How many-body correlations and $\alpha$-clustering shape $^6$He

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The Borromean $^6$He nucleus is an exotic system characterized by two halo neutrons orbiting around a compact $^4$He (or $\alpha$) core, in which the binary subsystems are unbound. The simultaneous reproduction of its small binding energy and extended matter and point-proton radii has been a challenge for ab initio theoretical calculations based on traditional bound-state methods. Using soft nucleon-nucleon interactions on chiral effective field theory potentials, we show that supplementing the model space with $^4$He+$n+n$ cluster degrees of freedom largely solves this issue. We analyze the role played by the $\alpha$-clustering and many-body correlations, and study the dependence of the energy spectrum on the resolution scale of the interaction.

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Introduction. Achieving a comprehensive and unified treatment of many-body correlations and clustering in atomic nuclei constitutes a frontier for contemporary nuclear theory. A light exotic nucleus that has been challenging our understanding of such complex phenomena based on nucleonic degrees of freedom and high-quality models of their interactions (i.e., within an ab initio framework) is Helium-6 ($^6$He). This is a prominent example of Borromean quantum ‘halo’, i.e., a weakly-bound state of three particles ($\alpha+n+n$) otherwise unbound in pairs, characterized by “large probability of configurations within classically forbidden regions of space” [1]. In the last few years, its binding energy [2] and charge radius [3] have been experimentally determined with high precision. The $^6$He ground state (g.s.) is also of great interest for tests of fundamental interactions and symmetries. Precision measurements of its $\beta$-decay half life have recently taken place [4] and efforts are under way to determine the angular correlation between the emitted electron and neutrino [5]. To date, traditional ab initio bound-state calculations can successfully describe the interior of the $^6$He wave function [6–10], but are unable to fully account for its three-cluster asymptotic behavior. At the same time, the only ab initio study of $\alpha+n+n$ dynamics naturally explains the asymptotic configurations, but underbids the $^6$He g.s. owing to missing many-body correlations [11, 12]. As a result, a comprehensive description of the $^6$He g.s. properties is still missing.

In this Letter we present a study of the $^6$He g.s. in which both six-body correlations and clustering are successfully addressed by means of the no-core shell model with continuum (NCSMC) [13]. This approach, introduced to describe binary processes starting from two [14, 15] and later three-body [16–18] Hamiltonians, is here generalized to the treatment of three-cluster dynamics. We further explore the role of six-body correlations in the description of the low-lying $\alpha+n+n$ continuum, required to accurately evaluate the $^4$He($2n,\gamma$)$^6$He radiative capture (one of the mechanisms by which stars can overcome the instability of the five- and eight-nucleon systems and create heavier nuclei [19]) and of the $^3$He($^3$H,2n)$^6$He reaction contributing to the neutron yield in inertial confinement fusion experiments [20, 21].

Approach. In the NCSMC, the $A$-nucleon wave function of a system characterized by a core+$n+\nu$ asymptotic in the total angular momentum, parity and isospin channel $J^P$ is written as the generalized cluster expansion

$$|\Psi^{J^P}\rangle = \sum_\lambda c_\lambda^{J^P}|\lambda J^P\rangle + \sum_\nu \int dx dy x^2 y^2 G_\nu^{J^P}(x, y) \hat{A}_\nu |\Psi^{J^P}\rangle,$$

where $c_\lambda^{J^P}$ and $G_\nu^{J^P}(x, y)$ are, respectively, discrete and continuous variational amplitudes to be determined, $|\lambda J^P\rangle$ is the square-integrable (antisymmetric) solution for the $\lambda$-th energy eigenstate of the system obtained within the $A$-body harmonic oscillator (HO) basis of the no-core shell model (NCSM) [22],

$$|\Phi^{J^P}_{\nu,xy}\rangle = \left[ (|A-2\lambda J^P T_c\rangle (|n\rangle |\nu\rangle)) |s_{nn} T_{nn}\rangle \right]^{(ST)} \times (Y_{\nu} (\bar{\eta}_{nn}) Y_{\nu} (\bar{\eta}_{n,nn})) |L\rangle^{(J^P T)} \delta(x - \bar{\eta}_{nn}) \delta(y - \bar{\eta}_{n,nn})$$

are continuous microscopic-cluster states [11] describing the organization of the nucleons into an $(A-2)$-nucleon core and two neutrons $|\nu\rangle$, and $\hat{A}_\nu$ is an appropriate intercluster antisymmetrizer introduced to preserve the Pauli exclusion principle. The core eigenstates are also computed in the NCSM, employing the same HO frequency $\hbar \Omega$ and consistent number of quanta above the lowest energy configuration $N_{\text{max}}$ used for the $A$-nucleon system. The states of Eq. (2) are labeled by the quantum numbers $\nu = \{ A-2 \lambda J^P T_c; s_{nn} T_{nn} S \ell_x \ell_y L \}$. Furthermore, $\bar{\eta}_{n,nn} = \bar{\eta}_{n,nn} \bar{\eta}_{n,nn}$ and $\bar{\eta}_{nn} = \bar{\eta}_{nn} \bar{\eta}_{nn}$ are Jacobi relative coordinates proportional to the separation between the center of mass (c.m.) of the core and that of
the residual two neutrons, and to the neutrons’ relative position, respectively.

Similar to the binary-cluster case [15], upon orthogonalization of expansion (1), we obtain the unknown \( c_\alpha \) and \( G^{\nu}_{\alpha} \) amplitudes by solving the Schrödinger equation in the model space spanned by the basis states \( |AAJ^{\nu}T\rangle \) and \( |\Phi_{J^{\nu}T}\rangle \). However, given the additional relative coordinate, in the three-cluster case we first express the continuous amplitudes in the orthogonalized expansion (i.e., the relative-motion wave functions) in terms of the hyperradius \( \rho = \sqrt{x^2 + y^2} \) and hyperangle \( \alpha = \arctan \frac{y}{x} \) and expand them in the hyperangular basis \( \phi^{\ell_{\alpha}}_{K} \) analogously to Ref. [11]. The \(^6\)He g.s. energy and wave function \( |\Psi_{g.s.}\rangle \), as well as the matrix elements of the \( \alpha+n+n \) scattering matrix are found by matching the orthogonalized form of expansion (1) with the known asymptotic behavior of the wave function using an extension of the microscopic \( R \)-matrix method on Lagrange mesh [15, 23–27]. We obtain convergence of the hyperangular expansion and \( R \)-matrix method using the same parameters as in Refs. [11, 12]. We then analyze the hyperradial components of the \( \alpha+n+n \) relative motion and preferred spatial configurations within the g.s. of \(^6\)He. To this end, we perform a projection of \( |\Psi_{g.s.}\rangle \) into the orthogonalized cluster basis (2), i.e.,

\[
\sum_{\nu} \int dx' dy' x'^2 y'^2 N_{\nu_{\nu'}}(x, y, x', y) \langle \Psi_{g.s.}|A_{\nu}|\Phi_{\nu_{\nu'}}\rangle = \frac{1}{\rho^{3/2}} \sum_{K} \tilde{a}_{K}(\rho) \phi^{\ell_{\alpha}}_{K}(\alpha),
\]

where \( N_{\nu_{\nu'}}(x, y, x', y') \) is the overlap between the antisymmetrized states (2) [11]. Finally, we obtain the matter \((r_{m})\) and point-proton \((r_{pp})\) root-mean-square (rms) radii by computing the square root of the expectation values on the g.s. wave function of the operators

\[
r^{2}_{m} = \frac{1}{A} \sum_{i=1}^{A} r_{i}^{2} = \frac{1}{A} \rho^{2} + \frac{A-2}{A} r^{2}_{m}^{(c)},
\]

and

\[
r^{2}_{pp} = \frac{1}{Z} \sum_{i=1}^{A} r_{i}^{2} \left( 1 + \frac{r^{(3)}_{i}}{2} \right) = r^{2}_{pp} + R^{2}(c),
\]

respectively. Here \( Z \) is the total number of protons, \( r^{(3)}_{i} \) is the third component of isospin, and \( r_{i} \) the distance from the \( A \)-nucleon c.m. of the \( i \)th nucleon, \( r^{2}_{m}^{(c)} \) and \( r^{2}_{pp} \) are \( \text{core operators defined analogously to Eqs. (4) and (5), respectively, and } R^{(c)} = \sqrt{\frac{2}{A-2}} l_{c,n} \text{ is the distance between the c.m. of the core and that of the whole system. The expressions on the far right-hand side of Eqs. (4) and (5) are used to compute the matrix elements involving the microscopic-cluster portion of the basis and were specifically derived for core+n+n partitions. In particular, the formulation of Eq. (5) is only valid for the present case of isospin \( T_{z} = 0 \) core. A more detailed account of the formalism will follow in a separate publication [28].}

\textbf{Results.} We start from the chiral N\(^3\)LO nucleon-nucleon (NN) interaction of Ref. [29] softened via the similarity renormalization group (SRG) method [30–32], which minimizes momentum components above a given resolution scale \( \Lambda \). In particular we work with \( \Lambda = 2.0 \text{ fm}^{-1} \). In nuclei up to mass number \( A = 6 \) this momentum resolution leads to binding energies close to experiment despite the omission of the three-nucleon (3N) components of the SRG-transformed chiral Hamiltonian [33], and has been shown to induce negligible (less than 1\%) two- and higher-body corrections of the \(^3\)H and \(^4\)He matter radii computed with bare operators [34]. In the interest of showing the vast improvement of the present approach over the use of expansions based exclusively on \( \alpha+n+n \) microscopic-cluster states, we also perform calculations with the even softer \( \Lambda = 1.5 \text{ fm}^{-1} \) resolution scale adopted in our earlier studies of Refs. [11, 12]. Calculations for \( \Lambda = 1.5 \text{ and } 2.0 \text{ fm}^{-1} \) were carried out using the same \( \hbar \Omega = 14 \) and 20 MeV HO frequencies of Refs. [11, 12] and [17], respectively. All results were obtained including only the \( J^{\pi}_{c}=0^{+}0 \) g.s. of the \( \alpha \) particle and the first four, three and two square-integrable eigenstates of the six-nucleon system for the \( J^{\pi} = 0^{+}, 1^{\pm} \) and 2\(^{+}\) channels, respectively.

As shown in Table I, convergence for the \(^6\)He g.s. energy computed within the NCSMC is achieved within less than 10 keV for \( \Lambda = 1.5 \text{ fm}^{-1} \), and the result is in excellent agreement with the infinite-space extrapolation of the NCSM [11]. This and the good agreement with the accurate extrapolated value of Ref. [8] give us reason to believe that convergence is achieved in the largest model space considered also for the harder (\( \Lambda = 2.0 \text{ fm}^{-1} \)) interaction. In general, the \(^4\)He(g.s.)+n+n degrees of freedom efficiently account for the onset of clustering already

\begin{table}[h]
\centering
\begin{tabular}{|l|c|c|c|c|c|}
\hline
\multicolumn{6}{|c|}{Table I. Computed \(^6\)He g.s. energies in MeV for the \( \Lambda = 1.5 \text{ and } 2.0 \text{ fm}^{-1} \) interactions as a function of the absolute HO model space size \( N_{\text{tot}} = N_{0} + N_{\text{max}} \), where \( N_{0} \) is the number of quanta shared by the nucleons in their lowest configuration. For the \(^4\)He(g.s.)+n+n calculation of Ref. [11], \( N_{0} = 0 \). However, for the p-shell \(^6\)He nucleus within the NCSM and NCSMC, \( N_{0} = 2 \). The last two rows show NCSM extrapolated results, and the experimental value, respectively.}\n\hline
\( N_{\text{tot}} \) & \multicolumn{2}{c|}{Ref. [11]} & \multicolumn{2}{c|}{NCSM} & \multicolumn{2}{c|}{NCSMC} \\
\hline
& \( \Lambda = 1.5 \text{ fm}^{-1} \) & \( \Lambda = 2.0 \text{ fm}^{-1} \) & \( \Lambda = 1.5 \text{ fm}^{-1} \) & \( \Lambda = 2.0 \text{ fm}^{-1} \) & \( \Lambda = 1.5 \text{ fm}^{-1} \) & \( \Lambda = 2.0 \text{ fm}^{-1} \) \\
\hline
6 & -29.81 & -27.71 & -30.02 & -26.44 & -28.64 \\
8 & -28.62 & -28.95 & -29.69 & -27.70 & -28.81 \\
10 & -28.70 & -29.45 & -29.86 & -28.37 & -28.97 \\
12 & -28.70 & -29.66 & -29.86 & -28.72 & -29.17 \\
\hline
\infty & -29.84(4) & -29.20(11) & -29.268 & & & \\
\hline
\end{tabular}
\end{table}
in small model spaces. Conversely, the square-integrable eigenstates supply many-body correlations that are not accounted for in a microscopic-cluster expansion including only the g.s. of $^4$He, such as the one shown in the first column of the table (note that $^6$He is unbound in the analogous calculations for $\Lambda = 2.0$ fm$^{-1}$). As shown in Fig. 1(a), the $^4$He(g.s.$)+n+n$ portion of the basis serves also the important role of providing the correct asymptotic behavior and extended configurations of the hyper-radial motion typical of a Borromean halo such as $^6$He.

The projection over the orthogonalized microscopic-cluster basis of Eq. (3) captures 97% of the original NCSMC solution, confirming the $\alpha+n+n$ picture of the $^6$He g.s. To visualize its spatial structure, we present in Fig. 1(b) the contour plot of the associated probability distribution. This displays the characteristic dominance of the “di-neutron” configuration (two neutrons about 2 fm apart orbiting the core at a distance of about 3 fm) over the “cigar” picture (two neutrons far from each other with the $\alpha$ particle in between) already seen in numerous previous studies [8, 11, 23, 35–38]. While these structures are already captured by the square-integrable portion of the basis [see Fig. 1(c)], they are more spatially extended in the full calculation.

The rms matter and point-proton radii obtained from the computed NCSMC g.s. wave functions using the more ‘realistic’ $\Lambda = 2.0$ fm$^{-1}$ momentum resolution are shown together with the corresponding two-neutron separation energy ($S_{2n}$) in Fig. 2 and summarized in Table II. Also shown as shaded bands are the accurate $S_{2n}$ measurement of Ref. [2], the range of experimental matter radii spanned by the the values and associated error bars of Refs. [39–41], and the bounds for the point-proton radius as evaluated in Ref. [7] from the charge radius reported in Ref. [3]. All three observables exhibit a considerably weaker dependence on the size of the HO basis compared

**TABLE II.** Summary of the results presented in Fig. 2, with $\Lambda_{\text{low}}$ in units of fm$^{-1}$. See text for further details.

|          | $S_{2n}$ (MeV) | $r_m$ (fm) | $r_{pp}$ (fm) |
|----------|----------------|------------|---------------|
| NCSMC ($N_{\text{max}} = 10$) | 0.94(5) | 2.43(2) | 1.88(2) |
| NCSM [8] ($N_{\text{max}} = \infty$) | 0.95(10) | — | 1.820(4) |
| EIHH [7] ($\Lambda_{\text{low}} = 2.0$) | 0.82(4) | 2.33(5) | 1.804(9) |
| Exp. | 0.975 | 2.32(10) | 1.938(23) |
to the results obtained within the NCSM (also shown in the figure as dashed red lines). While the NCSMC is not a variational method, given our previous analysis of the binding energy we are confident that the results for the largest model space are reasonably close to convergence. An estimate of our uncertainties, based on both the convergence of the two-neutron emission threshold $E_{th}(α+n+n)$ and the influence of $^6\text{He}$ square-integrable states beyond the g.s. is reported in Table II and shown in Fig. 2 for the largest model space. There, the theoretical $S_{2n}$ is closest to its empirical value, and the computed $r_m$ and $r_{pp}$ radii are, respectively, at the upper end and just below the lower bound of their experimental bands. More interestingly, our point-proton radius is substantially larger than both the extrapolated value of Sääf et al., which “calls for further investigations” [8], and the effective interaction hyperspherical harmonics (EIHH) result of Bacca et al. [7]. This latter calculation, based on the $V_{\text{low}}(N^3\text{LO})$ NN interaction, also yields a matter radius smaller than ours though within the experimental bounds. The present combination of $S_{2n}$ and $r_{pp}$ values are more in line with the Green’s function Monte Carlo results of Ref. [6], based on $NN+3\text{N}$ forces constrained to reproduce the properties of light nuclei including $^6\text{He}$.

With the present approach we are also able to quantify how the polarization of the $α$ core affects the low-lying continuum of $^6\text{He}$, a question that had been left unanswered by our previous study [12]. At the level of the $^4\text{He}+n+n$ scattering eigenphase shifts obtained for the $Λ = 1.5$ fm$^{-1}$ momentum resolution, the most significant effect is observed for the first $J^P = 2^+$ resonance, which becomes much sharper (with a width of $Γ = 15$ keV) and is shifted to lower energies (with the new centroid at 0.536 MeV). This behavior, indicative of a likely influence of the chiral $3\text{N}$ force on this state, can be seen in Fig. 3, which compares results obtained with (NCSMC) and without (cluster basis) coupling of $^6\text{He}$ square-integrable eigenstates. The effect in other partial waves is much more moderate. In particular, the $1^−$ eigenphase shift does not change significantly, excluding core-polarization effects as the possible origin of a low-lying dipole mode. A summary of the resonance centroids and widths (shown as shaded areas) extracted [43, 44] from the computed $Λ = 1.5$ and 2.0 fm$^{-1}$ positive-parity eigenphase shifts is presented and compared with experiment [42] in Fig. 4. Also shown, for the softer interaction, are extrapolated [45] energy levels (and their uncertainties) obtained within the NCSM by treating the $^6\text{He}$ excited states as bound states (note that the NCSM does not yield resonance widths). Clearly, such an approximation is only justified for the very narrow $2^+_1$ resonance. The two SRG resolution scales produce a qualitatively similar picture, with the harder interaction leading to higher-lying and wider resonances (see also Fig. 3).

Conclusions. We presented a study of $^6\text{He}$ in which both six-body correlations and $\alpha+n+n$ clustering are successfully addressed in the context of the no-core shell model with continuum, providing a comprehensive description of the g.s. and low-lying energy continuum of this nucleus. While the inclusion of $3\text{N}$ forces (currently underway) remains crucial to restore the formal unitarity of the adopted SRG transformation of the Hamiltonian and arrive at an accurate description of the spectrum as a whole, the present results demonstrate that rms matter and point-proton radii compatible with experiment can be obtained starting from a soft two-body Hamiltonian that reproduces the $^6\text{He}$ small binding energy. We conclusively show that a significant portion of the binding energy of the $^6\text{He}$ g.s. and the narrow width of the $2^+_1$ resonance are an effect of many-body correlations that, in a
microscopic-cluster picture, can be interpreted as a consequence of excitations of the α core. This work sets the stage for the \textit{ab initio} study of the $^6$He $\beta$-decay half-life and $^4$He($2n, \gamma$)$^6$He radiative capture, and is a stepping stone in the calculation of the $^3$H($^3$H, $2n$)$^6$He fusion.

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