Ab initio open core shell model for nuclear structure

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Ab Initio Open Core Shell Model for Nuclear Structure

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Abstract. The SU(3) symmetry-adapted version of the No-Core Shell Model (NCSM), which reduces to the Elliott SU(3) Model in its $0\hbar\omega$ limit, is described and shown to be effective in providing an efficient description of low-lying eigenstates of $^{12}$C and $^{16}$O. A symmetry-guided framework is suggested based on our recent findings of low-spin and high-deformation dominance in realistic NCSM results. This holds promise to significantly enhance the reach of ab initio shell models.

1. Significance of an ab initio symmetry-adapted open-core shell model
The dual challenge of understanding the strong interaction that precludes perturbative treatments, and the complexities of the quantum many-particle nuclear system that admit, for example, correlated phenomena and cluster sub-structures, places extraordinary demands on both physics and computational science. We aim to achieve significantly enhanced reach beyond that of the current no-core shell model (NCSM) by exploiting our knowledge of dominant symmetries, first of the interaction itself and then of those that emerge as a result of the many-body dynamics.

Ab initio approaches, which build upon a ‘first principles’ foundation, afford tremendous impact on advancing the frontiers of nuclear physics in multiple arenas, bridging from fundamental interactions and quantum chromodynamics (QCD) considerations to the physics of many-nucleon systems, including astrophysics and cosmology applications. Such approaches are crucial for achieving predictive power from fundamental input, and hence are vital for advancing energy applications as well as for gaining an understanding of nucleosynthesis and related nuclear reactions that are key to understanding the structure of atomic nuclei at a fundamental level.

It is important to acknowledge the impact the current ab initio NCSM (or open-core shell model, OCSM, for low $N_{\text{max}}$ cutoff parameter) has already had on achieving a better understanding of the structure of light nuclei, from the deuteron up through $^{16}$O and even for some selected cases beyond (e.g., see [1, 2] for NCSM and cluster NCSM/RGM results). However, it is also important to understand the limitations of the NCSM approach as currently implemented. Specifically, the combinatorial growth in the size of the basis or ‘model spaces’ that one encounters as a function of the $N_{\text{max}}$ total $\hbar\Omega$ excitations, and the associated computational complexity and storage requirements this implies, means extending its reach relies on the availability of ever-larger and more powerful HPC resources. Unfortunately, the $N_{\text{max}}$ values that can currently be accommodated, even if extended by 2 or 4 units to 10 or 12$\hbar\Omega$ for ‘$p$-shell’...
nuclei, fall short of what is required to take into account the presence of collective modes reflected in enhanced transition rates and cluster configurations. We aim to overcome this limitation, and achieve, for the first time, a unified microscopic description of low-lying states that reflect the close interplay of particle-hole modes, $\alpha$ clustering and collective rotational dynamics.

The symmetry-adapted OCSM (SA-OCSM) [3] advances the NCSM concept by recognizing that special symmetries often dominate the dynamics, and this means that physically relevant eigenstates can be described by a relatively few collective basis states that correspond to a special linear combination of a large number of NCSM basis states. (The SA-OCSM states can be obtained through a unitary transformation from the $m$-scheme basis used in the conventional shell model.) Hence, within the SA-OCSM framework, the growth of the model space can be managed by winnowing the model space to only physically relevant states as determined through symmetry considerations. The underlying concept of this framework is illustrated in our proof-of-principle study [3, 4] that exploits symplectic $Sp(3, \mathbb{R})$ symmetry and its SU(3) subgroup symmetry in an analysis of large-scale nuclear physics applications for $^{12}$C and $^{16}$O. What one learns from the outcome of these studies is that typically a small fraction of the full model space (Fig. 1), several orders of magnitude less than that of the corresponding NSCM approach, suffices to represent most of the physics – typically 90% or more as measured by projecting NCSM results onto a symmetry-adapted equivalent basis and noting that only a small subset of the full space contributes to the low-dynamics.

**Figure 1.** NCSM space dimension as a function of the $N_{\text{max}}$ model space compared to that of the $Sp(3, \mathbb{R})$ subspace of the most dominant symplectic basis states: (a) $J = 0, 2$, and 4 for $^{12}$C, and (b) $J = 0$ for $^{16}$O.

The significance of the symplectic $Sp(3, \mathbb{R})$ symmetry for a microscopic description of a quantum many-body system of interacting particles [5, 6] follows from the physical relevance of its 21 generators$^1$. Specifically, the generators are directly related to the particle momentum ($p_{s\alpha}$) and coordinate ($q_{s\beta}$) operators and constructed as $\sum_s p_{s\alpha} p_{s\beta}$, $\sum_s (q_{s\alpha} p_{s\beta} \pm q_{s\beta} p_{s\alpha})$, and $\sum_s q_{s\alpha} q_{s\beta}$ with $\alpha, \beta = x, y, z$ for the 3 spatial directions and $s = 1, ..., A$ running over the nucleons. These generators realize important observables, such as the many-particle kinetic energy $\sum_{s, \alpha} p_{s\alpha}^2 / 2m$, the mass quadrupole moment and angular momentum operators, together with multi-shell collective vibrations and vorticity degrees of freedom for a description of rotational dynamics in a continuous range from irrotational to rigid rotor flows.

$^1$ While in its quantal realization the $Sp(3, \mathbb{R})$ symmetry is known to realize the famous Bohr-Mottelson collective model (1975 Physics Nobel Prize), it is interesting to note that in its classical realization the symplectic $Sp(3, \mathbb{R})$ symmetry underpins the dynamics of rotating bodies and, for example, the $Sp(3, \mathbb{R})$ model has been used to describe the rotation of deformed stars and galaxies [7].
The symplectic generators can be written as SU(3) tensor operators in terms of the harmonic oscillator raising \((b^{(1)}_{10})\) and lowering \((b^{(0)}_{01})\) operators,

\[
A_{LM}^{(20)} = \frac{1}{\sqrt{2}} \sum_{n=1}^{A} \left[ b_{n}^{(1)}_{10} \times b_{n}^{(1)}_{10} \right]_{LM}^{(20)} \\
C_{LM}^{(11)} = \sqrt{2} \sum_{n=1}^{A} \left[ b_{n}^{(1)}_{10} \times b_{n}^{(0)}_{01} \right]_{LM}^{(11)} \\
H_{00}^{(00)} = \sqrt{3} \sum_{n=1}^{A} \left[ b_{n}^{(1)}_{10} \times b_{n}^{(0)}_{01} \right]_{00}^{(00)} + \frac{3}{2} A
\]

with \(B_{LM}^{(02)} = (-)^{C-M}(A_{LM}^{(20)})^{\dagger}\). The eight operators \(C_{LM}^{(11)}\) generate the SU(3) subgroup of \(Sp(3, \mathbb{R})\) and are related to the angular momentum operator \(L_{1q}\) and the Elliott algebraic quadrupole moment tensor \(Q_{2q}\) as follows,

\[
C_{1q}^{(11)} = L_{1q}, \quad q = 0, \pm 1 \\
C_{2q}^{(11)} = \frac{1}{\sqrt{3}} Q_{2q}, \quad q = 0, \pm 1, \pm 2.
\]

The deformation-related \((\lambda \mu)\) set of quantum numbers labels SU(3) irreducible representations, irreps. Consequently, SU(3)-symmetric states (and hence symplectic basis states that are built on these) bring forward important information about nuclear shapes and deformation in terms of \((\lambda \mu)\), for example, \((00)\), \((\lambda 0)\) and \((0 \mu)\) describe spherical, prolate and oblate shapes, respectively.

A basis of a symplectic irrep is constructed by acting with symmetrically coupled polynomials in the symplectic raising operators, \(A^{(20)}\), on a set of basis states of a symplectic bandhead, \(|\sigma; S_{\sigma}\rangle\), which is a Sp(3, \(\mathbb{R}\)) lowest-weight state,

\[
|\sigma n \rho \omega \kappa (LS_{\sigma})JM_{J}\rangle = \left[ \left[ A^{(20)} \times A^{(20)} \ldots \times A^{(20)} \right]^{n} \times |\sigma; S_{\sigma}\rangle \right]_{\kappa (LS_{\sigma})JM_{J}}^{\rho \omega},
\]

where \(\sigma \equiv N_{\sigma} (\lambda_{\sigma} \mu_{\sigma})\) labels Sp(3, \(\mathbb{R}\)) irreps, \(n \equiv N_{n} (\lambda_{n} \mu_{n})\), \(\omega \equiv N_{\omega} (\lambda_{\omega} \mu_{\omega})\), and \(N_{\omega} = N_{\sigma} + N_{n}\) is the total number of oscillator quanta related to the eigenvalue, \(N_{\omega} \Omega\), of the three-dimensional harmonic oscillator Hamiltonian. The symplectic structure divides the full space into Sp(3, \(\mathbb{R}\)) irreps (multi-shell “vertical” cones). The structure accommodates particle-hole (p-h) configurations in a natural way and in this way spans the entire space. The Sp(3, \(\mathbb{R}\)) symmetry provides for a further organization of the SU(3) basis of the SA-OCSM, which like the latter, also spans the entire space.

2. Symmetry-guided framework

The symmetry-guided framework of the SA-OCSM utilizes a natural preference towards low-spin and high-deformation dominance as revealed in realistic NCSM wavefunctions. Specifically, our recent study [8] showed that for the 6\(\hbar\Omega\) NCSM results for \(^{12}\text{C}\) using the effective N\(^{3}\)LO interaction (and similarly for other interaction choices, such as JISP16) with \(\hbar\Omega=15\text{ MeV}\) (Fig. 2), proton (neutron) spin values \(S_{p} (S_{n}) = 0 \text{ and } 1\) are sufficient to describe about 99% of the converged \(J = 0^{+}, 2^{+},\) and \(4^{+}\) \(^{12}\text{C}\) NCSM eigenvectors. The residual 1% involves time/memory consuming higher-spin and consequently less relevant configurations. Hence, retaining only the relevant proton (neutron) spin values allows one, with the same computer resources, to accommodate the full basis within the selected spin spaces up through higher
Winnowing considerations of this type illustrate that the SA-OCSM offers a systematic framework for down-selecting to physically relevant and manageable subspaces associated with full NCSM based on spin and deformation selection, which are complementary and mutually reinforcing. This is illustrated in Fig. 4, where a manageable (e.g., $N_{\text{max}} = 6$) NCSM many-body space is schematically shown (a) together with an associated manageable space within the symmetry-guided framework that underpins the SA-OCSM (b). In the SA-OCSM structured approach, the space is first separated into proton and neutron subspaces and then, in keeping with the $LS$ coupling foundation of the SA-OCSM, this is further organized according to the total proton spin ($S_\nu$) and neutron spin ($S_\pi$) coupled to total spin ($S$). This decomposition enables one to trim the space to the dominant low-spin configurations.

These spin spaces can be further organized into SU(3) structures, each of which realizes a
nuclear shape deformation (represented as ‘ellipsoids’ in Fig. 4). Since typically configurations of maximum spatial deformation dominate, only a percentage of the proton(neutron)/spin subspace need be further considered (green ‘ellipsoids’) to accommodate the physically most significant configurations, including particle-hole excitations that are important for a description of clustering modes, in higher \( h \Omega \) model spaces (e.g., \( N_{\text{max}} = 10 − 12 \) in Fig. 4). And beyond these, the Sp(3, \( \mathbb R \)) symplectic symmetry can guide an extension of model spaces to incorporate even higher \( h \Omega \) values (e.g., \( N_{\text{max}} = 14 − 16 \) in Fig. 4) [3] required to gain convergence of the lowest bound \( 0^+ \) states in light nuclei (green cones in Fig. 4).

An illustrative example for the symmetry-guided framework of the SA-OCSM is shown in Fig. 5 for the case of the \( N \sim Z \) pf-nucleus \( ^{64}\text{Ge} \) of astrophysical significance. The figure shows the combinatorial (near-exponential) growth of the full NCSM space (blue squares). Employing spin considerations, the full space can be reduced roughly by an order of magnitude while achieving considerable decrease in computing intensity because low-spin configurations typically have a simpler structure than for higher ones. In the example of Fig. 5, we chose to retain only proton (neutron) spin values \( S_\pi = 0 \) and 1 (\( S_\nu = 0 \) and 1) coupled to total spin \( S = 0 \), 1 and 2 (no restrictions, red diamonds). Further reductions of several order of magnitude can be achieved by selecting SU(3) proton (neutron) modes according to their shape deformation with the most deformed structures playing the foremost role in nuclear collectivity. As for the spin, the selected proton SU(3) configurations are coupled to the selected neutron configurations to yield the total number of many-body states (yellow, green and purple triangles). Beyond these winnowing considerations, only reduced matrix elements of the associated highest-weight states need to be calculated and stored because the associated coupling coefficients can be computed ‘on the fly’.

For shell models that employ restricted model spaces a suitable Hamiltonian renormalization,
which is properly derived from realistic nucleon-nucleon interactions tied to QCD, is required in order to preserve predictive capabilities. A novel approach, the Similarity Renormalization Group (SRG) [9], which was recently adopted in nuclear physics and continues to enjoy successes in, e.g., condensed matter and high energy physics, decouples spaces that are relevant for the regime of nuclear dynamics from highly-energetic irrelevant configurations. Moreover, reflecting the symmetries in play for the SA-OCSM, we suggest a SU(3)-based SRG renormalization [10], which is suitable for SU(3)-adapted shell model calculations. This is because the SRG in a SU(3) basis results in a unitarily transformed $NN$ interaction that respects the SU(3) symmetry, that is, a (near-)diagonal Hamiltonian in the basis used. In addition, while an important but challenging part of the SRG approaches is to properly account for the many-body forces induced during the renormalization (in order to preserve the unitarity of the SRG transformations), the use of symmetries, e.g. highest-weight states and reduced matrix elements, plays a crucial role in addressing this issue.

In short, the SA-OCSM builds upon a proton-neutron formalism in a $LS$ coupling scheme with the proton/neutron spaces organized into subspaces of definite spin and further into spatial SU(3) representations that key to deformation, and for even higher $\hbar\Omega$ model spaces, into symplectic Sp(3, $\mathbb{R}$)⊃SU(3) structures. The symmetry-guided framework utilizes the physical relevance at each level of the structured space, namely, low-spin and high-deformation dominance together with most important patterns of symplectic excitations. This approach will open up an entire region of the periodic table to investigation with ab initio methods with forefront predictive capabilities.

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