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Ab initio No-core Shell Model Calculations in a SU(3)-based Coupling Scheme

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Abstract. We use powerful algorithms of computational group theory to perform ab initio configuration-interaction calculations in a SU(3)-based symmetry-adapted many-particle basis. We demonstrate that eigenfunctions for the low-lying states of $^6$Li, $^8$Be, $^{12}$C, and $^{16}$O exhibit a strong dominance of low proton, neutron, and total intrinsic spins that carry the same spatial deformation as the leading symplectic Sp(3, R) irreducible representations. Our findings imply that only a small fraction of the complete model space is needed to model nuclear collective dynamics, deformation, and α-particle clustering even if one uses modern realistic interactions that do not preserve SU(3) symmetry. This in turn points to the importance of using a symmetry-adapted framework, one based on a LS coupling scheme with the associated spatial configurations organized according to deformation.

1. Introduction
Theoretical advances achieved in recent years in the development of realistic nuclear potential models [1, 2, 3, 4] along with progress in high performance computing have placed ab initio many-particle approaches [5, 6, 7] at the frontier of nuclear structure explorations. The ab initio methods are built on fundamental principles and therefore hold promise to provide predictive capabilities essential for a description of the 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) [5] is a prominent ab initio method that has achieved a good description of low-lying states and associated spectroscopic properties up through p-shell nuclei [8, 9, 10]. The NCSM typically employs the Lanczos algorithm to solve the eigenvalue problem for a realistic Hamiltonian. Matrix elements of the Hamiltonian are calculated in a many-particle basis of m-scheme states, which are constructed as an antisymmetrized product of the harmonic oscillator single-particle wave functions, and carry the z-component of the total angular momentum along with the total parity as good quantum numbers. The main limitation of this approach, and the predictive power thereof, is inherently coupled with the combinatorial growth in the size of the many-particle model space with increasing nucleon numbers and expansion in the number of single-particle levels in the model space.

We developed an innovative ab initio model, the symmetry-adapted no-core shell model (SA-NCSM), which utilizes a many-particle basis that exploits the physically relevant SU(3)⊃SO(3)
group-subgroup chain. The significance of the SU(3) group for a microscopic description of the nuclear collective dynamics can be readily seen from the fact that it is the symmetry group of the Elliott model \cite{11}, and a subgroup of the Sp(3, \mathbb{R}) symplectic model of nuclear collective motion \cite{12, 13}. The concept of symmetry-adapted many-particle basis represents a powerful tool that allows one to winnow a model space to correlations indispensable for modeling important modes of nuclear collective dynamics, specifically nuclear deformation and cluster substructures, thereby overcoming the scale explosion bottleneck of ab initio nuclear structure computations. Hence, SA-NCSM framework holds promise to expand dramatically the reach of current ab initio approaches toward describing heavier mass nuclei with unprecedented accuracy.

2. \textit{Ab initio} Calculations in a SU(3) Symmetry-Adapted Basis

The basis states of the SA-NCSM are constructed in the proton-neutron formalism and are labeled by the physical SU(3)\.sampl SO(3) subgroup chain quantum numbers (\(\lambda\mu\))\(\kappa L\), and by proton, neutron, and total intrinsic spins \(S_p\), \(S_n\), and \(S\). The orbital angular momentum \(L\) is coupled with \(S\) to the total angular momentum \(J\) and its projection \(M_J\). Each basis state is thus labeled in the SU(3)-scheme as

\[
\ket{\tilde{\alpha}(\lambda\mu)\kappa L; S_p S_n S; JM_J},
\]

where the deformation-related \((\lambda\mu)\) set of quantum numbers labels SU(3) irreducible representations (irreps) and brings forward important information about nuclear shapes and deformation. For example, \((00)\), \((\lambda 0)\) and \((0\mu)\) describe spherical, prolate and oblate shapes, respectively. The label \(\kappa\) distinguishes multiple occurrences of the same \(L\) value in the parent irrep \((\lambda\mu)\). The symbol \(\tilde{\alpha}\) schematically denotes the additional quantum numbers needed to unambiguously distinguish between irreps carrying the same \(S_p S_n S(\lambda\mu)\) quantum numbers. These irreps compose a well-defined subspace with a unique feature that allows for the complete separation of intrinsic and center-of-mass degrees of freedom. The size of these subspaces is typically several orders of magnitude smaller than the full \(N\hbar\Omega\) space, where the \(m\)-scheme basis also allows for an exact factorization of center-of-mass degrees of freedom. The decomposition of the SA-NCSM model space of \(^6\text{Li}\) up through \(N_{\text{max}} = 12\) model space is depicted in Fig. 1.

The SA-NCSM implements a set of powerful algorithms \cite{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. This allows for both the evaluation of the Hamiltonian matrix elements, and the use of the resulting eigenvectors to evaluate other experimental observables. The underlying principle behind the SA-NCSM computational kernel is a SU(3)-type Wigner-Eckhart theorem, which allows the problem to be factorized into SU(3) reduced matrix elements ($r_{mes}$) 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 $r_{mes}$ by the repetitive application of a SU(3)-type reduction formula for $r_{mes}$ of operators acting on the two independent, proton and neutron subsystems.

3. Results
We first calculate binding energies and low-lying eigenstates of $^6$Li, $^8$Be, $^{12}$C, and $^{16}$O nuclei using the JISP16 bare nucleon-nucleon (NN) interaction, for a wide range of HO energies $\hbar \Omega$ and the maximal full $N_{max}$ model spaces attainable by the current implementation of the SA-NCSM approach. The resulting wave functions are then employed to obtain physical observables such as mass rms radii, electric quadrupole moments, magnetic dipole moments, reduced electromagnetic

Figure 2. Probability distribution of proton, neutron, and total intrinsic spin components ($S_p, S_n, S$) across their Pauli-allowed spatial deformations ($\lambda \mu$) [horizontal axis] in the ground $1^+$ state of $^6$Li obtained for $N_{\text{max}} = 10$ and $\hbar \Omega = 20$ MeV.
Figure 3. Probability distribution of $(S_p, S_n, S)$ spin components across their Pauli-allowed spatial deformations $(\lambda \mu)$ in the ground $0^+$ state of $^8$Be obtained for $N_{\text{max}} = 8$ and $\hbar \Omega = 22.5$ MeV. The area of each circle is proportional to the total probability of $k\hbar \Omega$ states carrying the same $S_p S_n S(\lambda \mu)$ quantum numbers normalized with respect to the total probability of $k\hbar \Omega$ $S_p = 0$ $S_n = 0$ $S = 0$ $(4 + k 0)$ stretched-states.

B(E2) and B(M1) transition strengths. Direct comparison of the SA-NCSM outcomes with the results of analogous $m$-scheme based NCSM calculations reveals agreement typically to within the numerical precision of four significant figures, and thereby unambiguously confirming the validity of $ab\ initio$ SA-NCSM approach, and the correctness of our implementation of it.

The expansion of nuclear wave functions in a physically relevant SU(3)-scheme basis is illuminating salient features that emerge from the complex dynamics of strongly interacting many-particle systems. To investigate the nature of the most important many-particle correlations, we enumerate the probability distribution of intrinsic spin $(S_p, S_n, S)$ and deformation-related $(\lambda \mu)$ quantum numbers for the low-lying $T = 0$ states of $^6$Li, members of the ground-state rotational band in $^8$Be and $^{12}$C, and the ground state of $^{16}$O. Figure 2 shows the probability distribution of intrinsic spins across their Pauli-allowed deformations in the ground state of $^6$Li. This figure illustrates a facet common to low-energy $ab\ initio$ solutions we study: a hitherto unrecognized simple mixing pattern of intrinsic spins and SU(3) spatial quantum numbers.

We observe that over 99% of the SA-NCSM eigenstates is typically accounted for by a small fraction of intrinsic spin combinations. For instance, the lowest-lying $T = 0$ eigenstates in $^6$Li are almost entirely realized in terms of configurations characterized by the following intrinsic spin $(S_p, S_n, S)$ triplets: $(\frac{3}{2}, \frac{3}{2}, 3)$, $(\frac{1}{2}, \frac{3}{2}, 2)$, $(\frac{3}{2}, \frac{1}{2}, 2)$, $(\frac{1}{2}, \frac{1}{2}, 0)$ and $(\frac{1}{2}, \frac{1}{2}, 1)$ with the last carrying over 90% of the eigenstate. Similarly, the ground state band in $^8$Be and $^{12}$C along with the ground state of $^{16}$O are dominated by many-particle configurations carrying the total intrinsic spin of protons and neutrons equal to zero and one with the highest probability due to the dominant $S_p = S_n = S = 0$ configurations.
The mixing of $(\lambda \mu)$ spatial quantum numbers in the lowest-lying $T = 0$ eigenstates in $^6\text{Li}$, the ground state band in $^8\text{Be}$ and $^{12}\text{C}$ along with the ground state of $^{16}\text{O}$, induced by the SU(3) symmetry breaking terms of realistic interactions, exhibits a remarkably regular pattern. One of its key features is the preponderance of a single $0\hbar\Omega$ SU(3) irrep, the so-called leading irrep, that is, the one characterized by the largest value of the second order SU(3) Casimir invariant, $\hat{C}_2$, and hence corresponding to a large intrinsic quadrupole deformation. For instance, the low-lying $T = 0$ states of $^6\text{Li}$ project at 40%-70% level onto the prolate-like $0\hbar\Omega$ SU(3) irrep (20), as illustrated in Fig. 2 for the ground state. Qualitatively similar dominance of the leading $0\hbar\Omega$ SU(3) irreps (40), (04), and (00), associated with prolate, oblate, and spherical shapes is observed for the investigated eigenstates of $^8\text{Be}$, $^{12}\text{C}$, and $^{16}\text{O}$, respectively. Such clear prominence of the $p$-shell states with the highest spatial symmetry points to the fact that the effective quadrupole-quadrupole interaction of Elliott SU(3) model of nuclear rotations is realized naturally within the framework of the modern realistic NN interactions.

Our analysis reveals that the dominant SU(3)-scheme states at each $k\hbar\Omega$ subspace are typically those with $(\lambda \mu)$ quantum numbers such that

$$\lambda + 2\mu = \lambda_0 + 2\mu_0 + k \quad k = 2, 4, \ldots,$$

(2)

where $\lambda_0$ and $\mu_0$ denote labels of a leading SU(3) irrep at the $k = 0$, $0\hbar\Omega$ level. We conjecture that such an intriguing mixing pattern of SU(3) quantum numbers reflects the presence of an underlying symplectic $\text{Sp}(3, \mathbb{R})$ symmetry of microscopic nuclear collective motion that governs the low-energy structure of both even-even and odd-odd $p$-shell nuclei. This can be seen from the fact that the core excitations with $(\lambda \mu)$ deformation shapes satisfying condition (2) can be determined from the leading SU(3) irrep $(\lambda_0 \mu_0)$ through a successive application of a specific subset of the $\text{Sp}(3, \mathbb{R})$ symplectic $2\hbar\Omega$ raising operators. This subset is composed of $\hat{A}_{zz}, \hat{A}_{zx},$ and $\hat{A}_{xx}$ operators that distribute two oscillator quanta in $z$ and $x$ directions, but none in $y$ direction, thereby inducing SU(3)-scheme configurations with ever-increasing values of the Casimir invariant $\hat{C}_2$. These three operators are the generators of the $\text{Sp}(2, \mathbb{R}) \subset \text{Sp}(3, \mathbb{R})$ subgroup [17], and give rise to a hierarchy of deformation shapes that are energetically favored by an attractive quadrupole-quadrupole interactions [13]. Furthermore, there is an apparent hierarchy among states that fulfill condition (2). In particular, the $k\hbar\Omega$ configurations with $(\lambda_0 + k, \mu_0)$, the so-called stretched-states, carry a very noticeably higher probability than the others, as can be readily seen in Fig. 2 and Fig. 3. For instance, the $(2 + k 0)$ stretched-states contribute at 85% level to the ground state of $^6\text{Li}$. The sequence of the stretched-states, that is, the states with the highest possible deformations, can be formed from many-nucleon correlations of a leading SU(3) irrep by application of the $\hat{A}_{zz}$ operator, which is the generator of $\text{Sp}(1, \mathbb{R}) \subset \text{Sp}(2, \mathbb{R}) \subset \text{Sp}(3, \mathbb{R})$ subgroup. The important role of the stretched-configurations for the description of the rotational bands in $N = Z$ even-even nuclei of was recognized heretofore using a simplistic microscopic Hamiltonian [18]. Here, for the first time, we establish its presence in the framework of the $\textit{ab initio}$ nuclear structure study.

The revealed pattern of intrinsic spin and deformation mixing supports a symmetry guided truncation of the $N_{\text{max}}$ model space. Clearly, one can take advantage of the physical relevance of the SU(3)-scheme basis to winnow the full space down to the most relevant configurations that support the strongest many-nucleon correlations of the system using the underlying $\text{Sp}(1, \mathbb{R}) \subset \text{Sp}(2, \mathbb{R}) \subset \text{Sp}(3, \mathbb{R})$ symmetry considerations. As noted previously, this truncation, while significantly reducing the size of the model space, also preserves the ability to factor out exactly the spurious center-of-mass degrees of freedom.

4. Conclusion
We have developed a novel approach that capitalizes on advances being made in $\textit{ab initio}$ methods while exploiting exact and partial symmetries of nuclear many-body system. Using
this approach we have demonstrated that the low-lying eigenstates of $^6$Li, $^8$Be, $^{12}$C, and $^{16}$O, which were obtained using the JISP16 NN interaction, exhibit a strong dominance of few intrinsic spin components and carry an intriguingly simple pattern of dominant deformations. This demonstrates an important role of the symplectic $\text{Sp}(3,\mathbb{R})$ symmetry in light nuclei while reaffirming the value of the simpler $\text{SU}(3)$ model upon which it is based. The SA-NCSM thus offers a systematic framework for down-selecting many-body correlations to physically relevant and manageable subspaces based on spin and deformation selection, while preserving the ability to factorize the center-of-mass degrees of freedom exactly.

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References
[1] Shirokov A, Vary J, Mazur A and Weber T 2007 Phys. Lett. B 644 33
[2] Wiringa R B, Stoks V G J and Schiavilla R 1995 Phys. Rev. C 51 38
[3] Entem D R and Machleidt R 2003 Phys. Rev. C 68 041001
[4] Epelbaum E 2006 Prog. Part. Nucl. Phys 57 65
[5] Navrátíl P, Vary J P and Barrett B R 2000 Phys. Lett. 84 5728
[6] Pieper S C, Varga K and Wiringa R B 2002 Phys. Rev. C 66 044310
[7] Wnuk M, Dean D J, Gour J R, Hjorth-Jensen M, Kowalski K, Papenbrock T and Piecuch P 2005 Phys. Rev. Lett. 94 212501
[8] Navrátil P, Quaglioni S, Stetcu I and Barrett B R 2009 J. Phys. G: Nucl. Part. 36 083101
[9] Roth R and Navrátíl P 2007 Phys. Rev. Lett. 99 092501
[10] Navratil P, Gueorguiev V, Vary J P, Ormand W and Nogga A 2007 Phys. Rev. Lett. 99 042501 LANL ArXiV: Nucl-Th 0701038
[11] Elliott J P 1958 Proc. Roy. Soc. A 245 128
[12] Rosensteel G and Rowe D 1977 Phys. Rev. Lett. 38 10
[13] Rowe D 1985 Reports on Progr. in Phys. 48 1419
[14] Draayer J P, Leschber Y, Park S C and Lopez R 1989 Comput. Phys. Commun. 56 279
[15] Bahri C and Draayer J 1994 Comput. Phys. Commun. 83 59
[16] Akiyama Y and Draayer J 1973 Comput. Phys. Commun. 5 405
[17] Peteron D R and Hecht K T 1980 Nucl. Phys. A 344 361
[18] Arickx F 1976 Nucl. Phys. A 268 347