No-core Symplectic Model:
Exploiting Hidden Symmetry in Atomic Nuclei

J P Draayer[1]**, K D Launey**[1]**, T Dytrych**[1,2]**, A C Dreyfuss**[1]**, R B Baker**[1] **and M E Miora**[3]

[1] Dept. of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA
[2] Nuclear Physics Institute, 250 68 Řež, Czech Republic
[3] Rollins College, Winter Park, FL 32789, USA

Abstract.   We report on recent developments within the framework of the no-core symplectic shell model (NCSpM) that complements the no-core shell model (Navrátil, Vary, and Barrett) by exploiting the algebraic features of the symplectic shell model (Rowe and Rosensteel) while also allowing for high-performance computing applications, but in highly truncated, physically relevant subspaces of the complete space. The leading symplectic symmetry typically accounts for 70% to 90% of the structure of the low-lying states, a result that is only moderately dependent on the details of the selected inter-nucleon interaction. Examples for ^{6}Li, ^{12}C, ^{16}O, and ^{20}Ne are shown to illustrate the efficacy the NCSpM, and as well the strong overlap with cluster-like and pairing configurations that dominate the dynamics of low-lying states in these nuclei.

1. Introduction

The no-core shell model (NCSM) is a complete hamiltonian-based microscopic theory for studying the structure of atomic nuclei [1, 2]. The simplest implementation of the NCSM ignores all symmetries except for time reversal, parity and translational invariance; it is ideally suited for straightforward high performance computing (HPC) applications. The symplectic shell model [3, 4], developed by Rowe and Rosensteel, which predates the NCSM, establishes an algebraic framework that enables a partitioning of the complete space into physically relevant subspaces that respect rotational invariance and exposes important dynamical symmetries. In particular, in one limit the symplectic model reduces to Bohr-Mottelson theory [5], while in another it reduces to the Elliott model [6, 7].

That symplectic $\text{Sp}(3, \mathbb{R})$ symmetry is an important symmetry of atomic nuclei can be traced to the fact that, within a microscopic framework that relates to particle position and momentum coordinates, it naturally describes rotations and vibrations of equilibrium deformation (or a set of a reasonable number of deformed configurations). The existence of the symmetry and its slight symmetry breaking has been recently confirmed in light nuclei from first principles in the *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [8, 9]. The SA-NCSM capitalizes on exact as well as partial symmetries that underpin the structure of nuclei and provides remarkable insight into how simple symmetry patterns emerge in the many-body nuclear dynamics from first principles. Complementary to this, a fully microscopic no-core symplectic shell model (NCSpM) [10], by employing the symplectic symmetry and schematic interactions, can reach model spaces beyond the reach of any *ab initio* theory, thereby making possible to probe the
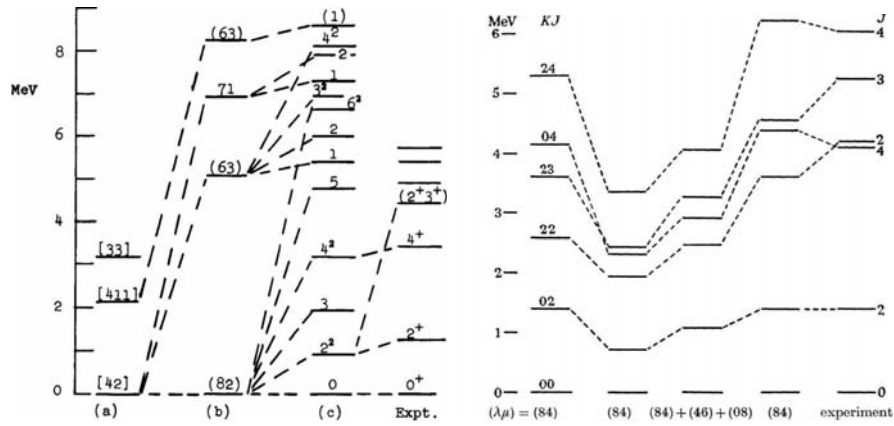
Figure 1. Elliott's SU(3) model applied to sd-shell nuclei. Left panel: Spectrum of ^{22}Ne (a) with a Majorana potential, (b) with the addition of the second-order SU(3) Casimir invariant, C_2^{su3}, and (c) with the Majorana potential plus an attractive $Q \cdot Q$ interaction [or (b) with the addition of L^2]. Figure taken from [15]. Right panel: Spectrum of ^{24}Mg with a Gaussian central force. Figure taken from [7]. The vertical axis in both figures represents energy in MeV. Note the importance of the most deformed SU(3) configuration $(8\,2)$ in ^{22}Ne and $(8\,4)$ in ^{24}Mg for reproducing the experimental low-lying states.

physics, e.g., of the challenging ^{12}C Hoyle state and its rotational band, as well as negative-parity states, together with highly deformed intermediate-mass nuclei. The NCSpM reveals the nature of collectivity with outcomes that corroborate the results of earlier studies [4, 11, 12]. It provides a description of bound states in terms of a relatively small fraction of the complete space when the latter is expressed in an $(LS)J$ coupling scheme with the spatial configurations further organized into irreducible representations (irreps) of SU(3) and then into irreps of the embedding $Sp(3, \mathbb{R})$. The SU(3) plays a key role as shown by the seminal work of Elliott [6, 7] (Fig. 1). The SU(3)-symmetry dominance has been also observed in heavier nuclei, where pseudo-spin symmetry and its pseudo-SU(3) complement have been shown to play a similar role in accounting for deformation in the upper pf and lower sdg shells, and in particular, in strongly deformed nuclei of the rare-earth and actinide regions [13], as well as in many other studies (e.g., [14]).

Concurrently to collective approaches, particle-driven models have been developed, following the success of the independent-particle model of Mayer and Jensen [16, 17]. One of the most successful is the *ab initio* NCSM discussed above. It adopts the harmonic oscillator (HO) single-particle basis characterized by the $\hbar\Omega$ oscillator strength and limited by the $N_{\max}$ cutoff, which is defined as the maximum number of HO quanta allowed in a many-body basis state above the minimum for a given nucleus. It divides the space in "horizontal" HO shells dictated by particle-hole excitations (complementary to a "vertical" space organization in the symplectic model dictated by collectivity). The NCSM has achieved remarkable descriptions of low-lying states of s- and p-shell light nuclei [1, 18], and is further augmented by several techniques, such as NCSM/RGM [19], Importance Truncation NCSM [20] and Monte Carlo NCSM [21]. This supports and complements results of other first-principle approaches, such as Green's function Monte Carlo (GFMC) [22], Coupled-cluster (CC) method [23], In-medium SRG [24], and Lattice Effective Field Theory (EFT) [25], along with the symmetry-adapted no-core shell model (SA-NCSM) [8] that combines both particle-driven and collective concepts.

2. Exploiting hidden symmetries
2.1. Simple pattern formation from first principles
The *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [8] adopts the first-principle concept and utilizes many-particle basis states that are organized with respect to the physically

relevant, deformation-related $\mathrm{SU(3)}_{(\lambda\,\mu)} \overset{\kappa}{\supset} \mathrm{SO(3)}_L$ subgroup chain (for reviews, see [9, 26]), that is, it is a no-core shell model with SU(3)-coupled basis states (hence, the SA-NCSM results obtained in a complete $N_{\max}$ space are equivalent to the $N_{\max}$ NCSM results). This allows the full model space to be down-selected to the physically relevant space.
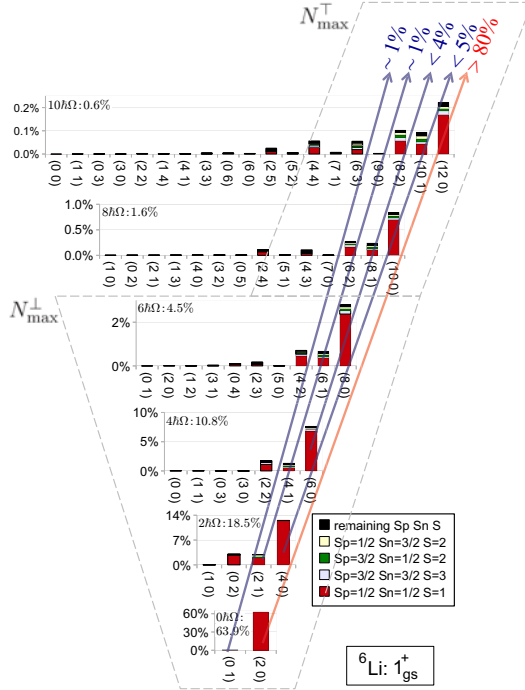

Figure 2. Probability distributions for proton, neutron, and total intrinsic spin components $(S_p S_n S)$ across the Pauli-allowed deformation-related $(\lambda\,\mu)$ values for the 1^+ ground state of ^{6}Li, calculated in 12 HO shells with the JISP16 bare interaction ($\hbar\Omega = 20$ MeV). The concentration of strengths to the far right demonstrates the dominance of collectivity. This supports a *symmetry-guided* model space selection, which implies inclusion of the full space up through $N^\perp_{\max}$, and a subset of deformation/spin configurations beyond this, up through $N^\top_{\max}$, labeled as $\langle N^\perp_{\max}\rangle N^\top_{\max}$. The projection onto symplectic vertical slices (with probability $\geq 1\%$) is schematically illustrated for ^{6}Li by arrows and clearly reveals the preponderance of a single symplectic irrep (vertical cone). Figure adapted from Ref. [8].

   The *ab initio* SA-NCSM results for p-shell nuclei reveal a dominance of configurations of large deformation in the $0\hbar\Omega$ subspace. For example, the *ab initio* $N_{\max} = 10$ SA-NCSM results with the bare JISP16 realistic interaction [27] (similarly, for the bare N^{3}LO realistic interaction [28]) for the 1^+ ground state (*g.st.*) and its rotational band for ^{6}Li (similarly for ^{6}He, ^{8}Be, and ^{12}C) reveal the dominance of the leading $0\hbar\Omega$ $(2\,0)$ irrep and its symplectic excitations (Fig. 2). The outcome points to a remarkable feature common to the low-lying states of nuclei that has heretofore gone unrecognized in other first-principle studies; namely, the emergence, without a priori constraints, of simple orderly patterns that favor strongly deformed configurations and low spin values. This feature confirms the dominant role the SU(3) and Sp(3, $\mathbb{R}$) symmetries play in nuclear dynamics and is central to expanding the reach of first-principle studies to heavier nuclei [29]. For example, model spaces that expand up to 20 HO shells for ^{12}C are feasible and en route to be employed. This allows the SA-NCSM to advance an extensible microscopic framework for studying nuclear structure and reactions that capitalizes on advances being made in *ab initio* methods while exploiting symmetries found to dominate the dynamics.

2.2. The elusive Hoyle state and negative-parity states in ^{12}C
The Hoyle state was predicted based on observed abundances of heavy elements in the universe [32] and has attracted much recent attention both in theory (e.g., see [25, 33, 34]) and experiment (e.g., [35–37]). The findings of the no-core symplectic shell model (NCSpM) inform key features of the primary physics responsible for the emergent phenomena of large deformation and alpha-cluster substructures in ^{8}Be and ^{12}C [10, 38], as well as enhanced collectivity in intermediate-mass nuclei, such as ^{20}O, ^{20,22,24}Ne, ^{20,22}Mg, and ^{24}Si [39] (Fig. 3).
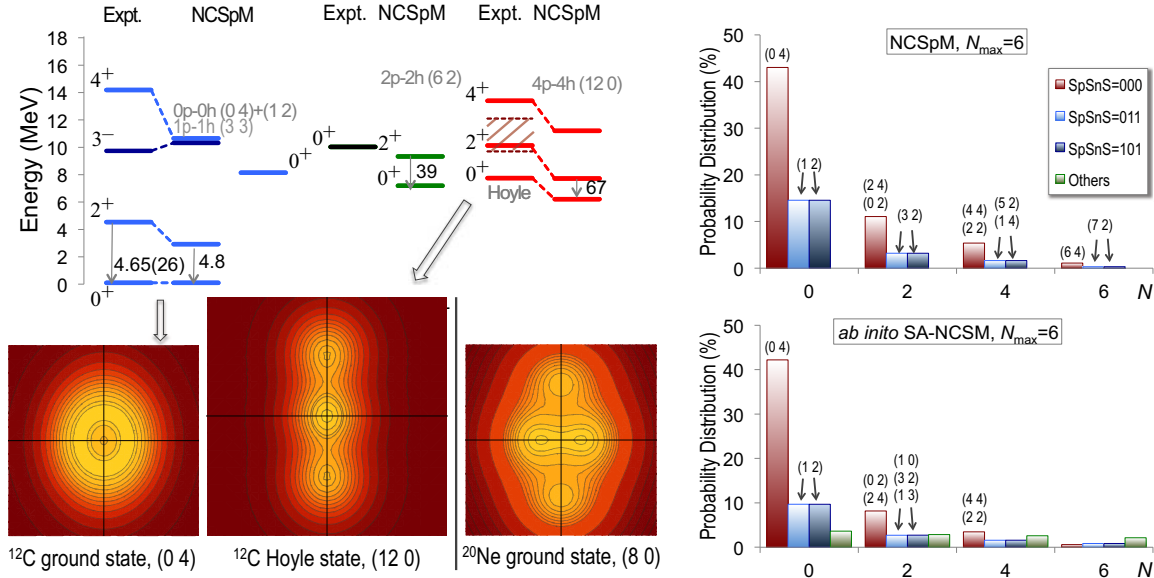
Figure 3. Left: ^{12}C energy spectrum (in MeV) and $B(E2)$ rates (in W.u.) calculated by the NCSpM using the schematic interaction of Eq. (1) with the bare JISP16 NN and 5 symplectic irreps (shown above each band) expanded up to $N_{max} = 20$, and compared to experiment ("Expt.") [30]. One-body density profiles *in the intrinsic frame* reveal a torus-like shape for the ^{12}C 0^+_{gs} and overlapping clusters in the Hoyle state. Right: Probability distribution across total HO quanta excitations for the ^{12}C 0^+_{gs} – close similarity is observed for NCSpM (top) and SA-NCSM (bottom) for $N_{max} = 6$ and $\hbar\Omega = 18$ MeV [10]. Dominant ($\geq 1\%$) SU(3) modes are also shown. Very similar results are obtained for 2^+_1 and 4^+_1 [31].

The NCSpM is a fully microscopic no-core shell model that can be employed in model spaces beyond current NCSM limits. It uses a symplectic Sp$(3,\mathbb{R})$ basis but is not limited to Sp$(3,\mathbb{R})$-preserving interactions. The NCSpM employed within a full model space up through a given N_{max} coincides with the NCSM for the same N_{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_{max} model space. We employ a Hamiltonian with an effective interaction derived from the long-range expansion of the two-body central nuclear force,

$$H_{eff} = H_0 + \frac{\chi}{2}\frac{\left(e^{-\gamma Q\cdot Q} - 1\right)}{\gamma} + V^{SB}_{NN}, \qquad (1)$$

where V^{SB}_{NN} is a symmetry-breaking term applied to symplectic bandheads (we adopt either a spin-orbit term, $-\kappa \sum^A_{i=1} l_i \cdot s_i$, or a realistic interaction, such as the bare interactions, JISP16 [27] or chiral N3LO [28] NN). The Sp$(3,\mathbb{R})$-preserving part of the Hamiltonian includes: the spherical HO potential, which together with the kinetic energy yields the HO Hamiltonian, $H_0 = \sum^A_{i=1}\left(\frac{\mathbf{p}^2_i}{2m} + \frac{m\Omega^2 \mathbf{r}^2_i}{2}\right)$, and the important $\frac{1}{2}Q\cdot Q = \frac{1}{2}\sum_s q_s \cdot (\sum_t q_t)$ interaction, which realizes the physically relevant interaction of each particle with the total quadrupole moment of the nuclear system (for a valence shell and very small γ, the Elliott model is recovered). The considerable average contribution, $\langle Q\cdot Q\rangle$, of $Q\cdot Q$ is removed [40]. We take the coupling constant χ to be proportional to $\hbar\Omega$ and, to leading order, to decrease with the total number of HO excitations, as shown by Rowe [41] based on self-consistent arguments.

The NCSpM outcome reveals a quite remarkable agreement with the experiment and *ab initio* results (Fig. 3) [10]. Energies and eigenstates for ^{12}C were calculated for $\hbar\Omega = 18$ MeV given by the empirical estimate $\approx 41/A^{1/3} = 17.9$ MeV. The results are shown for $N_{\max} = 20$, which we found sufficient for convergence. This $N_{\max}$ model space is further reduced by selecting the five most relevant symplectic irreps, extended up through $N_{\max} = 20$ (6.6×10^3 positive-parity basis states). In comparison to experiment (Fig. 3), the outcome for $\gamma = -1.71 \times 10^{-4}$ reveals that the lowest 0^+, 2^+, and 4^+ states of the 0p-0h symplectic irreps closely reproduce the *g.st.* rotational band, while the lowest 0^+ states of the $4\hbar\Omega$ 4p-4h $(12\,0)$ and the $2\hbar\Omega$ 2p-2h $(6\,2)$ irreps are found to lie close to the Hoyle state and the 10-MeV 0^+ resonance, respectively. The NCSpM successfully reproduces the 3^- state by the $1\hbar\Omega$ $(3\,3)$, as well as other observables, such as mass rms radii, electric quadrupole moments and $B(E2)$ transition strengths (Fig. 3). The model is also applicable to the low-lying states of ^{8}Be and *sd*-shell nuclei without any adjustable parameters [38,39]. This suggests that the fully microscopic NCSpM model has indeed captured an important part of the underlying physics and informs key features of the interaction and structure primarily responsible for the formation of such simple patterns.
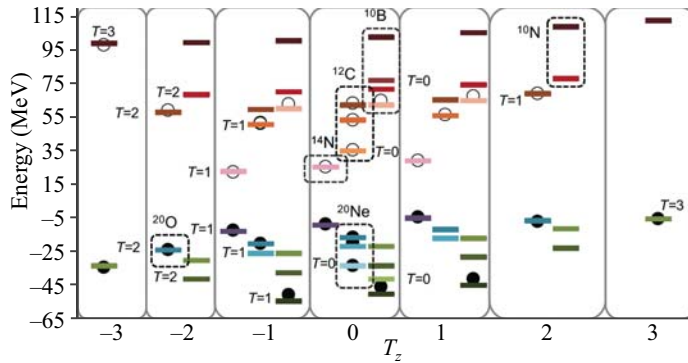

Figure 4. Exact solutions (lines) for a pairing Hamiltonian with experimentally deduced non-degenerate single-particle energies, like-nucleon and proton-neutron isovector pairing, proton-neutron isoscalar term, and a Coulomb potential, as compared to experimental 0^+ states (circle).

In addition, for the nuclei under consideration, we explore the formation of like-nucleon and proton-neutron (pn) isovector pairs together with pn isoscalar correlations, of importance to two-nucleon correlations in break-up reaction channels. These investigations are carried forward in the framework of exact pairing plus a mean field with single-particle energies (s.p.e.) that are empirically derived (in general, they can also be determined in a mean-field approach, including density functional theory for heavy nuclei, and in a spherical shell model). The method provides, for the first time, exact solutions when non-degenerate s.p.e. and the challenging pn correlations are considered, based on recent mathematical developments [42,43]. Results for light up through medium-mass nuclei ($10 \leq A \leq 62$) are found to remarkably agree with experiment [44] (see Fig. 4 for selected *p*- and *sd*-shell nuclei including the deformed ^{20}Ne). The outcome suggests that enhanced deformation does not preclude pair formation – indeed, collective modes appear to remain dominant even in the presence of pairing (see also [45, 46]), while the most noticeable effect of the latter is typically in reducing the moment of inertia.

In short, we have demonstrated the emergence of orderly patterns in nuclei from first principles, with associated hidden symmetry exploited, in turn, in the NCSpM. We have illustrated the efficacy of the NCSpM to gain new insights into the microscopic structure of nuclei, as well as into cluster-like and pairing correlations.

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