameters that discretizing them on grids leads to an enormous dimension of at least  $10^{10}$ . Thus we test a number of candidate bases with the stochastic variational method [2, 3]. We select the best one among them and increase the basis dimension one by one until a convergence is reached. This procedure is expensive as far as computer time is concerned, but no other viable methods are at hand to get converged solutions for the present problem.

### 3 Results

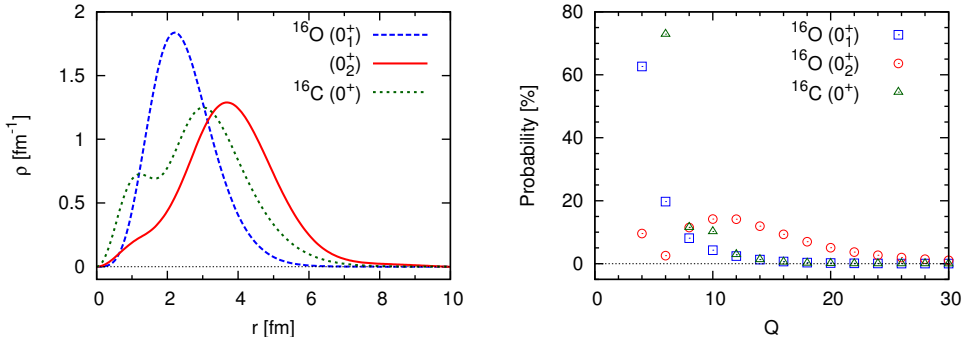
The left panel of Fig. 1 displays the calculated energy curves of the ground ( $0_1^+$ ) and first excited ( $0_2^+$ ) states of  $^{16}\text{O}$  as well as the ground state of  $^{16}\text{C}$  as a function of the number of basis functions. Convergence is very slow and more than 9000 basis states are needed. This number is very large compared to a four-nucleon system with the same  $NN$  interaction that requires only few tens of basis states [2]. The most basis states are used for eliminating the forbidden states.

The right panel of Fig. 1 plots the components of the forbidden states in the  $A = 16$  wave functions. The components gradually decrease as increasing the basis dimension. The values are around  $10^{-4}$  at 4000 basis dimension which corresponds to the ground state energy of  $^{16}\text{O}$  crosses the  $^{12}\text{C}+\alpha$  threshold. The case of  $^{16}\text{C}$  is easier than that of  $^{16}\text{O}$  because the valence neutrons do not form a strongly bound cluster. The energy curve of  $^{16}\text{C}$  is converged at 7000 basis states and the energy appears very closely to the experiment. When the valence nucleons form a cluster, the basis states may have a large overlap with the forbidden states, and thus more basis states are needed to get a converged solution. In fact, the components of the forbidden states decrease monotonically beyond 4000 basis in the case of  $^{16}\text{C}$ , whereas the two  $0^+$  states in  $^{16}\text{O}$  show some oscillatory behaviors. For the ground state, the components decrease and show a rapid rise from 4000 basis. After the peak, they decrease again. For the excited state, the behavior is opposite to that of the ground state. The components decrease up to about 6000 basis and increase gradually. Finally, the two  $0^+$  states appear below  $^{12}\text{C}+\alpha$  threshold and their energies are both remarkably close to experiment.

To see the spatial correlations in the  $A = 16$  system, we display, in the left panel of Figure 2, the density distributions of the valence nucleons,  $\rho(\mathbf{r}) = \sum_{i=1}^4 \langle \Psi_{00} | \delta(|\mathbf{r}_i - \mathbf{x}_5| - r) | \Psi_{00} \rangle$ , where the  $\mathbf{x}_5$  is the center-of-mass coordinate. For the ground state of  $^{16}\text{O}$  shows single-peaked structure, which is



**Figure 1.** Left: Energy curves for the  $A = 16$  systems. The calculated thresholds and experimental energies are plotted with thin lines. The figure is plotted based on the data of Ref. [1]. Right: Components of the forbidden states for the  $A = 16$  systems as a function of the number of basis dimensions.



**Figure 2.** Left: Density distributions of the valence nucleons of the  $A = 16$  systems. Right: Occupation probability of the numbers of the total HO quanta,  $Q$ . The figure is plotted based on the data of Ref. [1].

consistent with the configuration of  $(0p_{1/2})_v^2(0p_{1/2})_\pi^2$  dominance. Double-peaked structure of the  $^{16}\text{C}$  may be due to the configuration of either  $(0p_{1/2})_v^2(1s_{1/2})_v^2$  or  $(0p_{1/2})_v^2(0d_{j=2})_v^2$ . For the first excited state of  $^{16}\text{O}$ , the peak position is located beyond the surface of  $^{12}\text{C}$  ( $\sim 3.3$  fm) showing somewhat dilute distribution, which may not be expressed by simple shell model configurations.

For a quantitative discussion of the clustering degree, the spectroscopic amplitude of  $^{16}\text{O}$  was calculated in Ref. [1]. For the ground state, the amplitude peaks at inside of  $^{12}\text{C}$ , and a spectroscopic factor of the  $^{12}\text{C}+\alpha$  is small (0.105), whereas the  $^{12}\text{C}+\alpha$  cluster model calculation gives 0.300 [7]. In such a case, the  $\alpha$ -cluster is strongly distorted. Here 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 and peaked at the touching distance of  $^{12}\text{C}+\alpha$ , showing very long tail which suggests the well developed cluster structure. The spectroscopic factor is 0.680 which is in agreement with the value of the  $^{12}\text{C}+\alpha$  calculation, 0.679. The phase space of the first excited state of  $^{16}\text{O}$  is exhausted by the  $^{12}\text{C}+\alpha$  cluster component.

It is interesting to calculate the probability distribution of the total HO quanta  $Q$  in our wave functions. The right panel of Fig. 2 plots the HO quanta for the ground states of  $^{16}\text{C}$  and  $^{16}\text{O}$ , and first excited states of  $^{16}\text{O}$ . Oscillator frequency is set to be the same as the forbidden states in the  $^{12}\text{C}$  core. For the ground state of  $^{16}\text{C}$ , the distribution starts with  $Q = 6$ , which may correspond to the configuration of either  $(0p_{1/2})_v^2(1s_{1/2})_v^2$  or  $(0p_{1/2})_v^2(0d_j)_v^2$ . The distribution diminishes rapidly with increasing  $Q$ . For the ground state of  $^{16}\text{O}$  the distribution starts with  $Q = 4$ , which may correspond to the configuration of  $(0p_{1/2})_v^2(0p_{1/2})_v^2$ . The distribution also diminishes rapidly with increasing  $Q$ . For both the ground states of  $^{16}\text{O}$  and  $^{16}\text{C}$  a few major shell configurations are required to cover more than 90% of the model spaces, therefore the states may be described with the shell model picture.

As predicted by the cluster model [7], the distribution of the first excited state of  $^{16}\text{O}$  is quite different from these states. Since the ground state exhausts the  $Q = 4$  component, the component for the excited state becomes small approximately 10%. The HO quanta are peaked at  $Q = 12$  and widely distributed showing still undiminished probability at  $Q = 30$ . If we can cover the HO model space up to the peak position  $Q = 12$ , accumulated probability is still 47%. Therefore, it is practically difficult to describe such a state by the HO basis with the usual major shell truncation. One needs at least  $Q = 26$  to cover more than 90% of our model space which is not feasible at present.

## 4 Summary and conclusions

A  $^{12}\text{C}$ +four-nucleon five-body model is applied to the  $A = 16$  systems. The full five-body Schrödinger equation with Pauli constraint is solved by superposing many CG states prescribed with the stochastic variational method. The calculated total binding energies for the ground state and first excited states of  $^{16}\text{O}$  are obtained consistently with the experimental values. The ground state exhibits a shell model like structure, whereas our analyses suggest the first excited states has a well developed  $^{12}\text{C}+\alpha$  cluster structure. The probability distributions of the total harmonic-oscillator quanta also support our pictures and show the difficulty in describing the  $0_2^+$  state with the ordinary major shell truncation of the harmonic-oscillator basis. Future plans include an application to the other  $J^\pi$  states as well as an extension of the model with heavier doubly closed shell core.

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