Symmetry-Adapted Ab Initio Open Core Shell Model Theory

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Abstract. By using only a fraction of the model space, we gain further insight – within a symmetry-guided no-core shell model framework – into the many-body nuclear dynamics that gives rise to important single-particle configurations together with correlated highly-deformed and alpha-cluster structures. We show results of the novel\textit{ab initio} symmetry-adapted no-core shell model for large-scale nuclear structure computations. In addition, we use the symmetry patterns unveiled in these results to explore ultra-large model spaces.

1. Introduction
The major progress achieved during the recent years in high performance computing and in the internucleon interactions derived from first principles [1, 2] have placed \textit{ab initio} many-body approaches at the frontier of nuclear structure explorations [3, 4, 5, 6, 7]. The ultimate goal of \textit{ab initio} nuclear structure modeling is to establish a link between the underpinning principles of Quantum Chromodynamics (quark/gluon considerations) and properties of atomic nuclei, and in doing so, to use the predictive capabilities toward providing reliable descriptions of nuclei far off the valley of stability. This, in turn, yields highly accurate nuclear wave functions, which are key ingredients to calculating observables for nuclei and reactions in extreme environments, from the interiors of stars to the core of nuclear reactors.

We present first results of an innovative \textit{ab initio} model, the symmetry-adapted no-core shell model (SA-NCSM) [8, 9]. It utilizes an SU(3)-symmetric basis, which is related – via a unitary transformation – to the three-dimensional harmonic oscillator (HO) many-body basis (m-scheme) used in the no-core shell model (NCSM) [3, 7]. In particular, we show that \textit{ab initio} SA-NCSM calculations for p-shell nuclei in full space (equivalent to the NCSM results) reveal a clear Sp(3, R) symplectic structure with no \textit{a priori} restrictions to the symplectic symmetry. This, in turn, allows the growth of the model space within the SA-NCSM framework to be managed by winnowing to only physically relevant states as determined through symmetry considerations, thereby overcoming a prime bottleneck of the NCSM – the combinatorial growth of many-body basis with number of nucleons and model space truncation, $N_{\text{max}}$. As a complementary study, we examine the significance of employing ultra-large model spaces, much beyond the current
\( N_{\text{max}} \) limit. Specifically, we employ the no-core symplectic model (NCSpM) that utilizes the \( \text{Sp}(3, \mathbb{R}) \) symplectic basis, which can also be obtained via a unitary transformation from the NCSM \( m \)-scheme basis. We start with selected \( \text{Sp}(3, \mathbb{R}) \) symplectic structures, those that are found most important in the \textit{ab initio} results, and in addition, we use a simple internucleon interaction with only one adjustable parameter. This enables one to accommodate, for the first time, shell-model basis spaces that are believed to be essential to achieve convergence of, e.g., alpha-cluster states. The results for \( ^{12}\text{C} \) reveal that a large-\( N_{\text{max}} \) model space is indeed the key to describe – in a NCSM framework – the ‘Hoyle’ state, the second 0\(^+\) state in \( ^{12}\text{C} \) at 7.65 MeV, that is of particular astrophysical interest.

2. \textit{Ab initio} SA-NCSM Results: Symmetry Patterns

The \textit{ab initio} SA-NCSM adopts the first-principle concept and utilizes a many-particle basis that is reduced with respect to the physically relevant SU(3)\( \supset \)SO(3) subgroup chain. The significance of the SU(3) group 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 \cite{10, 11, 12}, and a subgroup of the \( \text{Sp}(3, \mathbb{R}) \) symplectic model \cite{13}. By recognizing that the choice of coordinates, especially when deformed nuclear shapes dominate, is crucial, the SA-NCSM affords a solution in terms of coordinates that reflect symmetries inherent to the nuclear system. This allows the full model space to be down-selected to the physically relevant space.

The \( C^{(11)}_{\Delta M} \) translationally invariant (intrinsic) eight generators of the SU(3) group can be written in terms of particle position and momentum coordinates and are related to the angular momentum operator \( L_{1q} \), the in-shell quadrupole moment tensor \( Q_{2q} \), and the deformation-related \( \langle \lambda \mu \rangle \) 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 \( \langle \lambda \mu \rangle \), for example, \( (0 0) \), \( (\lambda 0) \) and \( (0 \mu) \) describe spherical, prolate and oblate shapes, respectively.

The conventional NCSM basis spaces are constructed using HO single-particle states and are characterized by the \( \hbar \Omega \) oscillator strength as well as by the cutoff in total oscillator quanta, \( N_{\text{max}} \), above the lowest energy configuration for a given nucleus. The basis states of the SA-NCSM for a given \( N_{\text{max}} \) are constructed in the proton-neutron formalism using also HO single-particle states and are labeled by the SU(3)\( \supset \)SO(3) subgroup chain quantum numbers \( \langle \lambda \mu \rangle \kappa L \), together with 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 \( |\gamma (\lambda \mu) \kappa L; (S_{\pi}S_{\nu})S; JM_{J} \rangle \). 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 \( \langle \lambda \mu \rangle \) and \( (S_{\pi}S_{\nu})S \) labels.

The \textit{ab initio} SA-NCSM results for \( p \)-shell nuclei, such as \( ^{6}\text{Li}, ^{8}\text{B}, ^{12}\text{C} \) and \( ^{16}\text{O} \), reveal a dominance of shapes of large deformation (typically large \( |\lambda - \mu| \)) in the \( 0\hbar \Omega \) subspace. Furthermore, we find that important SU(3) configurations are then organized into structures with \( \text{Sp}(3, \mathbb{R}) \) symplectic symmetry. As an example, for the ground state of \( ^{6}\text{Li} \) calculated using the bare JISP16 realistic interaction \cite{14} for \( N_{\text{max}} = 10 \) and \( \hbar \Omega = 20 \) MeV, results indicate a clear dominance of the spin configuration, \( \{S_{\pi} = 1/2, S_{\nu} = 1/2, S = 1\} \), and the most deformed shapes, \( (2 0) \), \( (4 0) \), \( (6 0) \), \( (8 0) \), \( (10 0) \), and \( (12 0) \) in each \( \hbar \Omega \) subspace \cite{15}. In the case of \( ^{6}\text{Li} \), the \( (2 0) \) symplectic irrep gives rise to \( (0 2) \), \( (2 1) \) and \( (4 0) \) configurations in the \( 2\hbar \Omega \) subspace, 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 ground and low-lying excited states of \( ^{8}\text{B}, ^{12}\text{C} \) and \( ^{16}\text{O} \). The outcome points to the fact that the relevant model space can be systematically down-selected and further
expanded to higher $N_{\text{max}}$. For example, only 11% of the total space dimension is needed to yield 99% of the matter rms radius and the $M1$ moment calculated in full space.

In short, 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.

3. NCSpM: Highly-Deformed Structures in Ultra-large Model Spaces

The NCSpM, while selecting the most relevant symplectic configurations, is employed to provide shell model calculations beyond current NCSM limits, namely, up through $N_{\text{max}} = 20$ for $^{12}$C, the model space we found sufficient for the convergence of results. Clearly, the NCSpM employed within a full model space up through a given $N_{\text{max}}$, will coincide 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 Sp(3, $\mathbb{R}$) irreps within the $N_{\text{max}}$ model space.

The basis states of an Sp(3, $\mathbb{R}$) irrep (slice) are built by $2\hbar\Omega$ 1-particle-1-hole (1p-1h) monopole or quadrupole excitations (one particle raised by two shells) over a bandhead together with a smaller $2\hbar\Omega$ 2p-2h correction for eliminating the spurious center-of-mass (CM) motion. The symplectic bandhead is the lowest-weight Sp(3, $\mathbb{R}$) state, which is defined by the usual requirement that the symplectic lowering operators annihilate it – in analogy to a $\{J, M_j = -J\}$ state for the case of the SU(2) group of angular momentum $J$. The bandhead is a SU(3)-coupled many-body state with a given nucleon distribution over the HO shells. The corresponding energy of HO quanta, $N_\sigma\hbar\Omega$, together with the bandhead shape serve to label the symplectic irrep [e.g., for $^{12}$C, one of the Sp(3, $\mathbb{R}$) irrep is $N_\sigma = 24.5$ (0 4) or, equally, $0\hbar\Omega$ (0 4)]. The basis states within an irrep are, in addition, specified by the number of HO excitation quanta above $N_\sigma$ and by the resulting ($\lambda\mu$) deformation of the bandhead due to these excitations [e.g., for the $^{12}$C $4\hbar\Omega$ (120)] irrep, the $n = 2$ basis states ($2\hbar\Omega$ excitations) include (140), (121), and (102) shapes, and so forth for higher $n$.

In this study we employ a very simple Hamiltonian with an effective interaction derived from the long-range expansion of the two-body central nuclear force,

$$H_{\text{eff}} = H_0 - \frac{\chi}{2} \gamma \left( e^{\gamma(Q.Q-(Q.Q)_{\text{init}})} - 1 \right),$$

where $\gamma$ includes the spherical HO potential (which together with the kinetic energy yields the HO Hamiltonian, $H_0$) and the $Q.Q$ quadrupole-quadrupole interaction not restricted to a single shell. For the latter term, the average contribution, $(Q.Q)_n$, of $Q.Q$ within a subspace of $n$ HO excitations is removed [16], that is, the trace of $Q.Q$ divided by the space dimension for a fixed $n$. Hence, the large monopole contribution of the $Q.Q$ interaction is removed, which, in turn, helps eliminate the considerable renormalization of the zero-point energy, while retaining the $Q.Q$-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 [10, 12]. We take the coupling constant $\chi = \hbar\Omega/(4\sqrt{N_fN_i})$ with $N$ for the initial (i) and final (f) many-body states, where the quantum number $N = N_\sigma + n$ is the total number of HO excitations. The decrease of $\chi$ with $N$, to leading order in $\lambda/N$, has been shown by Rowe [17] based on self-consistent arguments. It is important to note that such a model Hamiltonian (1) fixes the strength of the $Q.Q$-term by the value of $\hbar\Omega$, thereby rendering the eigenstates $\hbar\Omega$-independent.

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. The low-lying energy spectrum and eigenstates for $^{12}$C were calculated using the NCSpM with $H$ of Eq. (1)
for $\hbar \Omega = 18$ MeV given by the empirical estimate $\approx 41/A^{1/3} = 17.9$ MeV. 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 all multiples thereof up through $N_{\text{max}} = 20$ of total dimensionality of $4.5 \times 10^3$. In comparison to the experimental energy spectrum (Fig. 3), the outcome reveals that the lowest $0^+$, $2^+$, and $4^+$ states of the $0\hbar \Omega 0p-0h$ (04) symplectic irrep calculated for $\gamma = -1.71 \times 10^{-4}$ 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. It is interesting to point out that, for small $N_{\text{max}}$, the $0^+$ state of (62) appears much lower in energy compared to the $0^+$ state of (120). However, the latter starts to dramatically drop as $N_{\text{max}}$ increases and aligns with the $0^+$ state of (62) around $N_{\text{max}} = 12$, falling further down for larger $N_{\text{max}}$. Clearly, the mechanism of lowering the highly-deformed (120) emerges from the fact that sufficiently large model spaces allow for the collectivity to develop, thereby, making the $0^+$ state of (120) energetically favorable.

We note that the energy spectrum, calculated in the NCSpM and shown in Figure 3, is rescaled by an overall factor of $\sim 2$. This factor is determined by fixing the lowest $2^+$ by its experimental value. This, however, has no implications on the underlying physics, as an overall factor for $H$ does not change its properties and eigenstates, together with associated observables. For example, the $B(E2; 2^+ \rightarrow 0^+ g.s.)$ is calculated to be 5.12 W.u., also in a close agreement with the 4.65 W.u. experimental measurement. While the model includes an adjustable parameter, $\gamma$, this parameter only controls the decrease rate of the $Q.Q$ interaction with increasing $n$. The entire many-body apparatus is fully microscopic and no adjustments are possible. Hence, as $\gamma$ varies, there is only a small window of possible $\gamma$ values that, for large enough $N_{\text{max}}$, closely reproduces the relative positions of the three lowest $0^+$ states. As for the ground-state rotational band, the $\gamma$ parameter has almost no effect on the energies and transition rates.

In short, the present microscopic study with a schematic many-nucleon interaction shows how both collective and cluster-like structures emerge out of a no-core shell-model framework, which can extend to and take into account essential high-lying shell-model configurations.
4. Conclusion
We have presented first results of the SA-NCSM, a fully microscopic theory designed to accept QCD-inspired interactions. We are beginning to observe collective features in the structure of the calculated eigenstates, but not always at the excitation energies found in nature. We have also observed that a simple part of the long-range nuclear force is sufficient to bring such states to the measured energies provided that high-lying shell-model configurations are taken into account. Hence, we are well-positioned to link to QCD considerations, but also to begin to address in a focused way the origin of collective degrees of freedom in nuclei and the underlying physics, that is, the emergence of collectivity from fundamental principles.

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