HPC-enabled Nuclear Structure Studies – Description and Applications of the Symmetry-adapted No-Core Shell Model

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Abstract. By exploiting symmetries that enable the accounting of vital collective correlations in nuclei, we achieve significantly reduced dimensions for equivalent ultra-large model spaces, and hence resolve the scale explosion problem in nuclear structure calculations, i.e., the explosive growth in computational resource demands with increasing number of particles and size of the spaces in which they reside. As a result, we provide – with the help of High Performance Computing (HPC) resources – first solutions for selected benchmark calculations with remarkable findings of large-deformation and low-spin dominance in low-lying nuclear states. In the framework of a complementary symmetry-adapted study, one is able, facilitated by symmetry-preserving pieces of the inter-nucleon interaction, to accommodate unprecedented shell-model spaces critical to capture the physics governing the Hoyle state in $^{12}$C, thereby addressing a 60-year-old puzzle on the emergence of cluster substructures within a no-core shell model framework. All of these findings underline the key role of symmetries in nuclear structure studies.

1. Introduction
The $\textit{ab initio}$ symmetry-adapted no-core shell model (SA-NCSM) [1], which capitalizes on exact as well as partial symmetries that underpin the structure of nuclei, provides remarkable insight into how simple symmetry patterns emerge in the many-body nuclear dynamics from first principles. Furthermore, by recognizing that deformed configurations often dominate the low-lying nuclear states, the SA-NCSM provides a strategy – a symmetry-guided concept – for determining the nature of bound states of nuclei in terms of a relatively small subspace of the symmetry-reorganized complete model space, which opens new domains of nuclei for $\textit{ab initio}$ investigations, namely, the intermediate-mass region, including isotopes of Ne, Mg, and Si. This innovative symmetry-guided concept is discussed with a focus on emergent patterns in complex nuclei, in particular, in a fully microscopic no-core symplectic shell-model (NCSpM) study of the challenging $^{12}$C Hoyle state. This state was predicted based on observed abundances of heavy elements in the universe [2] and has attracted much recent attention both in theory (e.g., see [3–5]) and experiment [6–13]. The NCSpM findings inform key features of the primary physics responsible for the emergent phenomena of large deformation and alpha-cluster substructures in $^{8}$Be and $^{12}$C [14,15], as well as enhanced collectivity in intermediate-mass nuclei [16].
Figure 1. Elliott’s SU(3) model applied to $sd$-shell nuclei. Left panel: Spectrum of $^{22}$Ne (or $^{22}$Mg) (a) with a Majorana potential, (b) with the addition of the second-order SU(3) Casimir invariant, $C_{su}^2$, and (c) with the Majorana potential plus an attractive $Q \cdot Q$ interaction [or (b) with the addition of $L^2$]. Figure taken from [27]. Right panel: Spectrum of $^{24}$Mg with a Gaussian central force. Figure taken from [20]. The vertical axis in both figures represents energy in MeV. Note the importance of the most deformed SU(3) configuration $(8\ 2)$ in $^{22}$Ne and $(8\ 4)$ in $^{24}$Mg for reproducing the experimental low-lying states.

Specifically, the ab initio SA-NCSM, with results that corroborate and are complementary to those enabled within the framework of the no-core shell model (NCSM) [17], and which can be used to facilitate ab initio applications to challenging lower $sd$-shell nuclei, reveal that bound states of light nuclei are dominated by high-deformation and low-spin configurations [1]. The applicable symmetries reveal the nature of collectivity in such nuclei and provide a description of bound states in terms of a relatively small fraction of the complete space when the latter is expressed in an $(LS)J$ coupling scheme with the spatial configurations further organized into irreducible representations (irreps) of SU(3). That SU(3) plays a key role tracks with the seminal work of Elliott [18–20], see figure 1. The SU(3)-symmetry dominance has been also observed in heavier nuclei, where pseudo-spin symmetry and its pseudo-SU(3) complement have been shown to play a similar role in accounting for deformation in the upper $pf$ and lower $sdg$ shells, and in particular, in strongly deformed nuclei of the rare-earth and actinide regions [21], as well as in many other studies (e.g., see [22]). This is further reinforced by the fact that SU(3) also underpins the microscopic symplectic model [23, 24], developed by Rowe and Rosensteel, which provides a theoretical framework for understanding deformation-dominated collective phenomena in nuclei [24–26].

One of the most successful particle-driven models is the no-core shell model (NCSM), which, in principle, can straightforwardly accommodate any type of inter-nucleon interaction [17,28,29]. 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 many-body basis 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 microscopic symplectic model, which divides the space in vertical slices selected by collectivity-driven rules). The NCSM has achieved remarkable descriptions of low-lying states from the lightest \( s \)-shell nuclei up through \(^{12}\text{C}, ^{16}\text{O}, \) and \(^{14}\text{F}, \) and is further augmented by several techniques, such as NCSM/RGM [30], Importance Truncation NCSM [31] and Monte Carlo NCSM [32]. This supports and complements results of other first-principle approaches, such as Green’s function Monte Carlo (GFMC) [33], Coupled-cluster (CC) method [34], In-medium SRG [35], and Lattice Effective Field Theory (EFT) [5].

The next-generation \textit{ab initio} symmetry-adapted no-core shell model (SA-NCSM) [1] combines the first-principle concept of the NCSM with symmetry-guided considerations of the collectivity-driven models. The model and its recent findings are described in the next section.

2. Symmetry-guided concept

2.1. Simple pattern formation from first principles

The \textit{ab initio} symmetry-adapted no-core shell model (SA-NCSM) [1] adopts the first-principle concept and utilizes a many-particle basis that is reduced with respect to the physically relevant, deformation-related \( \text{SU}(3) \supset \text{SO}(3) \) subgroup chain (for a review, see [36]). This allows the full model space to be down-selected to the physically relevant space.

Figure 2. Probability distributions for proton, neutron, and total intrinsic spin components \((S_p, S_n, S)\) across the Pauli-allowed deformation-related \((\lambda \mu)\) values and for \(N\hbar\Omega\) subspaces for the calculated \(1^+\) ground state of \(^6\text{Li}\) obtained for \(N_{\text{max}} = 10\) and \(\hbar\Omega = 20\) MeV with the JISP16 bare interaction. The concentration of strengths to the far right demonstrates the dominance of collectivity in the calculated eigenstates.

The basis states of the SA-NCSM are based on HO single-particle states and for a given \(N_{\text{max}}\), are constructed in the proton-neutron formalism using an efficient construction based on powerful group-theoretical methods. The SA-NCSM basis states are related to the NCSM basis states through a unitary transformation (hence, the SA-NCSM results obtained in a complete \(N_{\text{max}}\) space are equivalent to the \(N_{\text{max}}\)-NCSM results). They are labeled by the SU\((3) \supset \text{SO}(3)\) subgroup chain quantum numbers \((\lambda \mu)\kappa L\), together with proton, neutron, and total intrinsic spins \(S_p, S_n, \) and \(S\). The orbital angular momentum \(L\) is coupled with \(S\) to the total orbital momentum \(J\) and its projection \(M_J\). Each basis state in this scheme is labeled schematically as \(|\vec{\gamma} (\lambda \mu)\kappa L; (S_p S_n S); JM_J|\). The label \(\kappa\) distinguishes multiple occurrences of the same \(L\) value.
in the parent irrep \((\lambda \mu)\), and \(\vec{\gamma}\) distinguishes among configurations carrying the same \((\lambda \mu)\) and \((S_pS_n)S\) labels.

The \textit{ab initio} SA-NCSM results for \(p\)-shell nuclei reveal a dominance of configurations of large deformation in the \(0\hbar\Omega\) subspace. For example, the \textit{ab initio} \(N_{\text{max}} = 10\) SA-NCSM results with the bare JISP16 realistic interaction \cite{37} (similarly, for the bare N\(^3\)LO realistic interaction \cite{38}) for the \(1^+\) ground state (\(g.st.\)) and its rotational band for \(^6\)Li reveal the dominance of the \(0\hbar\Omega\) component with the foremost contribution coming from the leading \((20)\) \(S = 1\) irrep (figure 2). Furthermore, we find that important SU(3) configurations are then organized into structures with Sp(3, \(\mathbb{R}\)) symplectic symmetry, that is, the \((20)\) symplectic irrep gives rise to \((40), (21),\) and \((02)\) 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 \(^6\)He, \(^8\)Be, and \(^{12}\)C.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Schematic illustration of the symmetry-guided concept for a model-space selection (P-space, shaded in magenta) and associated interaction renormalization. (a) Conventional NCSM in \(N_{\text{max}}\) model spaces specified by HO \(N\hbar\Omega\) many-body configurations, and (b) SA-NCSM in a \(\langle N^\perp_{\text{max}} \rangle N^\top_{\text{max}}\) model space reorganized in terms of SU(3)-coupled \(N\hbar\Omega\) many-body configurations; P-space includes all configurations up to \(N^\perp_{\text{max}}\) (small square), and large deformation/low-spin configurations at each \(N\hbar\Omega\) subspace together with symplectic excitations built upon largely deformed SU(3) configurations in lower \(N\hbar\Omega\) subspaces (intersection of horizontal and vertical light-magenta stripes). Typically, \(N^\perp_{\text{max}} \leq N_{\text{max}}\), while \(N^\top_{\text{max}}\) extends much beyond \(N_{\text{max}}\). As indicated along the diagonal, the percentage (tremendously enhanced for illustration) of selected configurations relative to the corresponding complete subspace decreases for higher \(N\hbar\Omega\).

The outcome points to a remarkable feature common to the low-lying states of nuclei that has heretofore gone unrecognized in other first-principle studies; namely, the emergence, without a priori constraints, of simple orderly patterns that favor strongly deformed configurations and low spin values. This feature confirms the dominant role the SU(3) and Sp(3, \(\mathbb{R}\)) symmetries play in nuclear dynamics and is central to expanding the reach of first-principle studies to heavier nuclei \cite{39}. In particular, this provides a strategy to determine a physically relevant P-space (that is, the model space used in calculations) that could be used for interaction renormalization and for SA-NCSM calculations (figure 3). Such a model space can thus accommodate important physics in low \(N\hbar\Omega\) subspaces (all configurations up to \(N^\perp_{\text{max}}\)) together with symplectic excitations thereof up through \(N^\top_{\text{max}}\) including symplectic irreps that start over largely deformed configurations in high \(N\hbar\Omega\) subspaces. Hence, model spaces, e.g., such as \(|6\rangle_{18}\) for \(^{12}\)C are feasible and en route}
to be employed. This allows the SA-NCSM to advance an extensible microscopic framework for studying nuclear structure and reactions that capitalizes on advances being made in ab initio methods while exploiting symmetries found to dominate the dynamics.

2.2. Applications to the elusive Hoyle state

The symmetry-guided concept shown in figure 3 is utilized and further understood in the framework of the no-core symplectic shell model (NCSpM) with applications to the low-lying nuclear structure of $^{12}$C [15]. This is a fully microscopic no-core shell model employed in a model space beyond current NCSM limits, namely, up through $N_{\text{max}}^T = 20$, that uses a symplectic $\text{Sp}(3, \mathbb{R})$ basis and $\text{Sp}(3, \mathbb{R})$-preserving interactions, while a nonpreserving spin-orbit interaction is applied to $0\hbar \Omega$ configurations. For example, results for the $\langle N_{\text{max}}^\bot = 0 \rangle N_{\text{max}}^T = 20$ model space are presented in Ref. [40].

The NCSpM employed within a full model space up through a given $N_{\text{max}}$ coincides with the NCSM for the same $N_{\text{max}}$ 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 $N_{\text{max}}^T$ model space.

We employ a very simple Hamiltonian with an effective interaction derived from the long-range expansion of the two-body central nuclear force together with a spin-orbit term,

$$H_{\text{eff}} = H_0 + \chi \left( \frac{e^{-\gamma Q \cdot Q} - 1}{\gamma} \right) - \kappa \sum_{i=1}^{A} l_i \cdot s_i. \quad (1)$$

This includes the $\text{Sp}(3, \mathbb{R})$-preserving terms: the spherical HO potential, which together with the kinetic energy yields the HO Hamiltonian, $H_0 = \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + \frac{m\Omega^2 r_i^2}{2} \right)$, and the important $\frac{1}{2} Q \cdot Q = \frac{1}{2} \sum s_i \cdot (\sum_{t} g_t)$ interaction, which realizes the physically relevant interaction of each particle with the total quadrupole moment of the nuclear system; the nonpreserving spin-orbit term is turned on only among symplectic bandheads. The average contribution, $\langle Q \cdot Q \rangle_n$, of $Q \cdot Q$ within a subspace of $n$ HO excitations is removed [41], that is, the trace of $Q \cdot Q$ divided by the space dimension for a fixed $n$. Hence, the large monopole contribution of the $Q \cdot Q$ interaction is removed, which, in turn, helps eliminate the considerable renormalization of the zero-point energy, 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 $\chi$ to be proportional to $\hbar \Omega$ and, to leading order, to decrease with the total number of HO excitations, as shown by Rowe [42] based on self-consistent arguments. The success
of such an effective nuclear interaction is not unexpected, as the spherical HO potential and the $Q,Q$ 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, $V^{(2)} = \sum_{i<j} V(r_{ij}/a) = \sum_{i<j} (\xi_0 + \xi_2 r_{ij}^2/a^2 + \xi_4 r_{ij}^4/a^4 + \ldots)$ [27], for a range parameter $a$.

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 [15]. The low-lying energy spectrum and eigenstates for $^{12}$C were calculated using the NCSpM with $H$ of equation (1) for $\hbar \Omega = 18$ MeV given by the empirical estimate $\approx 41/A^{1/3} = 17.9$ MeV and for $\kappa \approx 20/A^{2/3} = 3.8$ MeV (e.g., see [43]). The results are shown for $N_{\text{max}} = 20$, which we found sufficient to yield convergence. This $N_{\text{max}}$ model space is further reduced by selecting the most relevant symplectic irreps, namely, the spin-zero ($S = 0$) $0\hbar \Omega 0p-0h$ (04), $2\hbar \Omega 2p-2h$ (62), and $4\hbar \Omega 4p-4h$ (120) symplectic bandheads together with the $S = 1 0\hbar \Omega 0p-0h$ (12) and all multiples thereof up through $N_{\text{max}} = 20$ of total dimensionality of $6.6 \times 10^5$. In comparison to the experimental energy spectrum (figure 4), the outcome reveals that the lowest $0^+$, $2^+$, and $4^+$ states of the $0p-0h$ symplectic slices calculated for $\gamma = -1.71 \times 10^{-3}$ closely reproduce the $g.st.$ rotational band, while the calculated lowest $0^+$ states of the $4\hbar \Omega 4p-4h$ (120) and the $2\hbar \Omega 2p-2h$ (62) slices are found to lie close to the Hoyle state and the 10-MeV $0^+$ resonance (third $0^+$ state), respectively. The model successfully reproduces other observables for $^{12}$C that are informative of the state structure, such as mass rms radii, electric quadrupole moments and $B(E2)$ transition strengths (figure 4). The model we find is also applicable to the low-lying states of other $p$-shell nuclei, such as $^8$Be, as well as $sd$-shell nuclei without any adjustable parameters [14,16]. In particular, using the same $\gamma = -1.71 \times 10^{-4}$ as determined for $^{12}$C, we describe selected low-lying states in $^8$Be in an $N_{\text{max}} = 24$ model space with only 3 spin-zero $0\hbar \Omega$ (40), $2\hbar \Omega$ (60), and $4\hbar \Omega$ (80) symplectic irreps. Furthermore, we have successfully applied the NCSpM without any adjustable parameters to the ground-state rotational band of heavier nuclei, such as $^{20}$O, $^{20,22,24}$Ne, $^{20,22}$Mg, and $^{24}$Si [16]. 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, in the framework of the SA-NCSM, we show the emergence of orderly patterns from first principles. These patterns are linked to the SU(3) and symplectic Sp(3, $\mathbb{R}$) symmetries. This novel feature, in turn, enables the SA-NCSM – by using symmetry-dictated subspaces – to reach new domains of nuclear structure currently inaccessible by $ab$ initio calculations, such as isotopes of Ne, Mg, and Si. Furthermore, the symmetry-guided concept is illustrated in the NCSpM. This study, in addition, reveals that, to explain emergent simple patterns of deformation and clustering, shell-model spaces well beyond the current limits (up through 22 major HO shells for the Hoyle state) are vital to accommodate particle excitations that appear critical to highly-deformed spatial structures and the convergence of associated observables. The outcome also points to the importance of simple many-body interactions and of the long-range part of the $NN$ interaction, especially through its link to the HO potential and the interaction of individual particles with the total quadrupole moment of the nuclear system.

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References

[1] Dytrych T, Launey K D, Draayer J P, Maris P, Vary J P, Saule E, Catalyurek U, Sosonkina M, Langr D and Caprio M A 2013 Phys. Rev. Lett. 111 252501
[2] Hoyle F 1954 Astrophys. J. Suppl. Ser. 1 121
[3] Chernykh M, Feldmeier H, Neff T, von Neumann-Cosel P and Richter A 2007 Phys. Rev. Lett. 98 032501
[4] Khoa D T, Cuonga D C and Kanada-En’yo Y 2011 Phys. Letts. B 695 469
[5] Epelbaum E, Krebs H, Lee D and Meissner U G 2011 Phys. Rev. Lett. 106 192501
[6] Fynbo H O U et al. 2005 Nature 433 136
[7] Freer M et al. 2009 Phys. Rev. C 80 041303
[8] Hyldegaard S et al. 2010 Phys. Rev. C 81 024303
[9] Itoh M et al. 2011 Phys. Rev. C 84 054308
[10] Zimmerman W R, Destefano N E, Freer M, Gai M and Smit F D 2011 Phys. Rev. C 84 027304
[11] Raduta A R et al. 2011 Phys. Letts. B 705 65
[12] Zimmerman W R et al. 2013 Phys. Rev. Lett. 110 152502
[13] Marin-Lambarri D, Bijker R, Freer M, Gai M, Kokalova T, Parker D and Wheldon C 2014 Phys. Rev. Lett. 113 012502
[14] Launey K D, Dytrych T, Draayer J P, Tobin G K, Ferriss M C, Langr D, Dreyfuss A C, Maris P, Vary J P and Bahri C 2013 Proceedings of the 5th International Conference on Fission and properties of neutron-rich nuclei, ICFN5, November 4 - 10, 2012, Sanibel Island, Florida, edited by J. H. Hamilton and A. V. Ramagya (World Scientific, Singapore) p 29
[15] Dreyfuss A C, Launey K D, Dytrych T, Draayer J P and Bahri C 2013 Phys. Letts. B 727 511
[16] Tobin G K, Ferriss M C, Launey K D, Dytrych T, Draayer J P and Bahri C 2014 Phys. Rev. C 89 034312
[17] Navrátil P, Vary J P and Barrett B R 2000 Phys. Letts. B 5728
[18] Elliott J P 1958 Proc. Roy. Soc. A 245 128
[19] Elliott J P 1958 Proc. Roy. Soc. A 245 562
[20] Elliott J P and Harvey M 1962 Proc. Roy. Soc. A 272 557
[21] Bahri C, Draayer J and Moszkowski S 1992 Phys. Rev. Lett. 68 2133
[22] Zuker A, Retamosa J, Poves A and Carrion E 1995 Phys. Rev. C 52 R1741
[23] Rosensteel G and Rowe D J 1977 Phys. Rev. Lett. 38 10
[24] Rowe D J 1985 Reports on Progr. in Phys. 48 1419
[25] Bahri C and Rowe D J 2000 Nucl. Phys. A 662 125
[26] Draayer J, Weeks K and Rosensteel G 1984 Nucl. Phys. A419 1
[27] Harvey M 1968 Adv. Nucl. Phys. 1 67
[28] Maris P, Shirokov A M and Vary J P 2010 Phys. Rev. C 81 021301(R)
[29] BR Barrett P N and Vary J 2013 Prog. Part. Nucl. Phys. 69 131
[30] Navrátil P, Quaglioni S, Stetcu I and Barrett B R 2009 J. Phys. G: Nucl. Part. 36 083101
[31] Roth R and Navrátil P 2007 Phys. Rev. Lett. 99 092501
[32] Abe T, Maris P, Otsuka T, Shimizu N, Utsuno Y and Vary J 2012 Phys. Rev. C 86 054301
[33] Pieper S C, Varga K and Wiringa R B 2002 Phys. Rev. C 66 044310
[34] Wloch M, Dean D J, Gour J R, Hjorth-Jensen M, Kowalski K, Papenbrock T and Piecuch P 2005 Phys. Rev. Lett. 94 212501
[35] Tsukiyama K, Bogner S K and Schwenk A 2011 Phys. Rev. Lett. 106 222502
[36] Dytrych T, Srivatceva K D, Draayer J P, Bahri C and Vary J P 2008 J. Phys. G: Nucl. Part. Phys. 35 123101
[37] Shirokov A, Vary J, Mazur A and Weber T 2007 Phys. Letts. B 644 33
[38] Enenst D R and Machleidt R 2003 Phys. Rev. C 68 041001
[39] Dytrych T, Launey K D and Draayer J P 2014 McGraw-Hill Yearbook of Science and Technology Y140314
[40] Dreyfuss A C, Launey K D, Dytrych T, Draayer J P, Baker R, Deibel C and Bahri C 2014 to be submitted to Phys. Rev. C
[41] Rosensteel G and Draayer J P 1985 Nucl. Phys. A 436 445
[42] Rowe D J 1967 Phys. Rev. 162 866
[43] Bohr A and Mottelson B R 1969 Nuclear Structure vol 1 (Benjamin, New York)