Ab Initio Symmetry-Adapted No-Core Shell Model

J P Draayer, T Dytrych, and K D Launey
Department of Physics and Astronomy, Louisiana State University,
Baton Rouge, LA 70803, USA
E-mail: draayer@lsu.edu

Abstract. A multi-shell extension of the Elliott SU(3) model, the SU(3) symmetry-adapted version of the no-core shell model (SA-NCSM), is described. The significance of this SA-NCSM emerges from the physical relevance of its SU(3)-coupled basis, which – while it naturally manages center-of-mass spuriosity – provides a microscopic description of nuclei in terms of mixed shape configurations. Since typically configurations of maximum spatial deformation dominate, only a small part of the model space suffices to reproduce the low-energy nuclear dynamics and hence, offers an effective symmetry-guided framework for winnowing of model space. This is based on our recent findings of low-spin and high-deformation dominance in realistic NCSM results and, in turn, holds promise to significantly enhance the reach of ab initio shell models.

1. Introduction

A quintessential goal of theoretical nuclear physics is to provide a detailed explanation of the properties of the atomic nucleus based on knowledge of the strong force between its constituents. When this goal is achieved, it will be possible to predict structures of exotic nuclei and reactions that take place in extreme environments – from the interiors of stars to the core of nuclear reactors. With a view toward this goal, the ab initio symmetry-adapted no-core shell model (SA-NCSM) aims to expand dramatically the reach as well as the impact of current ab initio shell models toward accommodating heavier mass nuclei together with highly deformed and cluster sub-structures. By effectively ferreting out important interactions at the fundamental quantum level, the SA-NCSM holds promise to achieve predictions of nuclear properties with unprecedented accuracy and provide a deeper understanding of the underlying forces.

Currently, the no-core shell model (NCSM) is used to reproduce features of the deuteron up through $^{16}$O and even for some selected cases beyond (e.g., see Refs. [1, 2] for NCSM and cluster NCSM/RGM results). The symmetry-adapted no-core shell model (SA-NCSM) approach augments the NCSM concept by recognizing that the choice of coordinates, especially when deformed nuclear shapes dominate, is crucial and presents a solution in terms of coordinates that reflect symmetries inherent to nuclear systems. While the SA-NCSM states can be obtained through a unitary transformation from the $m$-scheme basis used in the NCSM, the growth of the model space within the SA-NCSM framework can be managed by winnowing to only physically relevant states as determined through symmetry considerations.
2. Significance of an \textit{ab initio} symmetry-adapted no-core shell model

The underlying symmetry of the SA-NCSM is the SU(3) group, a subgroup of the physically relevant symplectic Sp(3, \mathbb{R}) group, which underpins a shell model that is known to provide a microscopic formulation of the famous Bohr-Mottelson collective model and to be a multiple oscillator shell generalization of the successful Elliott SU(3) model \cite{3}. Indeed, the significance of the symplectic symmetry for a microscopic description of a quantum many-body system of interacting particles \cite{3} naturally emerges from the physical relevance of its 21 generators, which are directly related to the particle momentum and coordinate operators and realize important observables, such as the many-particle kinetic energy, the mass quadrupole moment and angular momentum operators, together with multi-shell collective vibrations and vorticity degrees of freedom for a description from irrotational to rigid rotor flows. The translationally invariant (intrinsic) SU(3) generators can be written in terms of the harmonic oscillator raising (\(b^\dagger(1 0)\)) and lowering (\(b(0 1)\)) operators,

\[
C^{(1 1)}_{LM} = \sqrt{2} \sum_i \left[ b^\dagger_i \times b_i \right]^{(1 1)}_{LM} - \frac{\sqrt{2}}{A} \sum_{s,t} \left[ b^\dagger_s \times b_t \right]^{(1 1)}_{LM},
\]

where the sums are over all \(A\) particles of the system. The eight operators \(C^{(1 1)}_{LM}\) generate the SU(3) subgroup of Sp(3, \mathbb{R}) and are related to the angular momentum operator \(L_{1q} = C^{(1 1)}_{1q}\), \(q = 0, \pm 1\) and the Elliott algebraic quadrupole moment tensor \(Q^{(1 1)}_{2q}\) (\(= \sqrt{3}C^{(1 1)}_{2q}\), \(q = 0, \pm 1, \pm 2\)). 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, \((0 0)\), \((\lambda 0)\) and \((0 \mu)\) describe spherical, prolate and oblate shapes, respectively. Using conventional labels, the SU(3)\(\times\)SU(S(2) basis of the SA-NCSM is given as, \(|\alpha(\lambda \mu)\kappa(LS)JM_J\rangle\) with \(\alpha\) labeling the many-body configuration and \(\kappa\) distinguishing multiple occurrences of the same \(L\) value in the parent configuration \((S\text{ and } J\) denote spin and total angular momentum, respectively). This basis can be obtained as a unitary transformation from the NCSM \(m\)-scheme basis and hence, spans the entire space.

(a) Number of states \hspace{2cm} (b) Number of highest-weight states

\begin{figure} [h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Number of (a) NCSM many-body states and (b) all single-shell SU(3)\(\times\)SU(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.}
\end{figure}

The SA-NCSM implements a fast method for calculating matrix elements of arbitrary two-body operators in the SU(3)\(\times\)SU(S(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,

\[
\left\{ \alpha'_\eta, a^\dagger_{\eta j} \right\}_{S_{\alpha j}}^{(\lambda_\eta, \mu_\eta)} \otimes \left\{ a_{\eta i} \otimes a_{\eta k} \right\}_{S_{\alpha i}}^{(\mu_{\alpha i}, \lambda_{\alpha i})} \right]_{\alpha\lambda_{\alpha j}}^{(\lambda_\alpha, \mu_\alpha)}. \tag{2}
\]

Here \(a^\dagger_{\eta j}\) and \(a_{\eta j}\) denote fermion creation and annihilation operators in the \(\eta\) major oscillator shell with SU(3) symmetry \((\eta=0)\) and \((\eta=\eta)\), respectively. It is a straightforward matter to generalize this expansion for a three-body operator. Exploiting the SU(3)×SU(3) 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'):

\[
\langle \alpha_f (\lambda_f \mu_f) S_f \left| \right| \left\{ a^\dagger_{\eta i} \otimes a^\dagger_{\eta j} \right\}_{S_{\alpha i}}^{(\lambda_\eta, \mu_\eta)} \otimes \left\{ a_{\eta i} \otimes a_{\eta k} \right\}_{S_{\alpha i}}^{(\mu_{\alpha i}, \lambda_{\alpha i})} \right]_{\alpha_o (\lambda_o \mu_o)}^{(\lambda_\alpha, \mu_\alpha)} || \alpha_i (\lambda_i \mu_i) S_i \rangle. \tag{3}
\]

As the SU(3) configurations in the SA-NCSM are constructed by coupling a sequence of the physically allowed single-shell SU(3) representations, the reduced matrix elements (3) can be extracted from the full matrix elements between the highest-weight states of the single-shell SU(3) representations (a SU(3) highest-weight state, which is annihilated by the raising SU(3) generators, is analogous to a \(|J, M_J = J\rangle\) 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 key pieces of information required to the single-shell SU(3) r.m.e., and this 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.

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 [4, 5] that exploits symplectic Sp(3,\(\mathbb{R}\)) symmetry and its SU(3) subgroup symmetry in an analysis of large-scale nuclear physics applications for \(^{12}\text{C}\) and \(^{16}\text{O}\). 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 NCSM 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. Low-spin and high-deformation dominance

The symmetry-guided framework of the SA-NCSM utilizes a natural preference towards low-spin and high-deformation dominance as revealed in realistic NCSM wavefunctions. Specifically, our recent study [6] 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 \(\hbar\Omega=15\) MeV (Fig. 2), proton (neutron) spin values \(S_{\pi} (S_{\nu}) = 0\) and 1 are sufficient to describe about 99% of the converged \(J = 0^+\) and \(2^+\) and \(4^+\) \(^{12}\text{C}\) NCSM eigenvectors. The residual 1% involves time/memory consuming higher-spin and consequently less relevant configurations. Similarly, contributions from high \(S_{\pi} (S_{\nu})\) proton (neutron) spin values are found negligible for the \(J = 1\) state of \(^{12}\text{C}\) shown in Fig. 3 for two JISP16 and N\(^3\)LO effective interactions for \(\hbar\Omega=15\) MeV. 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 $\hbar\Omega$ values.

Furthermore, in a proton-neutron formalism, the spin quantum numbers dictate, within a single shell, the spatial symmetry because the fermion statistics requires overall antisymmetry within each sector. Hence, low-spin implies maximum spatial symmetry, which is where one finds the SU(3) configurations of maximum spatial deformation. Indeed, for the $0^+_1$ ground state in $^{12}\text{C}$, calculated by NCSM with JISP16 interaction for $\hbar\Omega = 15$ MeV [5], the SU(3) states that correspond to the most deformed oblate shape realize the major component of this state (Fig. 4).

4. Symmetry-guided framework

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. This is illustrated in Fig. 5, 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-NCSM (b). 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 ($S$). This
Figure 4. Probabilities (specified by the area of the circles) for the symplectic states which make up the most important 0-particle-0-hole (0p-0h) (blue circles) and 2ℏΩ 2p-2h (empty circles) symplectic irreps, within the 0\(^+\) ground state in \(^{12}\text{C}\), calculated by NCSM with JISP16 interaction, ℏΩ = 15 MeV. The Sp(3, R) states are grouped according to their \((\lambda_ω, μ_ω)\) SU(3) symmetry, which is mapped onto the \((βγ)\) shape variables of the collective model.

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. 5). 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 ℏΩ model spaces (e.g., \(N_{\text{max}} = 10 – 12\) in Fig. 5). And beyond these, the Sp(3, R) symplectic symmetry can guide an extension of model spaces to incorporate even higher ℏΩ values (e.g., \(N_{\text{max}} = 14 – 16\) in Fig. 5) \textsuperscript{[4]} required to gain convergence of the lowest bound 0\(^+\) states in light nuclei (green cones in Fig. 5).

An illustrative example for the symmetry-guided framework of the SA-NCSM is shown in Fig. 6 for the case of the \(N ∼ Z\) 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. 6, we chose to retain only proton (neutron) spin values \(S_π = 0\) and 1 \((S_ν = 0\) 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) [7], 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-NCSM, we suggest a SU(3)-based SRG renormalization [8], 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-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 $Sp(3,\mathbb{R}) \supset SU(3)$ 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 \textit{ab initio} methods with forefront predictive capabilities.
Figure 6. Dimensions of various model spaces for $^{64}_{32}$Ge: conventional NCSM model spaces (blue squares) and reduced model space dimensions when only proton (neutron) $S_p$ ($S_n$) = 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 $N_{\text{max}}$.

5. 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. 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 towards heavier ones that will require symmetry guided winnowing decisions.

Supported by the U.S. National Science Foundation (PHY-0500291 & OCI-0904874), the U.S. Department of Energy (DE-SC0005248), and the Southeastern Universities Research Association (http://www.sura.org).

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