

Dynamics of nuclear four- and five-body systems with correlated Gaussian method

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Abstract. We report our recent applications of the correlated Gaussian (CG) method to nuclear four- and five-body systems: (I) Spin-dipole response functions of ^4He and (II) ^{16}O as a $^{12}\text{C}+n+n+p+p$ five-body model. The CG is flexible to describe complex few-nucleon dynamics. The above examples actually demonstrate the power of the CG, giving a simultaneous description of both four-nucleon bound and unbound states using a realistic nuclear force, and both shell- and cluster-configurations in the ground and first excited 0^+ states of ^{16}O .

1. Introduction

Since the wave function has all information of a non-relativistic quantum system, we try to solve the many-body Schrödinger equation as precise as possible within present computational resources. A correlated Gaussian (CG) method is powerful and flexible to 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 to not only in nuclear physics but also in other quantum mechanical fields (See recent review [1]). Here we present our progress and recent applications of the CG method to nuclear four- and five-body systems.

In the first topic, we calculate the spin-dipole (SD) response functions of ^4He [2] with a full four-body calculation using realistic nuclear forces. The excited states of ^4He are all in the continuum and are treated properly with the complex scaling method. The SD operator belongs to the first-forbidden transition induced by the weak interaction and is expected to play a significant role for neutrino- ^4He reactions. The SD operator can change the spin wave function of the ground state and has three possible multipoles. We show that these properties of the SD operator can be used to probe the role of noncentral forces, especially the tensor force.

The second topic is a $^{12}\text{C}+n+n+p+p$ five-body calculation for the spectrum of ^{16}O [3]. A simultaneous description of the ground and first excited 0^+ states of ^{16}O is one of the outstanding and challenging problems in nuclear theory. The ground state of ^{16}O has been recognized as having a doubly closed shell model configuration, and thus the first excited state is expected to have the negative parity state in accordance with the particle-hole excitation but actually observed as 0^+ state. Many theoretical works are devoted to understand this ‘mysterious’ state, however, the state has not been reproduced microscopically even in modern large scale



calculations [4]. Since a fully microscopic calculation is not practical at present, it is interesting to perform the five-body calculation without assuming an alpha cluster.

The paper is organized as follows: Section 2 briefly explain the CG method used in this paper. Two recent applications of the nuclear four- and five-body systems are presented in Section 3. In Section 3.1 the calculation of the SD strength functions are presented. We show the possibility to probe the tensor correlations with the SD excitations. Section 3.2 presents converged results of a ^{12}C +four-nucleon five-body calculation and discusses the coexistence of shell- and cluster-configurations in the spectrum of ^{16}O . Summary and conclusions are given in Section 4.

2. Correlated Gaussian method

A trial wave function in a variational method for nuclear few-body problems has to be flexible enough to cope with the short-range repulsion and strong tensor force as well as different types of structure and correlated motion of the particles. A total wave function with the angular momentum J , its z component M_J , parity π , and isospin quantum numbers T , M_T is expressed as a combination of various components of orbital and spin angular momenta. Here the basis function we use takes a general form in LS coupling scheme

$$\Phi_{(LS)JM_J, TM_T}^\pi = \mathcal{A}[\phi_L^\pi \times \chi_S]_{JM_J} \eta_{TM_T}, \quad (1)$$

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

For the spatial part of the basis function, ϕ_L^π , we use the CG. Let $\mathbf{x}=(\mathbf{x}_i)$ denote a set of the Jacobi coordinates excluding the center-of-mass coordinate. We express ϕ_L^π as a combination of CG [5, 6] and the two global vectors [7]

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

with a solid harmonic $\mathcal{Y}_\ell(\mathbf{r}) = r^\ell Y_\ell(\hat{\mathbf{r}})$. Here $\tilde{\mathbf{x}} A \mathbf{x} = \sum_{i,j} A_{ij} \mathbf{x}_i \cdot \mathbf{x}_j$ and $\tilde{u}_i \mathbf{x} = \sum_k (u_i)_k \mathbf{x}_k$, 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, $\tilde{u}_1 \mathbf{x}$ and $\tilde{u}_2 \mathbf{x}$, that are responsible for the rotational motion, as shown in Eq. (2). When a realistic nucleon-nucleon (NN) potential is used, the tensor force mixes different angular momentum components in the wave function. With the two global vectors, any L^π states but 0^- can be constructed with a suitable choice of L_1 and L_2 . The power of the CG basis of type (2) has been demonstrated by many examples [7, 8, 1]. An advantage of the CG is that it keeps its functional form under a linear transformation of the coordinates [5, 6], which is a key for describing both cluster and delocalized structure in a unified manner.

3. Application to nuclear four- and five-body systems

3.1. Electroweak response functions of ^4He

The Hamiltonian of four-nucleon system consists of two- and three-nucleon forces. As an NN potential, we employ the Argonne $v8'$ [9] ($\text{AV}8'$) potential which contain central, tensor and spin-orbit components. The central component includes a strong short-ranged repulsion near the origin. We add a phenomenological three-body interaction (3NF) [10] that is set to reproduce the binding energies of the three- and four-nucleon bound states.

A spin-dipole (SD) response function of interest is given by

$$S(p, \lambda, E) = \mathcal{S}_{f\mu} |\langle \Psi_f | \sum_{i=1}^4 [\boldsymbol{\rho}_i \times \boldsymbol{\sigma}_i]_{\lambda\mu} T_i^p | \Psi_0 \rangle|^2 \delta(E_f - E_0 - E) \quad \text{with} \quad \boldsymbol{\rho}_i = \mathbf{r}_i - \mathbf{x}_4, \quad (3)$$

where \mathbf{r}_i is i th nucleon coordinate, \mathbf{x}_4 is the center-of-mass coordinate of the four-nucleon system, and $\boldsymbol{\sigma}_i$ is i th nucleon spin. The SD operator is specified by $\lambda\mu$ with the angular momentum coupling of $\boldsymbol{\rho}_i$ and $\boldsymbol{\sigma}_i$. The superscript p of T_i^p distinguishes different types of isospin operators, isoscalar ($p = \text{IS}$) and isovector ($p = \text{IV0}$). The Ψ_0 (Ψ_f) is the ground (final) state of ${}^4\text{He}$ with the energy E_0 (E_f), and $\mathcal{S}_{f\mu}$ denotes a summation over all final states and μ . For the continuum wave function, we use a square-integrable (\mathcal{L}^2) basis function which does not satisfy a proper boundary condition of continuum state. To treat it properly, we use the complex scaling method (CSM) which is a widely used method for calculating the strength function in a nuclear system [11]. The accuracy of the CSM calculation crucially depends on how completely the \mathcal{L}^2 basis functions are prepared. We attempt at constructing the basis paying attention to two points: the sum rule of the electroweak strength functions and the decay channels [12, 2].

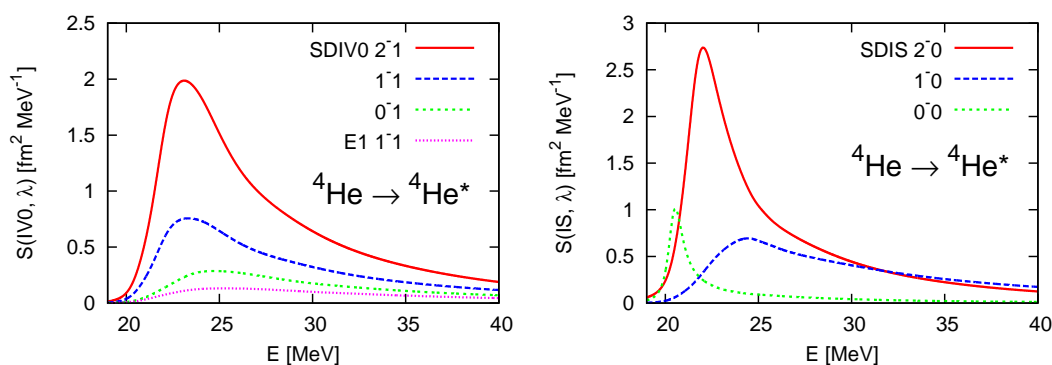


Figure 1. Left: Isovector SD strength functions of IV0 type and $E1$ strength function for ${}^4\text{He}$ as a function of excitation energy. The AV8' + 3NF potential is used. Right: The same plot as the left but isoscalar SD strength functions of IS type. The figures are plotted based on Ref. [2].

The left panel of Fig. 1 plots the SD strength functions of IV0 type with the AV8' + 3NF potential. For the sake of comparison, the electric dipole ($E1$) strength function is also plotted by choosing the $E1$ operator as $\sum_{i=1}^N \boldsymbol{\rho}_{i\mu} \frac{1}{2}(1 - \tau_z(i))$. As seen in the figure, the three SD strength functions show narrower widths at their peaks than the $E1$ strength function. Moreover their peak positions including the $E1$ case well correspond to the observed excitation energies of the four $T = 1$ negative-parity states of ${}^4\text{He}$ [13].

We display in the right panel of Fig. 1 the IS SD strength functions that reflect the $J^\pi T = \lambda^- 0$ continuum states of ${}^4\text{He}$. These IS SD strength functions, especially for the 0^- and 2^- cases, show much narrower distribution than the IV0 strength functions. These peak energies again appear to correspond to the observed $T = 0$ negative-parity levels in ${}^4\text{He}$. A close comparison between the IS and IV0 strength functions indicates that the 0^- case is noteworthy compared to the 1^- and 2^- cases in that the difference in the peak positions of the same J^- becomes much larger. As discussed in Refs. [8, 14], the reason for this is understood by analyzing the role played by the tensor force.

The resonance energy may be identified as the energy where the peak is located. We also estimate the decay width of the resonance by the difference of two excitation energies at which the strength becomes half of the maximum strength at the peak. The agreement between theory and experiment is very satisfactory [2]. The average deviation of the calculated resonance energies from experiment is less than 0.4 MeV for ${}^4\text{He}$ despite the fact that most of their widths are larger than 5 MeV. The estimated width is also in reasonable agreement with experiment.

Here we discuss the non energy-weighted sum rule (NEWSR) for the SD operator. The use of the closure relation enables us to express the NEWSR to the expectation value of the operator

$\sum_{\mu} \mathcal{O}_{\lambda\mu}^{p\dagger} \mathcal{O}_{\lambda\mu}^p$ with respect to the ground state Ψ_0 . It is convenient to express that operator as a scalar product of the space-space and spin-spin tensors, $\mathcal{Q}_{(\kappa)0}^p = \sum_{i,j=1}^A ([\boldsymbol{\rho}_i \times \boldsymbol{\rho}_j]_{\kappa} \cdot [\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j]_{\kappa}) T_i^{p\dagger} T_j^p$, where the rank κ can be 0, 1, and 2. With use of the above equation, the expression of the NEWSR is

$$m_0(p, \lambda) \equiv \int_0^{\infty} S(p, \lambda, E) dE = \sum_{\kappa=0}^2 U_{\lambda\kappa} \langle \mathcal{Q}_{(\kappa)0}^p \rangle. \quad (4)$$

The NEWSR is fully satisfied: the deviation of the NEWSR from the right hand side of Eq. (4) is less than 1%. This means that the basis functions prepared for the description of the SD excitation are sufficient enough to account for all the strength in the continuum. Among the three expectation values of $\langle \mathcal{Q}_{(\kappa)0}^p \rangle$ in Eq. (4), the $\kappa = 0$ term gives a dominant contribution to the NEWSR because the major component of the ground state of ${}^4\text{He}$ is $S = 0$ and it has a non-vanishing expectation value only for $\mathcal{Q}_{(0)0}^p$. In this limiting case $m_0(p, \lambda)$ is proportional to $U_{\lambda 0}$. Therefore the λ -dependence of the NEWSR turns out to be 1 : 3 : 5 for $\lambda = 0, 1, 2$, independently of p . The deviation from this ratio is due to the contributions of other $\mathcal{Q}_{(\kappa)0}^p$ terms, especially the $\kappa = 2$ term. Since the admixture of the $S = 2$ component is primarily determined by the tensor force, the deviation reflects the tensor correlations in the ground state. The term with $\kappa = 2$ is particularly interesting because it contains the tensor operator characteristic of the one-pion-exchange potential. Since $\langle \mathcal{Q}_{(2)0}^p \rangle$ is negative for $p = \text{IS}$, the ratio further increases from 1 : 3 : 5, which is approximately 1 : 4 : 7, whereas it is positive for $p = \text{IV0}$ and the ratio approximately reduces to 1 : 2 : 4.

As discussed above, $\langle \mathcal{Q}_{(\kappa)0}^p \rangle$ plays a central role to determine the NEWSR for the SD strength functions. Inverting the right hand side of Eq. (4) makes it possible to express $\langle \mathcal{Q}_{(\kappa)0}^p \rangle$ as a sum, over the multipole λ , of the NEWSR, $\langle \mathcal{Q}_{(\kappa)0}^p \rangle = \sum_{\lambda=0}^2 U_{\kappa\lambda}^{-1} m_0(p, \lambda)$, where U^{-1} is the inverse matrix of U . If the NEWSR for all λ are experimentally measured, the above equation indicates that $\langle \mathcal{Q}_{(\kappa)0}^p \rangle$ for all κ can be determined from experiment.

3.2. A ${}^{12}\text{C}+n+n+p+p$ five-body model for ${}^{16}\text{O}$

Let us move to the ${}^{16}\text{O}$ problem. A five-body system we consider here is characterized by the Hamiltonian which consists of an NN potential V_v for valence nucleons and a ${}^{12}\text{C}$ -nucleon (CN) potential V_{cv} . A central Minnesota (MN) potential [15] is employed as the NN potential. To fine tune the binding energy of the α particle, the potential strengths are multiplied by 0.9814. Symmetrized Woods-Saxon and its derivative forms are assumed for the CN potential, and their parameters are determined 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 [16]. Here we assume the harmonic oscillator (HO) wave functions of $0s_{1/2}$ and $0p_{3/2}$ as the occupied orbits of ${}^{12}\text{C}$. The HO frequency is set to be 16.0 MeV, which reproduces the size of the ${}^{12}\text{C}$ ground state. The core excitation is ignored in this calculation.

We express the wave function in terms of a linear combination of many CG states of Eq. (2). 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 [5, 6], choose the best one among them and increase the basis dimension one by one until a convergence is reached. This procedure costs expensively for computer time but no other viable methods are at hand to get converged solutions for the present problem.

The left panel of Fig. 2 displays the calculated energy curves of the ground (0_1^+) and first excited (0_2^+) states of ^{16}O 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 MN interaction that requires only few tens of basis states [5]. The most basis states are used for eliminating the forbidden states. This is because, when the valence nucleons are strongly correlated, the basis states may have a large overlap with the forbidden states, and thus more basis states are needed to get a converged solution. After the convergence two 0^+ states appear below $^{12}\text{C}+\alpha$ threshold and their energies are both remarkably close to experiment.

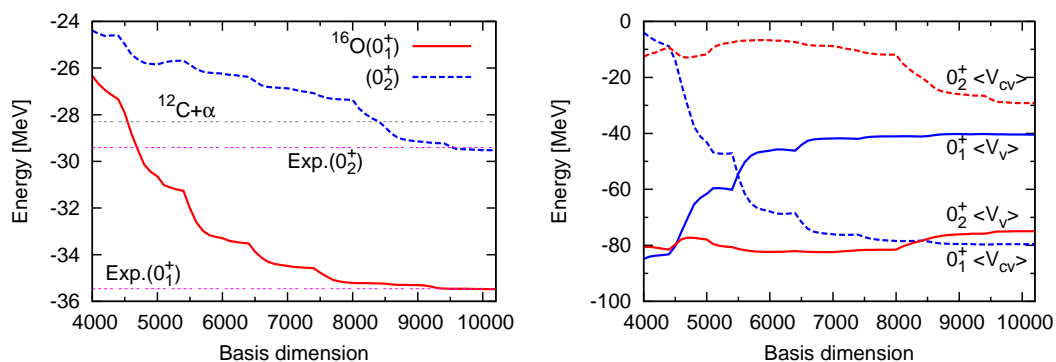


Figure 2. Left: Energy curves for the ground and excited 0^+ states of ^{16}O . The calculated $^{12}\text{C}+\alpha$ thresholds and experimental energies are plotted with thin lines. The figure is plotted based on the data of Ref. [3]. Right: Expectation values of V_{cv} and V_v of the two 0^+ states of ^{16}O as a function of the number of basis dimensions.

We found that the total energies for the ground and first excited 0^+ states of ^{16}O are in good agreement with experiment. The decomposition tells us information on the correlated structure of the valence nucleons. The right panel of Fig. 2 plots the expectation values of V_{cv} and V_v as a function of the number of basis dimensions. The energy curve for the 0_1^+ state changes drastically at 4000 to 6000 basis states where the energy crosses over the $^{12}\text{C}+\alpha$ threshold. We expect a phase transition from the cluster structure to shell-model like structure at this basis dimension. Beyond 8000 basis states where the energies are close to the convergence, the $\langle V_{cv} \rangle$ value turns out to be dominant. In the 0_1^+ state, the CN potential gives the major contribution to the energy $\langle V_{cv} \rangle = -79.55$ MeV, whereas $\langle V_v \rangle$ is approximately a half of it (-40.41 MeV). It is found that the $\langle V_v \rangle$ value is approximately a half of the NN contribution of the free alpha particle obtained with the MN potential (-85.22 MeV). The alpha particle is influenced and strongly distorted by the attraction, kinetic energy, and Pauli constraint from the core nucleus.

In the case of the 0_2^+ state, in contrast to the ground state, $\langle V_v \rangle$ is large, keeping a constant value shown in the right panel of Fig. 2. The converged $\langle V_{cv} \rangle$ is small -29.22 MeV compared to the contribution of the valence nucleons $\langle V_v \rangle = -74.92$ MeV, which is very close to that of the free alpha particle. This suggests that the 0_2^+ state has a well developed $^{12}\text{C}+\alpha$ structure as predicted by the cluster model [17]. It is interesting to note that $\langle V_{cv} \rangle$ of the 0_1^+ state is similar to $\langle V_v \rangle$ of the 0_2^+ state. Due to the balance of the core-nucleon and the valence nucleons contributions, the two 0^+ states appear at closely to each other, and thus the two different aspects coexist in the spectrum of ^{16}O .

For more quantitative discussion of the clustering degree, we calculate the $^{12}\text{C}+\alpha$

spectroscopic amplitude of ^{16}O defined by

$$y(r) = \frac{1}{r^2} \left\langle \phi_\alpha \phi_{I=0}(^{12}\text{C}) \delta(R-r) Y_{00}(\hat{\mathbf{R}}) \middle| \Psi_{00}(^{16}\text{O}) \right\rangle, \quad (5)$$

where $\Psi_{00}(^{16}\text{O})$, $\phi_{I=0}(^{12}\text{C})$, and ϕ_α are the wave functions of ^{16}O , ^{12}C core, and the free alpha particle obtained by a four-body calculation with the MN potential, respectively; and \mathbf{R} is a distance operator between the center-of-mass of the alpha and ^{12}C . The left panel of Fig. 3 displays the calculated spectroscopic amplitudes for the two 0^+ states of ^{16}O . At the short distances, we see some oscillations due to Pauli principle of $^{12}\text{C}+\alpha$. For the 0_1^+ state, the highest peak is located at around 4 fm. That is smaller than the touching distance of $^{12}\text{C}+\alpha$ (~ 5.9 fm). In such a case, the alpha particle may be distorted by the core nucleus. In fact, a spectroscopic factor $S_\alpha^2 = \int_0^\infty (ry(r))^2 dr$ is small (0.105), whereas the $^{12}\text{C}+\alpha$ cluster model calculation gives 0.300 [17]. 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 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}O is exhausted by the $^{12}\text{C}+\alpha$ cluster component.

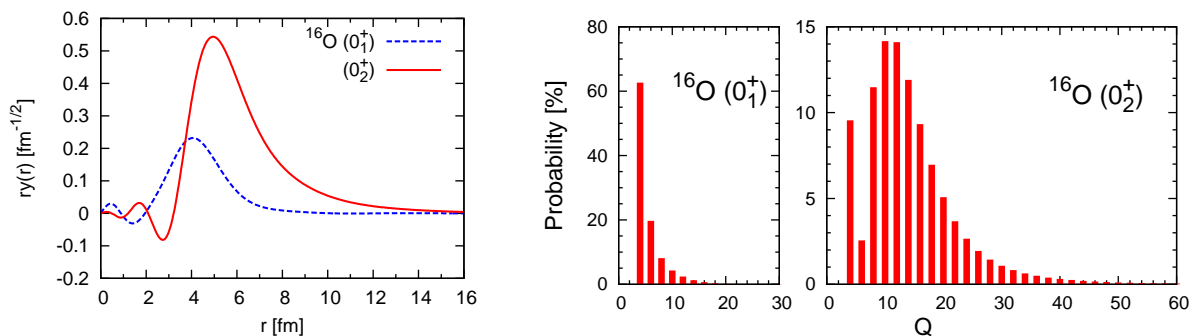


Figure 3. Left: Spectroscopic amplitude of the ground and excited 0^+ states of ^{16}O . Right: Decomposition of the ground and first excited states of ^{16}O wave functions into components having the harmonic oscillator quanta Q . The figures are plotted based on the data of Ref. [3].

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 harmonic oscillator (HO) quanta Q in our wave functions. The right panel of Fig. 3 plots the histogram of the HO quanta for the ground and first excited states of ^{16}O . 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 diminishes rapidly with increasing Q . Since a few major shell configurations 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 [17], the distribution of the first excited state of ^{16}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 again 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 second 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

Recent applications to nuclear four- and five-body problems have demonstrated the power of the explicitly correlated Gaussian (CG) method. Once the Hamiltonian is determined, the wave function of the system is accurately obtained and the model has no adjustable parameter.

First, the spin-dipole (SD) responses of ^4He are investigated based on the four-body calculation using a realistic nuclear force. Both the wave function of the ground state and the SD excitation are described accurately using the CG. The continuum states including two- and three-body decay channels are described with aid of the complex scaling method.

Experimental data that can directly be compared to the calculation are presently only the resonance parameters of the negative-parity levels of $A = 4$ nuclei. We find that peak position and width of the SD strength function corresponds well with experimental resonant energy and decay width, respectively. The non energy-weighted sum rule (NEWSR) of the SD strength function is investigated by relating it to the expectation values of three scalar products of the space-space and spin-spin tensors with respect to the ground state of ^4He . It turns out that our model space satisfies the NEWSR for each SD operator perfectly. The tensor operator of rank 2, $\mathcal{Q}_{(2)0}^p$, is sensitive to the D -state correlation in the ground state induced by the tensor force, and it is mainly responsible for distorting the ratio of the NEWSRs for the multipolarity $\lambda = 0, 1, 2$ from the uncorrelated ratio of $1 : 3 : 5$. An experimental observation of this ratio is desirable since it may lead us to reveal the degree of tensor correlations in the ground state.

In the second topic, we successfully describe the ground and first excited 0^+ states of ^{16}O in a single scheme, a ^{12}C +four-nucleon model. The ^{12}C -nucleon and NN potentials are chosen to reproduce low-energy properties of each subsystem. We solve the full five-body Schrödinger equation 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}O are obtained consistently with the experimental values. The ground state exhibits a shell model like structure. However, our analyzes suggest the first excited states has a well developed $^{12}\text{C}+\alpha$ cluster structure. The probability distributions of the harmonic oscillator quanta also support our pictures and show the difficulty to describe the 0_2^+ state with the ordinary major shell truncation of the harmonic oscillator basis. Possible and promising application is to extend our five-body model with heavier doubly closed shell core, that is, for example, ^{20}Ne , $^{44,52}\text{Ti}$, and ^{212}Po as is an interesting analogy to the ^{16}O problem.

Acknowledgments

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