Symmetry-adapted Ab Initio Theory for Many-body Correlations in Nuclei

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Abstract. We demonstrate that no-core shell-model results for low-lying states of light and medium mass nuclei, whether they are dilute or dense systems, reveal a strong dominance of low-spin and high-deformation configurations. This result is independent of whether the system Hamiltonian is phenomenological in nature or derived from a realistic interaction. It implies that only a small fraction of the complete model space is required for a description of such states, and this in turn points to the importance of using a symmetry-adapted, no-core shell-model framework for describing such nuclei, one based on an LS coupling scheme with the associated spatial configurations organized according to deformation.

These results confirm that the pioneering work of early developers of the field, J. P. Elliott with his SU(3) model and M. Moshinsky with his U(3) many-body oscillator work, extends to more open, multi-shell environments. Specifically, algebraic methods are both relevant in such an environment and they can be used to quell the combinatorial growth in dimensionality that comes with the addition of oscillator shells to a model space. Indeed, our findings demonstrate the utility of a symmetry-adapted, no-core shell-model approach, one that takes advantage of group theoretical as well as advanced computational methods. And importantly, what at first glance appear to be a daunting task – casting complex algebraic expressions of a symmetry-adapted scheme into a user-friendly and efficient shell-mode code, turns out to be not only doable, but a logical framework that embraces constructs that can be made to execute efficiently on massively parallel, multi-processor (and core) systems. Early results for some light p-shell nuclei are presented. In addition, we will show that the method can be extended to heavier nuclei of the sd-shell and beyond, including some cases of special astrophysical interest in the upper fp- and lower gds-shells, like isotopes of Ge, Se, and even Kr.

1. Introduction

Many-body correlations play an important role in nuclear dynamics and are key to understanding a variety of interesting phenomena observed in nuclear structure. Among these are alpha-cluster substructures and collective deformations that can strongly influence energy spectra and other properties of nuclei. Ironically, even these relatively easy-to-recognize features continue to resist microscopic solutions, challenging even the most sophisticated of ab initio shell model theories (e.g., see Refs. [1, 2, 3]). Such models, with their current relatively limited applicability to light nuclei and low-excitation structures, build on fundamental principles and should therefore offer predictive capabilities essential for a description of unstable and exotic nuclei, many of which are of high interest, e.g. in nucleosynthesis, but remain inaccessible even to experiment.
We offer a novel model, the \textit{ab initio} symmetry-adapted no-core shell model (SA-NCSM), that adapts the \textit{ab initio} (first principles) concept and in addition, utilizes the symmetries known to dominate the nuclear dynamics. Hence, the model holds promise to expand dramatically the reach as well as the impact of current \textit{ab initio} shell models toward describing – with unprecedented accuracy – heavier mass nuclei together with highly deformed and cluster substructures. This is achieved by recognizing that the choice of coordinates, especially when deformed nuclear shapes dominate, is crucial, and that the SA-NCSM affords solution in terms of coordinates that reflect symmetries inherent to nuclear systems. We present first results of the SA-NCSM that employs the SU(3) symmetry, which underpins the successful Elliott model \cite{4,5,6} and which is a subgroup of the Sp(3, \mathbb{R}) of the symplectic model \cite{7}. Indeed, these results confirm that the pioneering work of early developers of the field, J. P. Elliott with his SU(3) model \cite{8} and M. Moshinsky with his U(3) many-body oscillator work \cite{9}, extends to more open, multi-shell environments. While the SA-NCSM states can be obtained through a unitary transformation from the \textit{m}-scheme basis used in the NCSM – and hence, span the entire space, the growth of the model space within the SA-NCSM framework can be managed by winnowing operators, and the use of the resulting eigenvectors to evaluate other experimental observables. Any two-symmetry-adapted basis. This facilitates both the evaluation of the Hamiltonian matrix elements (currently up to two-body, but expandable to higher ranks) operators in the SU(3) irreducible representations, irreps, and bring forward important information about nuclear shapes and deformation, for example, (0 0), (\lambda 0) and (0 \mu) describe spherical, prolate and oblate shapes, respectively.

The SA-NCSM implements fast methods for calculating matrix elements of arbitrary (currently up to two-body, but expandable to higher ranks) operators in the SU(3)×SU(2) symmetry-adapted basis. This facilitates both the evaluation of the Hamiltonian matrix elements and the use of the resulting eigenvectors to evaluate other experimental observables. Any two-body operator can be expanded in terms of SU(3)-coupled fermion creation and annihilation operators,

\begin{equation}
\langle \alpha_f(\lambda_f \mu_f)S_f \mid \left\{ a_{\eta_j}^\dagger \otimes a_{\eta_j}^\dagger \right\}_{S_{\eta j}}^{(\lambda_\alpha \mu_\alpha)} \otimes \left\{ a_{\eta_i} \otimes a_{\eta_i} \right\}_{S_{\eta i}}^{(\mu_\alpha \lambda_\alpha)} \rangle_{\alpha\lambda\mu}\mid \alpha_i(\lambda_i \mu_i)S_i \rangle .
\end{equation}

Here \(a_{\eta_j}^\dagger\) and \(a_{\eta_j}\) denote fermion creation and annihilation operators in the \(\eta\) major oscillator shell with SU(3) symmetry \((\eta 0)\) and \((0 \eta)\), respectively. It is a straightforward matter to generalize this expansion to three-body (and higher ranks, if necessary) operators.

Exploiting the SU(3)×SU(2) symmetry of the SA-NCSM basis states, it suffices to evaluate the following SU(3)-reduced matrix elements, r.m.e. (‘i’ for ‘initial’, ‘f’ for ‘final’, ‘o’ for ‘operator’):

\begin{equation}
\langle \alpha_f(\lambda_f \mu_f)S_f \mid \left\{ a_{\eta_j}^\dagger \otimes a_{\eta_j}^\dagger \right\}_{S_{\eta j}}^{(\lambda_\alpha \mu_\alpha)} \otimes \left\{ a_{\eta_i} \otimes a_{\eta_i} \right\}_{S_{\eta i}}^{(\mu_\alpha \lambda_\alpha)} \rangle_{\alpha\lambda\mu}\mid \alpha_i(\lambda_i \mu_i)S_i \rangle.
\end{equation}

As the SA-NCSM SU(3) configurations are constructed by coupling a sequence of single-shell SU(3) irreps that are physically allowed, the reduced matrix elements \((2)\) can be extracted from matrix elements between the highest-weight states of the single-shell SU(3) irreps (a SU(3) highest-weight state, which is annihilated by the raising SU(3) generators, is analogous to a \(J,M_F = J\) state for the case of the SU(2) group).

This factorization of matrix elements into the product of single-shell SU(3) r.m.e. and the associated SU(3) coupling coefficient, which can be calculated ‘on the fly’, reduces the number of calculations.
of key pieces of information required to the single-shell SU(3) r.m.e., and these track with the number of single-shell SU(3) highest-weight states. Clearly, compared to the explosive growth of the number of NCSM many-body configurations with increasing $N_{\text{max}}$ cutoff (Fig. 1a), the number of single-shell highest-weight states of the SA-NCSM (Fig. 1b) is manageable even, e.g., for ‘$pf$-shell’ nuclei and beyond.

![Figure 1.](image_url) Number of (a) NCSM many-body states and (b) all single-shell SU(3) × SU$_3$(2) highest-weight states of the SA-NCSM many-body model space as a function of the $N_{\text{max}}$ many-body cutoff for several representative nuclei in the $p$, $sd$, and $pf$ shells.

Furthermore, within the SA-NCSM 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 [10, 11] 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, 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-energy dynamics.

### 3. Symmetry-guided framework

The SA-NCSM model offers a natural organization of the model space (Fig. 2). In particular, in the SA-NCSM structured approach, the space is first separated into proton and neutron subspaces and then, in keeping with the $LS$ coupling foundation of the SA-NCSM, this is further organized according to the total proton spin ($S_\nu$) and neutron spin ($S_\pi$) coupled to total spin ($S$). These spin spaces can be further organized into SU(3) structures, each of which realizes a nuclear shape deformation given by ($\lambda\mu$).

This SA-NCSM framework allows users to down-select from all possible configurations to a subset that tracks with an inherent preference of a system towards low-spin and high-deformation dominance as revealed in realistic NCSM wavefunctions. For example, for the $0^+$ ground state in $^{12}$C, calculated by NCSM with JISP16 interaction for $\hbar\Omega = 15$ MeV [11], the SU(3) states that correspond to the most deformed oblate shape realize the major component of this state. As for the low-spin dominance, our recent study [12] showed the preponderance of only proton (neutron) spin values $S_\pi$ ($S_\nu$) = 0 and 1 for the $6\hbar\Omega$ NCSM results for $^{12}$C using the effective
Figure 2. Many-body SA-NCSM configurations for $^6$Li organized into proton-, neutron- and total-spin [SU$_S$(2)] and shape [SU(3)] sectors up through $N_{\text{max}} = 2$.

N$^3$LO interaction (and similarly for other interaction choices, such as JISP16) with $\hbar\Omega=15$ MeV. Specifically, $S_x \times S_y \rightarrow S$ with $0 \times 0 \rightarrow 0$, $0 \times 1 \rightarrow 1$, $1 \times 0 \rightarrow 1$, and $1 \times 1 \rightarrow 2$ are sufficient to describe 98.75%, 98.72%, and 98.82% of the converged $J = 0^+_\text{gs}$, $2^+_1$, and $4^+_1$ $^{12}$C NCSM eigenvectors, respectively, with a dominance of about 80% of the $0 \times 0 \rightarrow 0$ configurations. The residual roughly 1% of the wavefunctions involves time/memory consuming higher-spin and consequently less relevant configurations. Retaining only the most 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 $\hbar\Omega$ values. And since typically configurations of maximum spatial deformation also dominate, only a percentage of the proton(neutron)/spin subspace need be further considered to accommodate the physically most significant configurations, including particle-hole excitations that are important for a description of clustering modes, in higher $\hbar\Omega$ model spaces. Beyond these, the Sp(3, $\mathbb{R}$) symplectic symmetry can guide an extension of model spaces to incorporate even higher $\hbar\Omega$ values \cite{10} required to gain convergence of the lowest bound $0^+$ states in light nuclei.

As an illustration, we note that the \textit{ab initio} SA-NCSM and the symmetry-guided framework was employed for the $1^+$ ground state of $^6$Li with JISP16 ($\hbar\Omega=11$ MeV). The model space included all the configurations up through $N_{\text{max}} = 4$ (full space) with the $N_{\text{max}} = 6$ subspace
restricted to only 19 SU(3) × SU_S(2) configurations. These first examples illustrate the remarkable result that only a fraction of the model space yields high (99.6% for $^6$Li) overlap with the corresponding NCSM wavefunctions and most (98.7%) of the corresponding binding energy.

The symmetry-guided framework of the SA-NCSM is especially crucial for reaching heavier nuclei. An illustrative example is shown in Fig. 3 for the case of the $N \sim Z$ pf-nucleus $^{64}$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. 3, 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'.

In short, the SA-NCSM 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 $\text{Sp}(3,\mathbb{R}) \supset \text{SU}(3)$ 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

![Figure 3. Dimensions of various model spaces for $^{64}$Ge: conventional NCSM model spaces (blue squares) and reduced model space dimensions when only proton (neutron) $S_\pi$ ($S_\nu$) = 0 and 1 values coupled to total spin 0, 1 and 2 are considered (red diamonds) and when beyond this only 25%, 10% and 5% of the most deformed proton (neutron) SU(3) configurations are retained (yellow, green and purple triangles, respectively) as a function of $N_{\text{max}}$.](image-url)
region of the periodic table to investigation with *ab initio* methods with forefront predictive capabilities.

4. Conclusion
The SA-NCSM advances an extensible microscopic framework for studying nuclear structure and reaction processes – strong as well as weak interaction dominated, that capitalizes on advances being made in *ab initio* methods while exploiting symmetries – exact and partial, known to dominate the dynamics. We have developed a symmetry-adapted shell model with the view toward exploring the properties of nuclei far from stability using externally provided realistic interactions derived from Quantum Chromodynamics (QCD) considerations.

Winnowing considerations of the type shown above illustrate that the SA-NCSM 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. The method is applied first for light systems so the currently available *ab initio* methods can be used to guide the development, but ultimately pushing toward heavier ones that require symmetry guided winnowing decisions.

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