Advances in the \textit{ab initio} description of nuclear three-cluster systems

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Abstract. We introduce the extension of the \textit{ab initio} no-core shell model with continuum to describe three-body cluster systems. We present results for the ground state of \textsuperscript{6}He and show improvements with respect to the description obtained within the no-core shell model and the no-core shell model/resonating group methods.

1 Introduction

The \textit{ab initio} no-core shell model/resonating group method (NCSM/RGM) was presented in \cite{1,2} as a technique that is able to describe both structure and reactions in light nuclear systems. Within this approach, the wave function is expanded in a continuous cluster basis using the resonating group method with realistic interactions and a consistent \textit{ab initio} description of the nucleon clusters.

The method was first introduced in detail for two-body cluster bases and has been shown to work efficiently in different systems \cite{1–4}. Later, the expansion of the method for three-cluster systems was introduced in \cite{5,6}. The capability of \textit{ab initio} methods to properly describe three-body cluster states is essential for the study of nuclear systems that present such configuration. This type of systems appear, e.g., in structure problems of two-nucleon halo nuclei such as \textsuperscript{6}He and \textsuperscript{11}Li, resonant systems such as \textsuperscript{5}H, and reactions with three fragments in their final state such as \textsuperscript{3}H(\textsuperscript{3}H,2n)\textsuperscript{4}He or \textsuperscript{3}He(\textsuperscript{3}He,2p)\textsuperscript{4}He.

Despite the success of the NCSM/RGM in describing the asymptotic behavior of the wave functions, it has been shown that it has limitations when it comes to accurately describe systems at short to medium ranges (up to about 5 fm for the \textsuperscript{6}He case). This is due to the fact that, in order to account for all many-body correlations, several excited states of the nuclear clusters must be included in the basis, resulting in an increase of the problem size that goes beyond current computational capabilities. This limitation has been overcome by introducing the \textit{ab initio} no-core shell model with continuum (NCSMC). With this method, the wave function is written as a superposition of both continuous NCSM/RGM cluster states and discrete eigenstates of the compound system obtained with the no-core shell model (NCSM). The latter eigenstates compensate for missing cluster excitations, improving the description of the wave function at short to medium range.

The NCSMC was first introduced in \cite{7,8} for binary systems. Its expansion to three-cluster systems was recently achieved and we show here the first results for the \textsuperscript{6}He ground state (g.s).

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Table 1. Energy (in MeV) for the NCSM $^4$He g.s. and the $^6$He g.s. using the NCSM/RGM, NCSM and NCSMC approaches in terms of the absolute HO model space size $N_{tot} = N_0 + N_{max}$, where $N_0$ is the number of oscillator quanta shared by the nucleons in their lowest configuration. For the NCSM, we also show the extrapolated value to $N_{max} \to \infty$ (the extrapolation was performed with an exponential fit).

| $N_{tot}$ | $^4$He | $^6$He | $^4$He | $^6$He |
|----------|-------|-------|-------|-------|
| 8        | 28.17 | 28.62 | 28.95 | 29.69 |
| 10       | 28.22 | 28.72 | 29.45 | 29.86 |
| 12       | 28.22 | 28.70 | 29.66 | 29.86 |
| Extrapolation | 28.230(5) | —     | 29.84(4) | —     |

2 Formalism

In the NCSMC, the ansatz for the three-cluster many-body wave function is given by

$$|\Psi^{JT}\rangle = \sum |A\lambda \ell^I T\rangle + \sum \int dx dy x^2 y^2 G^\nu (x, y, \lambda) \hat{A}_\nu |\Phi^{JT}_v\rangle,$$

where $c_\lambda$ and $G^\nu (x, y)$ are, respectively, discrete and continuous variational amplitudes, $|A\lambda \ell^I T\rangle$ are NCSM eigenstates of the compound nucleus labeled by the set of quantum number $\lambda$, $\hat{A}_\nu$ is an appropriate intercluster antisymmetrizer introduced to exactly preserve the Pauli exclusion principle, and

$$|\Phi^{JT}_v\rangle = \left[ \left( |A - a_23 \alpha_1 T_1\rangle \left( |a_2^2 T_2^2 T_2\rangle |a_3 \alpha_3 T_3^2 T_3\rangle \right)^{s_23} \right)^{(ST)} \left( Y_\ell (\hat{\eta}_{23}) Y_\nu (\hat{\eta}_{1,23}) \right)^{(L)} \right]^{(JT)},$$

are three-body cluster channels of total angular momentum $J$, parity $\pi$ and isospin $T$, where $\nu$ represents a set of quantum numbers that describes the channel within the cluster basis. Here, $|A - a_23 \alpha_1 T_1\rangle$, $|a_2 \alpha_2 T_2^2 T_2\rangle$ and $|a_3 \alpha_3 T_3^2 T_3\rangle$ denote the microscopic (antisymmetric) wave functions of the three nuclear fragments calculated within the NCSM. The Jacobi coordinates describing the relative positions of the clusters are denoted by $\hat{\eta}_{23} = \eta_{23} \hat{\eta}_{23}$ and $\hat{\eta}_{1,23} = \eta_{1,23} \hat{\eta}_{1,23}$.

We calculate the unknowns of the NCSMC wave function $|c_\lambda$ and $G^\nu (x, y)$ by solving the orthogonalized coupled equations obtained by projecting the Schrödinger equation on the model space spanned by NCSM eigenstates and the NCSM/RGM basis $|\Phi^{JT}_v\rangle$. Those equations are solved by means of the microscopic R-matrix method on a Lagrange mesh [9]. Details on the procedure will be available in [10].

3 Application to $^6$He

The lightest Borromean nucleus is $^6$He [11, 12], formed by an $^4$He core and two halo neutrons. It is, therefore, an ideal first candidate to be studied within a three-body formalism. Hence, it was used as a test case when the NCSM/RGM formalism for three-cluster dynamics was introduced in [5, 6] and here is studied again in order to perform a benchmark with such results. We describe the $^4$He core by its g.s. wave function and couple the three-cluster basis with the $^6$He g.s. eigenstate obtained through the NCSM.
Figure 1. Most relevant hyperradial contributions to the $^6$He g.s. wave function. Both the contribution from the NCSM wave function and the total NCSMC wave function are shown for a $N_{\text{max}} = 6$ model space. The figure shows how the addition of the three-cluster basis within the NCSMC compensates for the limitations of the NCSM to obtain an extended wave function characteristic of two-neutron halo nuclei. The hyperradial wave functions $u_{K\nu}(\rho)$ are the coefficients of the wave function when expanded in the hyperspherical basis, where $K$ represents the hypermomentum.

We use the same potential as in [5, 6], i.e., the similarity-renormalization-group (SRG) [13, 14] evolved potential obtained from the chiral N$^3$LO NN interaction [15] with $\Lambda_{\text{SRG}} = 1.5$ fm$^{-1}$. With this potential, the variational minimum for the NCSM $^6$He g.s. is found at an HO frequency of around $\hbar\Omega = 14$ MeV, which is used in this work for all calculations. With this soft potential the binding energy can be accurately computed by extrapolating (through an exponential fit) the NCSM results to $N_{\text{max}} \to \infty$, hence providing a good benchmark for the newly implemented NCSMC.

From Table 1, we can see that the NCSMC $^6$He g.s. energy quickly converges to the NCSM extrapolated value, unlike in the NCSM/RGM, i.e., using only the basis (2) in the expansion of the wave function. This is due to the fact that the $^6$He NCSM eigenstate takes into account the six-body correlations and $^4$He core polarization that are missing when considering the cluster basis alone. It is also important to note that, in contrast to the behavior offered by the NCSM, the NCSMC presents the correct extended asymptotic behavior of the wave function. In Fig 1 such comparison is shown in a preliminary calculation at an $N_{\text{max}} = 6$ model space.

Finally, we can also compare the probability densities from the $^6$He g.s. obtained with the NCSM/RGM and the NCSMC. In Fig. 2, such comparison is shown and it is interesting to find that while the two main configurations (di-neutron and cigar) appear to have the same probability within the NCSM/RGM, the di-neutron probability is enhanced when using the NCSMC. This asymmetry in the strength of the probability peaks is known to be a characteristic of $^6$He and these results show that it is a consequence of the additional six-body correlations.

4 Conclusions

The NCSMC uses an ansatz wave function that includes both an expansion in a continuous three-cluster basis and in a discrete basis of NCSM eigenstates. This provides a foundation that is capable of describing both short and long range characteristics of three-cluster systems. In the case of the $^6$He g.s., we could see that this approach provides both the correct binding energy and extended asymptotic behavior unlike the NCSM, that does provide the correct binding energy, but not the correct
Figure 2. Probability distribution of the $^6$He g.s. wave function in terms of the relative distance between the neutrons ($r_{nn}$) and the distance between the center of mass of the neutrons and the $^4$He ($r_{\alpha,nn}$). The di-neutron and cigar configurations appear to have the same probability within the NCSM/RGM (a), while the di-neutron probability is enhanced when using the NCSMC (b).

asymptotics, or the NCSM/RGM that does the opposite. Calculations in larger model spaces for both g.s. and continuum states of $^6$He are underway.

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