

Ab Initio No-core Shell Model Calculations in SU(3)-scheme Basis

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Abstract. The predictive power of ab initio approaches to nuclear structure depends critically on the choice of a realistic nuclear potential, and on the ability of a finite model space to describe multifaceted properties of atomic nuclei emerging from the underlying nuclear forces. We use powerful algorithms of the computational group theory to perform ab initio configuration-interaction calculations in the model space spanned by SU(3) symmetry-adapted many-body configurations. We demonstrate that the results for the ground states of ⁶Li, ⁷Li, ¹²C, and ¹⁶O exhibit a strong dominance of low proton, neutron, and total intrinsic spins, and carry the same spatial deformations as the leading symplectic Sp(3, \mathbb{R}) irreducible representations. We also find states dominated by the α -clustering correlations among the lowest lying 0^+ eigenstates of ¹²C and ¹⁶O. Our findings imply that only a small fraction of the complete model space is needed to model nuclear collective dynamics, deformations, and α -particle clustering even if one uses a modern realistic interactions that do not preserve SU(3) symmetry. This in turn points to the importance of using a symmetry-adapted CI framework, one based on an LS coupling scheme with the associated spatial configurations organized according to deformation.

1 Introduction

The ab initio approaches to studies of light atomic nuclei [1–3] represent forefront research area of contemporary nuclear structure physics. They are built on fundamental principles and therefore hold promise to provide predictive capabilities essential for a description of structure and reactions of unstable and exotic nuclei, many of which are of high interest, e.g. in nucleosynthesis, but remain inaccessible even to experiment.

The no-core shell model (NCSM) [1] is ab initio configuration-interaction (CI) method that has achieved a good description of low-lying states and nuclear reactions up through p-shell nuclei [4–7]. This method uses Lanczos algorithm to compute few lowest-lying eigenstates and eigenvalues of a realistic Hamiltonian matrix whose elements are calculated in an m -scheme basis, *i.e.* basis of Slater determinants constructed from single-particle wave functions of the harmonic oscillator. The main limitation of this approach, and its predictive power

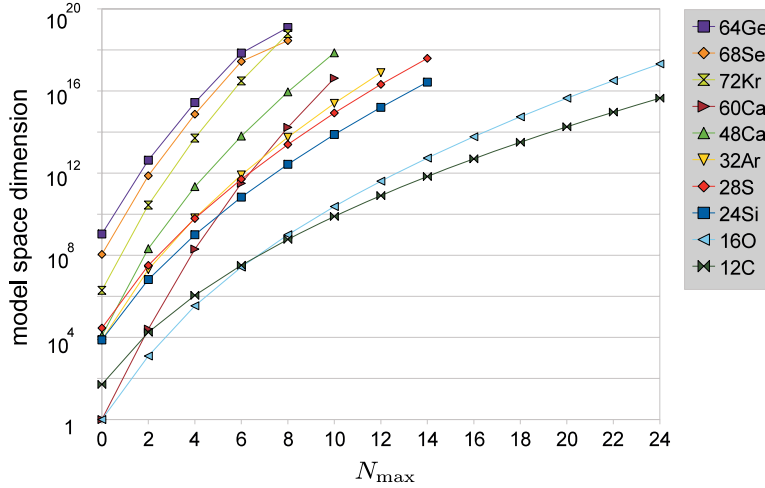


Figure 1. Number of NCSM many-body states as a function of the N_{\max} many-body cutoff for several representative nuclei in the p-, sd-, and pf-shells.

thereof, 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_{\max} as illustrated in Figure 1.

We offer a novel model, the ab initio symmetry-adapted no-core shell model (SA-NCSM), that adapts the ab initio concept and in addition, utilizes many-body basis that reduces the physically relevant $SU(3) \supset SO(3)$ subgroup chain. The significance of $SU(3)$ group for a microscopic description of the nuclear collective dynamics can be seen from the fact that it is the symmetry group of the Elliot model [8], and a subgroup of the $Sp(3, \mathbb{R})$ symplectic model [9]. Hence, the SA-NCSM holds promise to expand the reach as well as the impact of current 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 solution in terms of coordinates that reflect symmetries inherent to nuclear systems.

2 Ab Initio Calculations in $SU(3)$ Symmetry-Adapted Basis

The basis states of the 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_π , S_ν , 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 is thus labeled in the $SU(3)$ -scheme as

$$|\vec{\alpha} S_\pi S_\nu S(\lambda \mu) \kappa L J M_J\rangle, \quad (1)$$

where the deformation-related $(\lambda \mu)$ set of quantum numbers labels SU(3) irreducible representations, irreps, and bring forward important information about nuclear shapes and deformation. For example, (00) , $(\lambda 0)$ and (0μ) describe spherical, prolate and oblate shapes, respectively. The label κ distinguishes multiple occurrences of the same L value in the parent irrep $(\lambda \mu)$. Symbol $\vec{\alpha}$ schematically denotes the additional quantum numbers needed to unambiguously distinguish between irreps carrying the same $S_\pi S_\nu S(\lambda \mu)$ quantum numbers. These irreps compose a well defined subspace with a very unique ability to completely separate intrinsic and center-of-mass degrees of freedom. Size of these subspaces is typically several orders of magnitude smaller than the full $N\hbar\Omega$ space, where the m -scheme basis allows exact factorization of center-of-mass degrees of freedom. The decomposition of the SA-NCSM model space of ${}^6\text{Li}$ up through $N_{\text{max}} = 2$ model space is depicted in Figure 2.

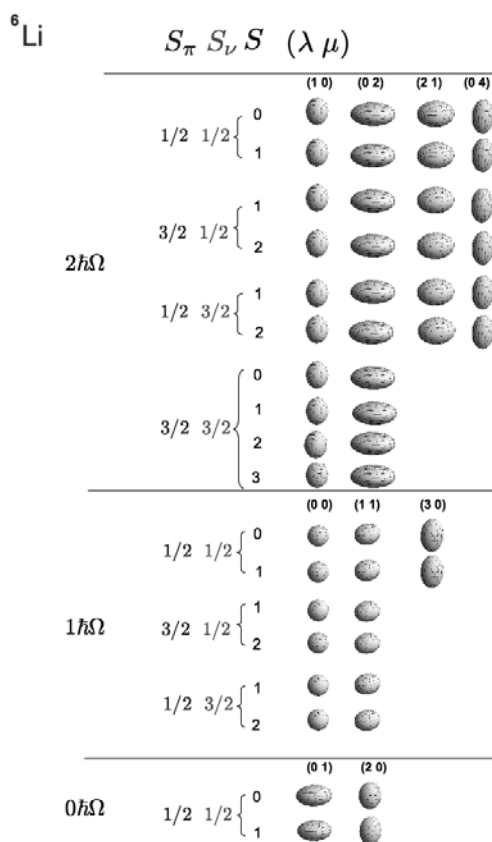


Figure 2. Pauli-allowed deformations $(\lambda \mu)$ and their proton, neutron, and total intrinsic spins $S_\pi S_\nu S$ for the many-body SU(3)-scheme configurations of ${}^6\text{Li}$ up through $N_{\text{max}} = 2$.

The SA-NCSM implements a set of powerful algorithms [10, 11], 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, which factorizes the problem into reduced matrix elements (*rmes*) and $SU(3)$ coupling/recoupling coefficients. While the latter can be computed using the publicly available library [12], the former is calculated from a set of single-shell *rmes* by the repetitive application of a $SU(3)$ -type reduction formula for *rmes* of operators acting on two independent subsystems. The algorithm is very general, and hence allows both, the evaluation of the Hamiltonian matrix elements, and the use of the resulting eigenvectors to evaluate other experimental observables.

3 Results

We calculated the lowest-lying wave functions and physical observables for ${}^6\text{Li}$, ${}^7\text{Li}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$, using the bare JISP16 potential [13] for $N_{\text{max}} = 6$ and $\hbar\Omega = 10$ MeV, and compare our results with those obtained by the *m*-scheme based NCSM approach. This stringent test yields the agreement up to 10^{-4} between the two ab initio approaches, and hence further validates the SA-NCSM approach.

3.1 Symmetry-Adapted Selection Scheme of SA-NCSM

In order to demonstrate efficacy of the symmetry-adapted selection scheme, we show ab initio SA-NCSM calculations for the ground state of ${}^6\text{Li}$ and ${}^7\text{Li}$ with the bare JISP16 interaction for $N_{\text{max}} = 6$ and $\hbar\Omega = 10$ MeV (Figure 3 and Figure 4). The model space includes all the configurations up through $N_{\text{max}} = 4$

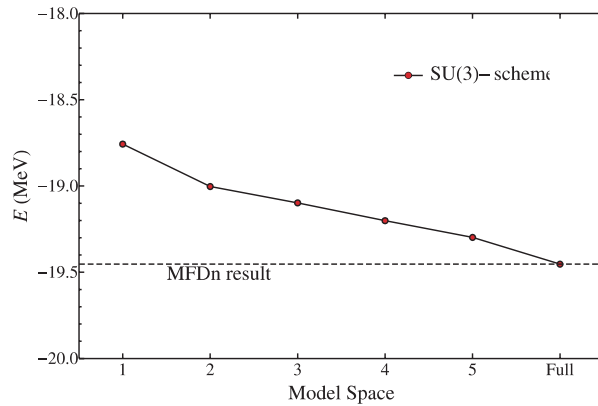


Figure 3. Ground-state binding energy of ${}^6\text{Li}$ for the model spaces (2) in comparison to the full $N_{\text{max}} = 6$ result of $SU(3)$ -shell and MFDn (vertical line).

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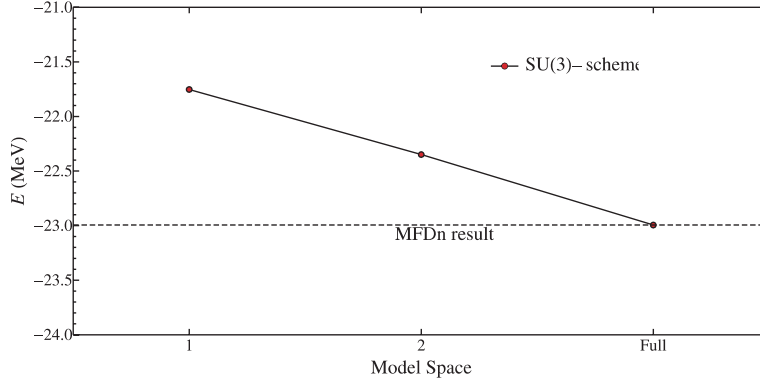


Figure 4. Ground-state binding energy of ${}^7\text{Li}$ for the model spaces (3) in comparison to the full $N_{\text{max}} = 6$ result of SU(3)-shell and MFDn (vertical line).

(full space) with the $N_{\text{max}} = 6$ subspace restricted to only a few SU(3) and S configurations. Definition of the symmetry selected model spaces for the ground state of ${}^6\text{Li}$,

$$\begin{aligned}
 1 & : \{N_{\text{max}} = 4\} \oplus A \\
 2 & : \{N_{\text{max}} = 4\} \oplus A \oplus B \\
 3 & : \{N_{\text{max}} = 4\} \oplus A \oplus B \oplus C \\
 4 & : \{N_{\text{max}} = 4\} \oplus A \oplus B \oplus C \oplus D \\
 5 & : \{N_{\text{max}} = 4\} \oplus A \oplus B \oplus C \oplus D \oplus E,
 \end{aligned} \tag{2}$$

where A, B, C, D, and E are sets of $(\lambda \mu)S_{\pi}S_{\nu}S$ subspaces defined in Table 1.

Table 1. Deformations and intrinsic spins of $6\hbar\Omega$ configurations of ${}^6\text{Li}$ utilized in model spaces (2).

S_{π}	S_{ν}	S	A	B	C	D	E
$\frac{1}{2}$	$\frac{1}{2}$	1	(2 0) (4 2) (6 1) (8 0)	(0 4)			
$\frac{3}{2}$	$\frac{1}{2}$	2	(4 2)	(8 0)	(6 1)		
$\frac{1}{2}$	$\frac{3}{2}$	2	(4 2)	(8 0)	(6 1)		
$\frac{3}{2}$	$\frac{3}{2}$	3	(4 2) (8 0)			(6 1)	
$\frac{1}{2}$	$\frac{1}{2}$	0		(6 1)			
$\frac{3}{2}$	$\frac{1}{2}$	1				(8 0)	(4 2)
$\frac{1}{2}$	$\frac{3}{2}$	1				(8 0)	(4 2)

Similarly, we define the two model spaces for the ground state of ${}^7\text{Li}$ as

$$\begin{aligned} 1 & : \{N_{\max} = 4\} \oplus A \\ 2 & : \{N_{\max} = 4\} \oplus A \oplus B \end{aligned} \quad (3)$$

where the subspaces A and B are specified in Table 2. These first examples illustrate the remarkable result that only a fraction of the model space yields high (e.g., 99.6% for ${}^6\text{Li}$) overlap with the corresponding NCSM wavefunctions and furthermore, most (98.7%) of the corresponding binding energy.

Table 2. Deformations and intrinsic spins of $6\hbar\Omega$ configurations of ${}^7\text{Li}$ utilized in model spaces (3).

S_π	S_ν	S	A	B
$\frac{1}{2}$	0	$\frac{1}{2}$	(1 1) (3 3) (5 2) (9 0) (7 1)	(3 0) (4 1)
$\frac{1}{2}$	1	$\frac{3}{2}$	(3 3) (5 2) (9 0) (7 1)	
$\frac{3}{2}$	1	$\frac{5}{2}$	(3 3)	(5 2) (7 1) (9 0)

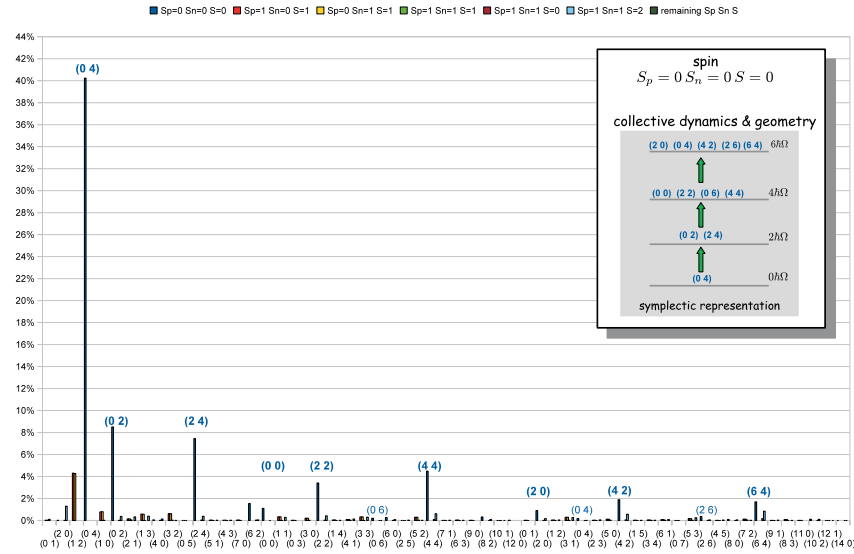


Figure 5. Probability distribution of the 0^+ ground state in ${}^{12}\text{C}$ over subspaces carrying $(\lambda\mu)$ spatial deformations and the six most important spin components $\{S_\pi, S_\nu, S\} \in \{[0, 0, 0], [1, 0, 1], [0, 1, 1], [1, 1, 1], [1, 1, 0], [1, 1, 2]\}$. The blue labels denote $\text{SU}(3)$ quantum labels of basis states of the leading $(0 4)$ $\text{Sp}(3, \mathbb{R})$ irrep. The wave function was obtained by SA-NCSM in $N_{\max} = 6$ model space using the JISP16 bare interaction with $\hbar\Omega = 10$ MeV.

3.2 Ground-state Structure of ^{12}C and ^{16}O

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 of the leading $(0\ 4)$ $S = 0$ symplectic irrep (Figure 5). Furthermore, we find that important SU(3) configurations are typically organized into structures with $\text{Sp}(3, \mathbb{R})$ 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 Figure 5, 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_{max} .

3.3 Structure of the Hoyle State

The ‘Hoyle’ state is 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

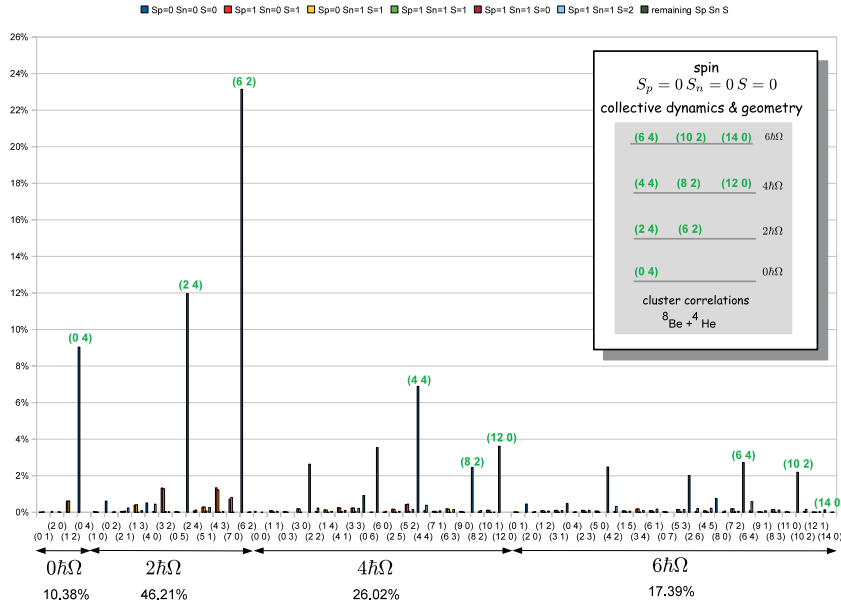


Figure 6. Probability distribution of the 0_6^+ state in ^{12}C over subspaces carrying $(\lambda\ \mu)$ spatial deformations and the six most important spin components $\{S_\pi, S_\nu, S\} \in [\{0, 0, 0\}, \{1, 0, 1\}, \{0, 1, 1\}, \{1, 1, 1\}, \{1, 1, 0\}, \{1, 1, 2\}]$. The green SU(3) labels denote physically allowed deformations of $^8\text{Be} + ^4\text{He}$ cluster basis states. The wave function was obtained by SA-NCSM in $N_{\text{max}} = 6$ model space using the JISP16 bare interaction with $\hbar\Omega = 10$ MeV.

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_{\max} much greater 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}C as obtained in $N_{\max} = 6$ SA-NCSM calculations using JISP16 are examined for characteristic $\text{SU}(3)$ configurations that could point to a cluster structure. These configurations, given in the insert of Figure 6, 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}C system. Among all excited 0^+ states, only the sixth 0^+ state, reveals a pronounced pattern predominantly comprised of the characteristic deformations (Figure 6). Hence, it is this state that is expected to converge to the 7.65-MeV 0^+ of ^{12}C for large N_{\max} spaces, where higher-lying configurations, such as (120), (140) and (160), are expected to grow in importance.

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. Windowing 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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