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Emergence of cluster structures and collectivity within a no-core shell-model framework

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Abstract. An innovative symmetry-guided concept, which capitalizes on partial as well as exact symmetries that underpin the structure of nuclei, is discussed. Within this framework, *ab initio* applications of the theory to light nuclei reveal the origin of collective modes and the emergence a simple orderly pattern from first principles. This provides a strategy for determining the nature of bound states of nuclei in terms of a relatively small fraction of the complete shell-model space, which, in turn, can be used to explore ultra-large model spaces for a description of alpha-cluster and highly deformed structures together with the associated rotations. We find that by using only a fraction of the model space extended far beyond current no-core shell-model limits and a long-range interaction that respects the symmetries in play, the outcome reproduces characteristic features of the low-lying 0^+ states in ^{12}C (including the elusive Hoyle state and its 2^+ excitation) and agrees with *ab initio* results in smaller spaces. This is achieved by selecting those particle configurations and components of the interaction found to be foremost responsible for the primary physics governing clustering phenomena and large spatial deformation in the ground-state and Hoyle-state rotational bands of ^{12}C . For these states, we offer a novel perspective emerging out of no-core shell-model considerations, including a discussion of associated nuclear deformation, matter radii, and density distribution. The framework we find is also extensible to negative-parity states (e.g., the 3^-_1 state in ^{12}C) and beyond, namely, to the low-lying 0^+ states of ^8Be as well as the ground-state rotational band of Ne, Mg, and Si isotopes. The findings inform key features of the nuclear interaction and point to a new insight into the formation of highly-organized simple patterns in nuclear dynamics.

1. Introduction

Approximate symmetries in atomic nuclei that favor large deformation in nuclear dynamics have been long recognized [1, 2, 3, 4, 5, 6, 7, 8, 9, 10], and only recently confirmed in the *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [11]. This study unveiled the orderly patterns associated with such symmetries in nuclear wavefunctions from first principles, without *a priori* symmetry constraints. These symmetries are utilized and further understood in the framework of the microscopic no-core symplectic model (NCSM) [12], which combines a long-range many-nucleon interaction that respects the symmetries in play together with a symmetry-mixing realistic nucleon-nucleon interaction derived from meson exchange theory (e.g., CD-Bonn [13]), chiral effective field theory (e.g., N³LO [14]), or *J*-matrix inverse scattering theory (JISP16 [15]). The findings of the present study point to a new insight, namely, understanding the mechanism and the primary physics responsible for the emergence of such simple structures from a no-core shell-model perspective.



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One of the most successful particle-driven models is the *ab initio* no-core shell model (NCSM) [16], which can accommodate any type of inter-nucleon interaction, including modern two- and three-nucleon realistic interactions. Specifically, for a general problem, the NCSM adopts the intrinsic non-relativistic nuclear plus Coulomb interaction Hamiltonian defined as follows:

$$H = T_{\text{rel}} + V_{NN} + V_{NNN} + \dots + V_{\text{Coulomb}}, \quad (1)$$

where the V_{NN} nucleon-nucleon and V_{NNN} 3-nucleon interactions are included along with the V_{Coulomb} Coulomb interaction between the protons. The Hamiltonian may include additional terms such as multi-nucleon interactions among more than three nucleons simultaneously and higher-order electromagnetic interactions such as magnetic dipole-dipole terms. It adopts the harmonic oscillator (HO) single-particle basis characterized by the $\hbar\Omega$ oscillator strength and retains many-body basis states of a fixed parity, consistent with the Pauli principle, and limited by a cutoff N_{max} . The N_{max} cutoff is defined as the maximum number of HO quanta allowed in a many-body basis state above the minimum for a given nucleus. It divides the space in “horizontal” HO shells and is dictated by particle-hole excitations (this is complementary to the NCSpM, which divides the space in vertical slices selected by collectivity-driven rules). It seeks to obtain the lowest few eigenvalues and eigenfunctions of the Hamiltonian (1). The NCSM has achieved remarkable descriptions of low-lying states from the lightest nuclei up through ^{12}C , ^{16}O , and ^{14}F [16, 17], and is further augmented by several techniques, such as NCSM/RGM [18], Importance Truncation NCSM [19] and Monte Carlo NCSM [20]. This supports and complements results of other first-principle approaches, such as Green’s function Monte Carlo (GFMC) [21], Coupled-cluster (CC) method [22], In-Medium SRG [23], and Lattice Effective Field Theory (EFT) [24].

However, using the established NCSM methods is not enough to reach the physics regime necessary for a description of largely deformed nuclear states, such as the ^{12}C Hoyle state that was predicted based on observed abundances of heavy elements in the universe [25], and which has attracted much recent attention both in theory (e.g., see [26, 27, 24]) and experiment ([28, 29, 30, 31, 32, 33, 34, 35]). In this study, we address this problem, within a no-core shell-model framework, by utilizing a small subset of symplectic $\text{Sp}(3, \mathbb{R})$ basis states [6, 7] (with the complete set yielding results equivalent to those of the NCSM), an $\text{Sp}(3, \mathbb{R})$ -preserving part of the long-range inter-nucleon interaction [12], together with the bare JISP16 interaction.

2. Collectivity and clustering in light nuclei

2.1. Orderly patterns unveiled in the *ab initio* SA-NCSM

The next-generation *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [11] combines the first-principle concept of the NCSM with symmetry-guided considerations of the collectivity-driven models. For the first time, we show the emergence – in the framework of the SA-NCSM from first principles – of orderly patterns that favor large deformation/low spin in nuclear wavefunctions [11]. These patterns are linked to the $\text{SU}(3)$ and its embedding symplectic $\text{Sp}(3, \mathbb{R})$ symmetry¹. For example, the *ab initio* $N_{\text{max}} = 8$ SA-NCSM results with the bare N^3LO (similarly, for JISP16) realistic interaction for the ^8Be 0^+ ground state (*g.st.*) and its rotational band reveal the dominance of the $0\hbar\Omega$ component with the foremost contribution coming from the leading (40) $S = 0$ irrep (Fig. 1a). Furthermore, we find that important $\text{SU}(3)$ configurations are then organized into structures with $\text{Sp}(3, \mathbb{R})$ symplectic symmetry, that is, the (40) symplectic irrep gives rise to (60), (41), and (22) configurations in the $2\hbar\Omega$ subspace and so on, and those configurations indeed realize the major components of the wavefunction in this subspace. Similar results are observed for other *p*-shell nuclei, such as ^6Li , ^6He , and ^{12}C . This further confirms the significance of the symplectic symmetry to nuclear dynamics.

¹ Deformation-related $(\lambda \mu)$ quantum numbers of $\text{SU}(3)$ can be linked to nuclear shapes, e.g., (00), (λ 0), and (0 μ) describe spherical, prolate, and oblate shapes, respectively

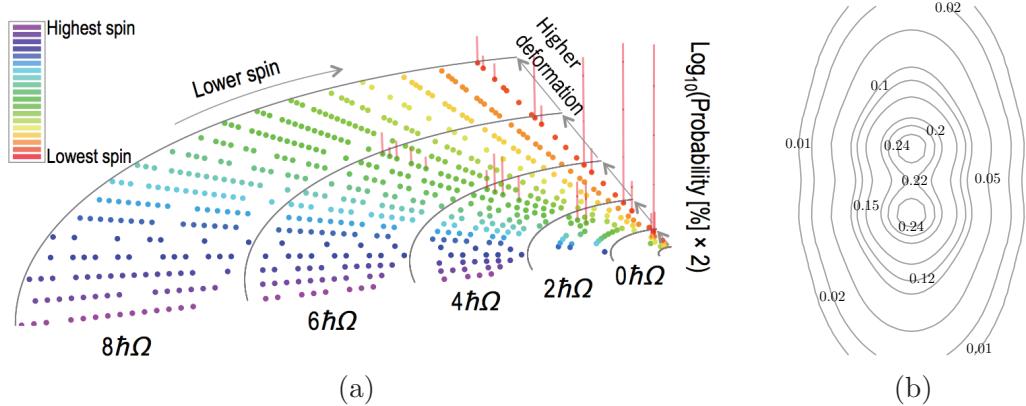


Figure 1. (a) Probability distribution across Pauli-allowed intrinsic spin and deformation configurations for the *ab initio* SA-NCSM 0^+ *g.st.* of ${}^8\text{Be}$ for $N_{\text{max}} = 8$ and $\hbar\Omega = 25$ MeV with the N³LO interaction. The concentration of strengths to the far right demonstrates the dominance of collectivity in the calculated eigenstates. This novel feature enables the SA-NCSM – by using symmetry-dictated subspaces – to reach new domains currently inaccessible by *ab initio* calculations, such as isotopes of Ne, Mg, and Si. (b) NCSpM matter-density profile of ${}^8\text{Be}$ for $N_{\text{max}} = 20$ and $\hbar\Omega = 20$ MeV [with H of Eq. (2) and JISP16 turned off].

The significance of the symplectic $\text{Sp}(3, \mathbb{R})$ symmetry for a microscopic description of a quantum many-body system of interacting particles has been recognized by Rowe and Rosensteel [6, 7]. Indeed, the 21 generators of $\text{Sp}(3, \mathbb{R})$ are directly related to the particle momentum ($p_{s\alpha}$) and coordinate ($r_{s\alpha}$) operators, with $\alpha = x, y$, and z for the 3 spatial directions and s labeling an individual nucleon, and realize important observables. Namely, $\text{Sp}(3, \mathbb{R})$ -preserving operators include: the many-particle kinetic energy $\sum_{s,\alpha} p_{s\alpha}^2/2m$, the HO potential, $\sum_{s,\alpha} m\Omega^2 r_{s\alpha}^2/2$, the mass quadrupole moment $Q_{(2\mathcal{M})} = \sum_s q_{(2\mathcal{M})s} = \sum_s \sqrt{16\pi/5} r_s^2 Y_{(2\mathcal{M})}(\hat{\mathbf{r}}_s)$, and angular momentum L operators, together with multi-shell collective vibrations and vorticity degrees of freedom for a description from irrotational to rigid rotor flows. The symplectic $\text{Sp}(3, \mathbb{R})$ symmetry underpins the symplectic shell model, which provides a microscopic formulation of the Bohr-Mottelson collective model [1] and is a multiple oscillator shell generalization of the successful Elliott SU(3) model [2]. The symplectic model with $\text{Sp}(3, \mathbb{R})$ -preserving interactions² has achieved a remarkable reproduction of rotational bands and transition rates without the need for introducing effective charges, while only a single $\text{Sp}(3, \mathbb{R})$ configuration is used [7, 9]. A shell-model study in a symplectic basis that allows for mixing of $\text{Sp}(3, \mathbb{R})$ configurations due to pairing and non-degenerate single-particle energies above a ${}^{16}\text{O}$ core [8] has found that using only seven $\text{Sp}(3, \mathbb{R})$ configurations is sufficient to achieve a remarkable reproduction of the ${}^{20}\text{Ne}$ energy spectrum as well as of $E2$ transition rates without effective charges.

2.2. Formation of clusters in ${}^{12}\text{C}$ in the hybrid NCSpM model

In this study, a fully microscopic no-core symplectic shell model, NCSpM, is explored to study low-lying 0^+ states and unnatural-parity states in ${}^{12}\text{C}$. As a new feature, the model utilizes a hybrid interaction, namely, a schematic many-nucleon $Q \cdot Q$ -type interaction [12] – which is $\text{Sp}(3, \mathbb{R})$ -preserving – plus the bare JISP16 nucleon-nucleon interaction – which is symmetry-breaking. The JISP16 has been successfully employed in *ab initio* NCSM calculations for the ${}^{12}\text{C}$ *g.st.* rotational band [36]. And while the coupling constants of the two-body part of the

² An important $\text{Sp}(3, \mathbb{R})$ -preserving interaction is $\frac{1}{2}Q \cdot Q = \frac{1}{2} \sum_s q_s \cdot (\sum_t q_t)$, as this realizes the physically relevant interaction of each particle with the total quadrupole moment of the nuclear system.

schematic interaction can be tied to realistic nucleon-nucleon interactions, we include many-nucleon interactions of a simple form ($e^{-\gamma Q \cdot Q}$) controlled by a parameter γ , the only adjustable parameter in the model. The study has revealed the importance of ultra-large shell-model spaces that are imperative to provide a successful description of the ^{12}C Hoyle state rotational band and the 3^- state, as well as low-lying states in nuclei from Be (Fig. 1b) to Si [12, 37].

The NCSpM employed within a full model space up through a given N_{\max} coincides with the NCSM for the same N_{\max} cutoff. However, in the case of the NCSpM, the symplectic irreps divide the space into ‘vertical slices’ that are comprised of basis states of a definite deformation ($\lambda \mu$). Hence, the model space can be reduced to only a few important configurations that are chosen among all possible $\text{Sp}(3, \mathbb{R})$ irreps within the N_{\max} model space. The NCSpM, while selecting the most relevant symplectic configurations, is employed to provide shell model calculations beyond current NCSM limits, namely, up through $N_{\max} = 20$ for ^{12}C , the model spaces we found sufficient for the convergence of results [12].

We employ a microscopic Hamiltonian given as,

$$H = T_{\text{rel}} + V_{NN} + V_{mN}^{\text{eff}} + \dots + V_{\text{Coulomb}}, \quad (2)$$

where T_{rel} is the relative kinetic energy. The V_{NN} is taken to be the bare JISP16 nucleon-nucleon interaction, which is turned on only among bandheads of symplectic irreps, introducing ‘horizontal’ mixing of all the states (up through the N_{\max} cutoff) within the symplectic vertical slices. The V_{mN}^{eff} effective many-nucleon interaction is taken to be,

$$V_{mN}^{\text{eff}} = V_0 + \frac{\chi}{2} \frac{(e^{-\gamma(Q \cdot Q - \langle Q \cdot Q \rangle_n)} - 1)}{\gamma}, \quad (3)$$

which simplifies to the two-body interaction, $V_0 - \frac{\chi}{2}(Q \cdot Q - \langle Q \cdot Q \rangle_n)$, in the $\gamma \rightarrow 0$ limit. The spherical HO potential, $V_0 = \sum_{i=1}^A \frac{m\Omega^2 \mathbf{r}_i^2}{2}$, and the $Q \cdot Q$ quadrupole-quadrupole interaction directly follow from the second and third term, respectively, in the long-range expansion of any two-body central force, e.g., like the Yukawa radial dependence, $V^{(2)} = \sum_{i < j} V(r_{ij}/a) = \sum_{i < j} (\xi_0 + \xi_2 r_{ij}^2/a^2 + \xi_4 r_{ij}^4/a^4 + \dots)$ [38], for a range parameter a . The $Q \cdot Q$ interaction is not restricted to a single shell. In addition, its average contribution, $\langle Q \cdot Q \rangle_n$, within an $n\hbar\Omega$ subspace is removed [39], where $\langle Q \cdot Q \rangle_n$ is the trace of $Q \cdot Q$ divided by the space dimension for a fixed number n of HO excitation quanta. This helps eliminate a considerable effect of $Q \cdot Q$ on the HO shell structure, while retaining the $Q \cdot Q$ -driven behavior of the wavefunctions. This Hamiltonian in its zeroth-order approximation (for parameter $\gamma \rightarrow 0$) and for a valence shell goes back to the established Elliott model. We take the coupling constant χ to be proportional to $\hbar\Omega$ and, to leading order, to decrease with the total number of HO excitations, as shown by Rowe [40] based on self-consistent arguments.

As the interaction and the model space are carefully selected to reflect the most relevant physics, the outcome reveals a quite remarkable agreement with the experiment (Fig. 2a). The low-lying energy spectrum and eigenstates for ^{12}C were calculated using the NCSpM with H of Eq. (2) for $\hbar\Omega = 18$ MeV given by the empirical estimate $\approx 41/A^{1/3}$ (e.g., see [1]). The results are shown for $N_{\max} = 20$, which we found sufficient to yield convergence. This N_{\max} model space is further reduced by selecting the most relevant symplectic irreps, namely, five symplectic bandheads and all symplectic multiples thereof up through $N_{\max} = 20$ of total dimensionality of about 10^4 . The five bandheads are, for positive-parity states, the spin-zero ($S = 0$) $0\hbar\Omega$ 0p-0h (0 4), $2\hbar\Omega$ 2p-2h (6 2), and $4\hbar\Omega$ 4p-4h (12 0) symplectic bandheads together with the $S = 1$ $0\hbar\Omega$ 0p-0h (1 2), and for negative-parity states, the 1p-1h (3 3) bandhead. In comparison to experiment (Fig. 2a), the outcome reveals that the lowest 0^+ , 2^+ , and 4^+ states of the 0p-0h symplectic slices calculated with JISP16 and V_{mN}^{eff} with $\gamma = -1.71 \times 10^{-4}$ closely reproduce the

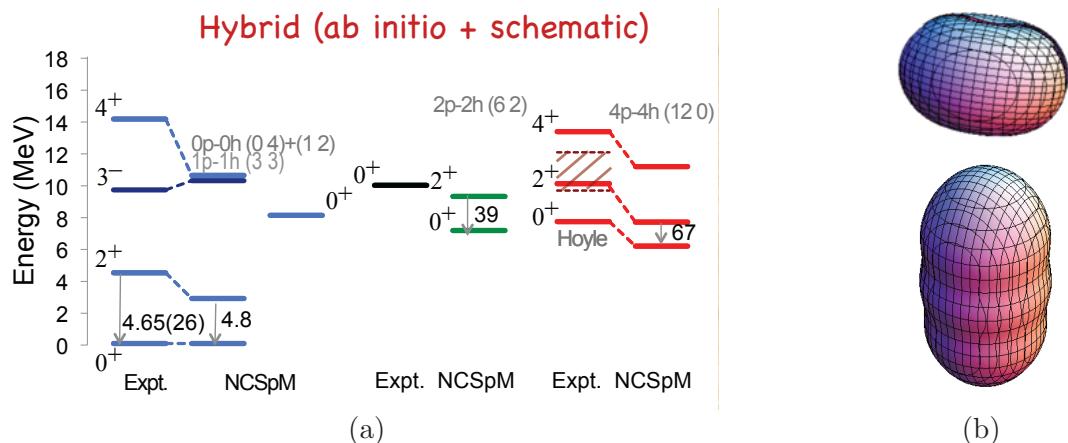


Figure 2. (a) ^{12}C energy spectrum calculated by the NCSpM using V_{mN}^{eff} with $\gamma = -1.71 \times 10^{-4}$ and the JISP16 in an $N_{\text{max}} = 20$ model space and compared to experiment (“Expt.”). Experimental data is from [41], except the latest results for 0_3^+ [31] and the states above the Hoyle state, 4^+ [42] and 2^+ [34] (with a shaded area showing the energy range from [29, 30, 31, 32, 33]). $B(E2)$ transition rates are in W.u. units. (b) NCSpM matter-density profile (with respect to the intrinsic frame) of the ^{12}C ground state (top) and the Hoyle state (bottom) showing the formation of three clusters in the Hoyle state within a no-core shell-model framework.

g.st. rotational band, indicating clear oblate shapes (Fig. 2b, top). In addition, the calculated lowest states of the $4\hbar\Omega$ 4p-4h (12 0) slice are found to lie close to the Hoyle-state rotational band, revealing alpha-clustering and prolate shapes (Fig. 2b, bottom). Furthermore, the lowest 0^+ of the $2\hbar\Omega$ 2p-2h (6 2) slice is found to lie around the 10-MeV 0^+ resonance (third 0^+ state), while the 1p-1h (3 3) slice is used to describe the lowest unnatural-parity 3^- state. The model successfully reproduces other observables for ^{12}C that are informative of the state structure, such as $B(E2)$ transition strengths (Fig. 2a), ground-state matter rms radius, $r_{\text{rms}}^{\text{NCSpM}} = 2.46$ fm compared to $r_{\text{rms}}^{\text{Expt}} = 2.43(2)$ fm, and the 2_1^+ electric quadrupole moment, $Q_{2_1^+}^{\text{NCSpM}} = +6.2$ efm 2 compared to $Q_{2_1^+}^{\text{Expt}} = +6(3)$ efm 2 . For the Hoyle state and its 2^+ excitation, theoretical calculations suggest matter rms radii, $r_{\text{rms}} = 2.95$ fm and $r_{\text{rms}} = 2.97$ fm, respectively.

While the model includes an adjustable parameter, γ in V_{mN}^{eff} , this parameter only controls the presence of many-body interactions that cannot be informed by existing realistic NN and NNN interactions. The entire many-body apparatus is fully microscopic and no adjustments are possible. Hence, as γ varies, there is only a small window of possible γ values that, for large enough N_{max} , closely reproduces the relative positions of the ^{12}C three lowest 0^+ states, as well as mass rms radii, electric quadrupole moments and $B(E2)$ transition strengths. This many-nucleon long-range interaction (V_{mN}^{eff}) is found to be foremost responsible for including alpha-particle correlations and for bringing the Hoyle state down in energy (Fig. 3a). However, using only V_{mN}^{eff} yields a compressed energy spectrum, which is remedied by a mixing of symplectic slices introduced by the bare JISP16. The spin-1 (1 1) component of JISP16 (or a spin-orbit-like term) is found to contribute the most to this effect (Fig. 3b), while the spin-2 tensor-force-like component of JISP16 appears to influence the ^{12}C energy spectrum only slightly (Fig. 3c). This outcome is in a close agreement with the results of Ref. [12], where the mixing of symplectic slices is successfully accounted for by an empirical spin-orbit force.

In addition, NCSpM eigenstates reveal a preponderance of the (0 4) $S = 0$ configuration and also (1 2) $S = 1$ configuration for the ^{12}C *g.st.* rotational band, further confirming an oblate shape. As shown in Fig. 3d for the 4^+ state, NCSpM results are in a close agreement with the *ab*

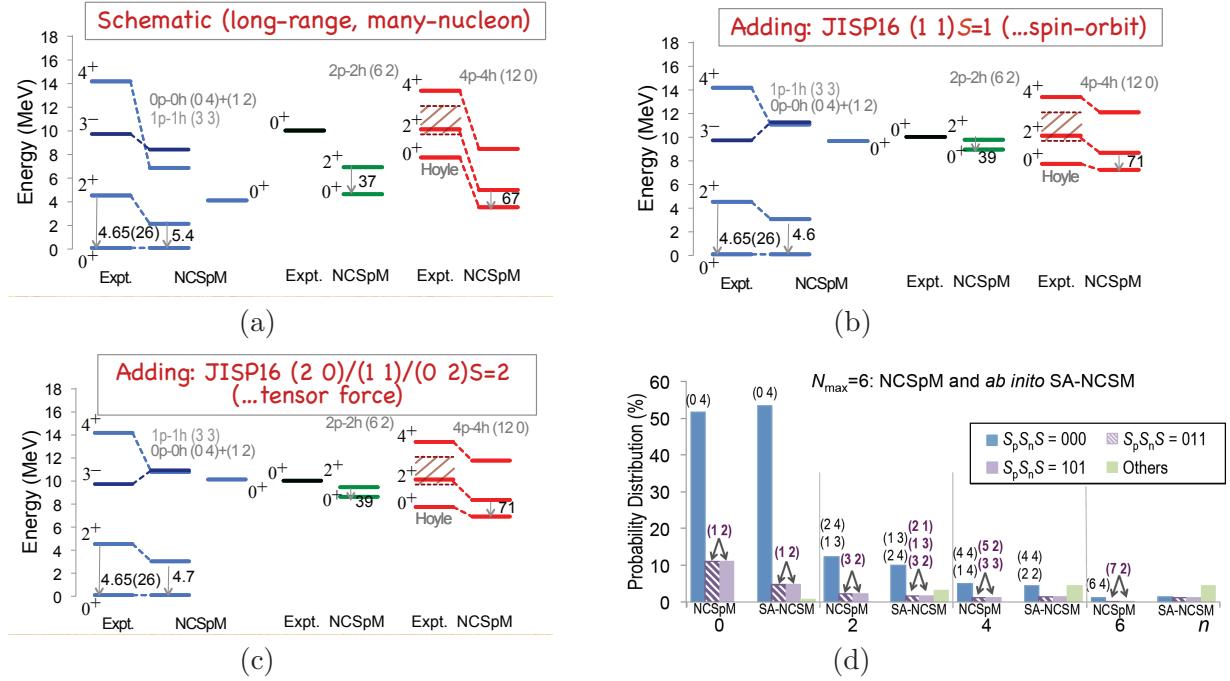


Figure 3. (a)-(c) Same as Fig. 2a, but showing the effect of various interaction components on the ^{12}C energy spectrum: (a) only V_{mN}^{eff} ; (b) $V_{mN}^{\text{eff}} + V_{NN}^{(11)S=1}$ [adding spin-orbit-like $(11)S = 1$ components of JISP16]; and (c) $V_{mN}^{\text{eff}} + V_{NN}^{(11)S=1} + V_{NN}^{(20),(11),(02)S=2}$ (with the addition of a JISP16 tensor force). (d) Close agreement of probability distributions for the ^{12}C 4_1^+ state (similarly, for the *g.st.* and 2_1^+) as calculated by NCSpM (left) and *ab initio* SA-NCSM with JISP16 (right) for $N_{\max} = 6$ and $\hbar\Omega = 18$ MeV, shown vs. the n total excitations and with dominant deformation modes, specified by $(\lambda \mu)$.

initio SA-NCSM in the reasonable $N_{\max} = 6$ model space. Furthermore, the outcome shows that among all possible configurations present in the SA-NCSM, only the states of the (0 4) and then (1 2) symplectic slices indeed appear dominant in the *g.st.* rotational band. The wavefunctions of the Hoyle-state rotational band can be obtained only in the NCSpM (for $N_{\max} = 20$) and are found to include shapes of very large prolate deformation, with the largest contribution of (16 0) (consistent with the prolate shape shown in Fig. 2b).

The outcome of the present analysis is not limited to ^{12}C . The model we find is also applicable to the low-lying states of other p -shell nuclei, such as ^8Be , as well as sd -shell nuclei without any adjustable parameters [37, 43]. In particular, using the same $\gamma = -1.71 \times 10^{-4}$ as determined for ^{12}C , we describe selected low-lying states in ^8Be in an $N_{\max} = 24$ model space with only 3 spin-zero $0\hbar\Omega$ (4 0), $2\hbar\Omega$ (6 0), and $4\hbar\Omega$ (8 0) symplectic irreps [37]. Furthermore, we have successfully applied the NCSpM without any adjustable parameters to the ground-state rotational band of heavier nuclei, such as ^{20}O , $^{20,22,24}\text{Ne}$, $^{20,22}\text{Mg}$, and ^{24}Si [43]. This suggests that the fully microscopic NCSpM model has indeed captured an important part of the physics that governs the low-energy nuclear dynamics and informs key features of the interaction and nuclear structure primarily responsible for the formation of such simple patterns.

In short, by utilizing symmetries that are found to underpin nuclear dynamics, we offer a novel framework, based on the no-core shell model, to further understand highly deformed states, exemplified by the Hoyle state and its rotational band, as well as unnatural-parity states.

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