Symmetry-Adapted *Ab Initio* Shell Model for Nuclear Structure Calculations

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Abstract. An innovative concept, the symmetry-adapted *ab initio* shell model, that capitalizes on partial as well as exact symmetries that underpin the structure of nuclei, is discussed. This framework is expected to inform the leading features of nuclear structure and reaction data for light and medium mass nuclei, which are currently inaccessible by theory and experiment and for which predictions of modern phenomenological models often diverge. We use powerful computational and group-theoretical algorithms to perform *ab initio* CI (configuration-interaction) calculations in a model space spanned by SU(3) symmetry-adapted many-body configurations with the JISP16 nucleon-nucleon interaction. We demonstrate that the results for the ground states of light nuclei up through $A = 16$ exhibit a strong dominance of low-spin and high-deformation configurations together with an evident symplectic structure. This, in turn, points to the importance of using a symmetry-adapted framework, one based on an LS coupling scheme with the associated spatial configurations organized according to deformation.

1. Introduction

With considerable progress made in recent years in the development of realistic two- and three-nucleon interactions (e.g., [1, 2, 3, 4]), *ab initio* approaches [5, 6, 7], which build on fundamental principles, have successfully described properties of light nuclei while establishing a link between few-nucleon interactions, linked to Quantum Chromodynamics (QCD) considerations, and many-body nuclear dynamics. The predictive power of these approaches to nuclear structure and reactions depends critically on the choice of the realistic interaction and on the ability of the underlying theory, while restricted to available computational resources, to describe multifaceted properties of atomic nuclei from single-particle effects to collective phenomena. For example, light nuclei with equal numbers of protons and neutrons ($N = Z$) and total particle numbers that are multiples of four ($4n$ systems) display a complex pattern in their low-lying energy spectra with certain states continuing to remain a challenge for *ab initio* techniques. An important example of such a configuration is the first excited $0^+$ state in $^{12}$C (with impact on stellar evolution and nucleosynthesis); another is the first excited $0^+$ state in $^{16}$O.

The no-core shell model (NCSM) [5] is an *ab initio* configuration-interaction (CI) method that has achieved a good description of low-lying states and nuclear reactions for nuclei up through the $p$ shell [8, 9, 10, 11]. This method uses the Lanczos algorithm to compute the lowest few eigenvalues and associated eigenstates of a realistic Hamiltonian matrix whose elements are...
calculated in an $m$-scheme basis, i.e. a basis of Slater determinants constructed from single-particle wavefunctions of the harmonic oscillator. The main limitation of this approach, and its predictive power, is inherently coupled with the combinatorial growth of the $m$-scheme basis with increasing nucleon number and maximal number of total harmonic oscillator quanta $N_{\text{max}}$.

We have developed a next-generation \textit{ab initio} model, the \textit{ab initio} symmetry-adapted no-core shell model (SA-NCSM), that adopts the first-principle concept, and capitalizes on exact and approximate symmetries of nuclei. Our goal is, using the SA-NCSM model, to reproduce and predict properties of heavy as well as light nuclei, starting with and building upon QCD-informed and inspired interactions. This study focuses on the following current and near-future developments:

- Exploit the existing NCSM technology to prove the method efficacy, revealing (or not) any inherent limitations.
- Explore the need (or not) for interaction renormalization, as well as for winnowing of the model space to physically relevant and tractable subspaces.
- Evaluate the extensibility of the theory and its characteristics vis-à-vis the current as well as emerging computational resources.
- Study the emergence of collective phenomena and tracking their evolution to fundamental features of the interaction.
- Apply the theory to studies of extreme phenomena known to be important to understanding nuclear systems.
- Extend the theory to include coupling to the continuum, and apply the results to studies of nuclear reactions.
- Develop a user friendly desktop version of the SA-NCSM code for simple applications as well as educational and training purposes.

The significance of the SU(3) group, used in the SA-NCSM to construct the many-body basis, for a microscopic description of the nuclear collective dynamics can be seen from the fact that it is the symmetry group of the Elliott model [12], and a subgroup of the Sp(3,$\mathbb{R}$) symplectic model [13]. Hence, the SA-NCSM holds promise to expand the reach as well as the impact of current \textit{ab initio} approaches toward describing heavier mass nuclei together with collective, 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 a solution in terms of coordinates that reflect symmetries inherent to the nuclear system. While the SA-NCSM states can be obtained through a unitary transformation from the $m$-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 to only physically relevant states as determined through symmetry considerations.

2. SU(3) Symmetry-Adapted Theoretical Framework

The basis states of the \textit{ab initio} SA-NCSM are constructed in the proton-neutron formalism and are labeled by the physical SU(3)$\supset$SO(3) subgroup chain quantum numbers $(\lambda \mu)\kappa L$, and by proton, neutron, and total intrinsic spins $S_\pi$, $S_\nu$, 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 $|\gamma(\lambda \mu)\kappa L; (S_\pi S_\nu)S; JM_J\rangle$, where the set of deformation-related $(\lambda \mu)$ quantum numbers labels irreducible representations (irreps) of SU(3) that bring forward important information about nuclear shapes and deformation. For example, (00), (0$\lambda$0) and (00$\mu$) describe spherical, prolate and oblate shapes, respectively. The label $\kappa$ distinguishes multiple occurrences of the same $L$ value in the parent irrep $(\lambda \mu)$, and $\gamma$ distinguishes among configurations carrying the same $(\lambda \mu)$ and $(S_\pi S_\nu)S$ labels.
Figure 1. Probability distribution of the lowest calculated $0^+$ state for $^{12}\text{C}$ over deformed subspaces labeled by $(\lambda \mu)$ for six of the most important spin components $\{S_x, S_y, S_z\} = \{0, 0, 0\}, \{1, 0, 1\}, \{0, 1, 1\}, \{1, 1, 1\}, \{1, 1, 0\}$ and $\{1, 1, 2\}$. Blue labels denote SU(3) quantum labels of basis states that belong to the leading $(0^4)$ symplectic Sp(3, R) irrep. The wavefunction was obtained using the $N_{\text{max}} = 6$ SA-NCSM with the JISP16 bare interaction and $\hbar \Omega = 10$ MeV.

The SA-NCSM implements a set of powerful algorithms [14, 15], which facilitate calculations of matrix elements of arbitrary (currently up to two-body, but expandable to higher-rank) operators in the SU(3)-scheme basis. The underlying principle behind the SA-NCSM computational kernel is a SU(3)-type Wigner-Eckhart theorem that enables a factorization of the problem into reduced matrix elements ($r\text{mes}$) and SU(3) coupling/recoupling coefficients. While the latter can be computed using the publicly available library [16], the former is calculated from a set of single-shell $r\text{mes}$ by the repetitive application of a SU(3)-type reduction formula for $r\text{mes}$ of operators acting on two independent subsystems. The resulting algorithm is very general; it allows for the evaluation of the Hamiltonian matrix elements and the use of the resulting eigenvectors to determine other experimental observables.

3. Results and Discussions

We calculated low-lying wavefunctions and some associated physical observables for $^6\text{Li}$, $^7\text{Li}$, $^{12}\text{C}$, and $^{16}\text{O}$, using the bare JISP16 interaction [1] for $N_{\text{max}} = 6$ and $\hbar \Omega = 10$ MeV, and compared our results with those obtained using the $m$-scheme based NCSM approach. To demonstrate the efficacy of the symmetry-adapted selection scheme of the SA-NCSM, ab initio SA-NCSM calculations for the ground state of $^6\text{Li}$ and $^7\text{Li}$ were carried out. The model space included all
Figure 2. Probability distribution of the calculated $0^+$ state for $^{12}$C over deformed subspaces labeled by $(\lambda \mu)$ for six of the most important spin components \(\{S_\pi, S_\nu, S\} = \{0, 0, 0\}, \{1, 0, 1\}, \{0, 1, 1\}, \{1, 1, 1\}, \{1, 1, 0\}\) and \{1, 1, 2\}. Green SU(3) labels denote physically allowed configurations of the $^8$Be$^+$$^4$He cluster basis states. The wavefunction was obtained using the $N_{\text{max}} = 6$ SA-NCSM with the JISP16 bare interaction and $\hbar \Omega = 10$ MeV.

the configurations up through $N_{\text{max}} = 4$ (full space) with the $N_{\text{max}} = 6$ subspace restricted to only a few SU(3) and S configurations. The outcome points to the remarkable result that only a small fraction of the model space ($19$ SU(3) configurations for $^6$Li and $15$ SU(3) configurations for $^7$Li) yields high overlap with the corresponding NCSM wavefunction and furthermore, most ($\sim 99\%$ for $^6$Li and $\sim 97\%$ for $^7$Li) of the corresponding binding energy.

In addition, the ab initio $N_{\text{max}} = 6$ SA-NCSM results for the $0^+$ ground state of $^{12}$C reveal the dominance of the $0\hbar \Omega$ component with the foremost contribution coming from the leading (0 4) $S = 0$ irrep (Fig. 1). We find that important SU(3) configurations are typically organized into structures with Sp(3, R) symplectic symmetry. For example, the (0 4) symplectic irrep gives rise to (0 2) and (2 4) configurations in the $2\hbar \Omega$ subspace, as shown in the insert of Fig. 1, and those configurations indeed realize the major components of the wavefunction in this subspace. This further confirms the significance of the symplectic symmetry to nuclear dynamics. Similar results are observed for the $0^+$ ground state of $^{16}$O. The outcome points to the fact that the relevant model space can be systematically selected and further expanded to higher $N_{\text{max}}$. Another interesting result is related to the ‘Hoyle’ state, the second $0^+$ state in $^{12}$C that lies at 7.65 MeV and is of particular astrophysical interest. However, its ab initio description still remains beyond the reach of traditional NCSM calculations. Due to the presence of alpha-
cluster structures, achieving convergence of this state requires ultra-large NCSM basis spaces for \( N_{\text{max}} \) considerably higher than the cutoffs currently considered. Nonetheless, in the SA-NCSM framework, it is now possible to identify the ‘Hoyle’ state and to study its structure. In particular, the lowest ten \( 0^+ \) states in \(^{12}\text{C} \) as obtained in \( N_{\text{max}} = 6 \) SA-NCSM calculations using the JISP16 interaction were examined for characteristic SU(3) configurations that could point to a cluster structure. These configurations, given in the insert of Fig. 2, can be easily understood in the framework of a microscopic cluster model, which builds upon \(^8\text{Be} + ^4\text{He} \) clusters and yields physically allowed deformations of the compound \(^{12}\text{C} \) system. Among all excited \( 0^+ \) states, only the sixth \( 0^+ \) state reveals a pronounced pattern predominantly comprised of the characteristic deformations (Fig. 2). Hence, it is this state that is expected to converge to the 7.65-MeV \( 0^+ \) of \(^{12}\text{C} \) for large \( N_{\text{max}} \) spaces, with higher-lying configurations, such as \((12 \, 0)\), \((14 \, 0)\) and \((16 \, 0)\) expected to grow in importance.

4. Conclusion
The SA-NCSM advances an extensible microscopic framework for studying nuclear structure and reactions that capitalizes on advances being made in \textit{ab initio} methods while exploiting symmetries – exact and partial, known to dominate the dynamics. We have developed a symmetry-adapted \textit{ab initio} shell-model code with the view toward exploring the properties of nuclei far from stability using externally provided realistic interactions derived from Quantum Chromodynamics (QCD) considerations. This, in turn, allows us to begin to address, in a focused way, the origin of collective degrees of freedom in nuclei, that is, the emergence of collectivity from fundamental principles.

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