

— Unraveling Mysteries of the Strong Interaction —
‘Top Down’ versus ‘Bottom Up’ Considerations

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Abstract

Ab initio theories that build on first principles are essential for understanding nuclear structure at a fundamental level and for providing reliable predictions of short-lived nuclei. While the *ab initio* symmetry-adapted no-core shell model (SA-NCSM) has unveiled a clear symmetry structure that emerges from first principles — an outcome that has only recently become feasible with the advent of high performance computing (HPC) facilities, these symmetries have been long recognized and have been key to successful algebraic models with the cornerstone approaches reviewed here. Utilizing these symmetries, we have found that a fully microscopic no-core symplectic model reproduces characteristic features of the low-lying 0^+ states in ^{12}C and ground-state rotational bands in p and sd -shell nuclei (from Be to Si). Such ‘top down’ algebraic considerations can hence inform ‘bottom up’ *ab initio* approaches by exposing emergent properties in terms of simple interaction forms that are likely to dominate nuclear structure.

Keywords: *Ab-initio symmetry-adapted no-core shell model; SU(3) coupling scheme; symplectic Sp(3,R) shell model; Hoyle state*

1 Introduction

The *ab initio* symmetry-adapted no-core shell-model (SA-NCSM), with results that corroborate and are complementary to those enabled within the framework of the no-core shell model¹ (NCSM) [1], and which can be used to facilitate *ab initio* applications to challenging lower sd -shell nuclei, reveal that bound states of light nuclei are dominated by high-deformation and low-spin configurations [2]. The applicable symmetries reveal the nature of collectivity in such nuclei and provide 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 of $SU(3)$. That $SU(3)$ plays a key role tracks with the seminal work of Elliott [3], and is further reinforced by the fact that $SU(3)$ also underpins the microscopic symplectic model [4, 5], which provides a theoretical framework for understanding deformation-dominated collective phenomena in atomic nuclei [6].

¹This talk is dedicated to James P. Vary on the occasion of his 70th birthday, and is given in recognition and celebration of his important contributions to nuclear physics, especially for his seminal and sustained leadership in the development of the no-core shell model.

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<http://www.ntse-2013.khb.ru/Proc/Draayer.pdf>.

While applications to p -shell and selected heavier nuclei [2, 7–9] illustrate the success of the *ab initio* approach, a very simple algebraic interaction, which reduces to the Elliott SU(3) model [3] in the single-shell limit, augmented by the SU(3) symmetry breaking spin-orbit interaction, reproduces characteristic features of the low-lying 0^+ states in ^{12}C as well as ground-state rotational bands in p and sd -shell nuclei (from Be to Si) [10, 11]. The study of ^{12}C includes the elusive first excited 0_2^+ state, known as the Hoyle state [12] that was predicted based on observed abundances of heavy elements in the universe, and which has attracted much recent attention [13–16]. An implication of the latter is that efforts to reproduce the structure of ^{12}C using a ‘bottom up’ *ab initio* effective interaction theory may benefit from ‘top down’ algebraic considerations that serve to expose emergent properties in terms of simple interaction forms that seem to dominate the structure of deformed nuclei, especially the 0^+ states of ^{12}C .

2 Shell models and collectivity-driven models

This section is dedicated to a short review of the major theoretical efforts that underpin development of the SA-NCSM and/or have advanced our understanding of particle- and collectivity-driven phenomena (Table 1). For a complete list of approaches that have made substantial contributions, we refer the reader to the review articles [6, 17, 18] and references therein.

In the 1950s, two simple models of nuclear structure were advanced that are complementary in nature, namely, the independent-particle model of Mayer and Jensen [19], and the collective model of Bohr and Mottelson [20]. The first of these, which is microscopic in nature, recognizes that nuclei can be described by particles independently moving in a mean field, with the harmonic oscillator (HO) potential being a very good first approximation to the average potential experienced by each nucleon in a nucleus. The second of these, which is collective in nature, recognizes that deformed shapes dominate the dynamics. For example, deformed configurations are found to be important even in a nucleus such as ^{16}O , which is commonly treated as spherical in its ground state, but 20% of the latter is governed by deformed shapes; in addition, the lowest-lying excited 0^+ states in ^{16}O and their rotational bands are dominated by large deformation [21]. Bohr and Mottelson offered a simple but important description of nuclei in terms of the deformation of the nuclear surface and associated vibrations and rotations.

The seminal work of Elliott [3, 22] focused on the key role of SU(3), the exact symmetry of the three-dimensional spherical HO. Within a shell-model framework, Elliott’s model utilizes an SU(3)-coupled basis that is related via a unitary transformation to the basis used in the conventional shell model. The new feature here is that SU(3) divides the space into basis states of definite $(\lambda\mu)$ quantum numbers of SU(3) linked to the intrinsic quadrupole deformation [23–25]. E. g., the simplest cases, (00) , $(\lambda 0)$, and (0μ) , describe spherical, prolate, and oblate deformation, respectively. For SU(3)-symmetric interactions, the model can be solved analytically. But regardless whether a simple algebraic interaction is used, such as $H = H_{\text{HO}} - \frac{\chi}{2} Q \cdot Q$ (see, e. g., Fig. 1, left), or an SU(3)-symmetry breaking interaction (see, e. g., Fig. 1, right), the results have revealed a striking feature, namely, the dominance of a few most deformed configurations. This has been shown for sd -shell nuclei, such as ^{18}Ne , ^{20}Ne , ^{22}Ne , ^{22}Mg , ^{24}Mg , and ^{28}Si , that have been known to possess a clear collective rotational structure in their low-lying states [22, 26]. It 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 [27].

Table 1: Major cornerstone theories in the development of two classes of nuclear structure models, starting with the Shell Model (SM) and the Collective Model (CM).

Particle Focus	Shape (Collectivity) Focus
<p>Shell Model Goepfert-Mayer & Jensen (1950s) [19] 1963 Nobel Prize: “... for their discoveries concerning nuclear shell structure ...”</p> <ul style="list-style-type: none"> ◦ Independent-particle model, spherical harmonic oscillator (HO) mean field plus $l \cdot s + l^2$ 	<p>Collective Model Bohr & Mottelson (1950s) [20] 1975 Nobel Prize: “... for the discovery of the connection between collective motion and particle motion in atomic nuclei and the development of the theory of the structure of the atomic nucleus based on this connection ...”</p> <ul style="list-style-type: none"> ◦ Descriptions in shape variables, β & γ (deformation, rotations, vibrations)
<p>Nilsson Model (1955) [28] ◦ Independent-particle model with a deformed HO mean field plus $l \cdot s + l^2$</p> <p>Pairing Model <i>Algebraic pairing</i>: Racah (1940s), Flowers (1950s), Kerman (1960s) [29–31] ◦ SU(2) for like particles (pp and nn pairs) and Sp(2) for pp, pn, nn pairs <i>Exact pairing</i>: ◦ Exact solutions to standard pairing in spherical/deformed mean field (Fig. 2, Guan & Pan (2012) [32]) ◦ <i>Complementary developments</i>: <i>Ab initio</i> Density Functional Theory (DFT) — first-principle informed, self-consistent mean-field theory plus correlation effects, UNEDF SciDAC Collaboration (2005–Present) [33]</p>	<p>Elliott SU(3)* Model (1958) [3] *SU(3) is the symmetry of the 3-D HO Discovery of dominance of a few most deformed configurations (Fig. 1) ◦ Shell model in SU(3)-adapted basis ◦ Valence shell ◦ SU(3)-conserving interactions ◦ SU(3)-breaking interactions: effective, surface-delta (SDI), $l \cdot s + l^2$, pairing (Fig. 3a, Vargas & Hirsch (2001) [36])</p> <ul style="list-style-type: none"> ◦ <i>Complementary developments</i>: Geometric Collective Model — with interactions in terms of β & $\cos 3\gamma$, Greiner (1969) [34] and Interacting Boson Model — algebraic, pairs approximated by bosons, Iachello (1975) [35]
<p><i>Ab initio</i> No-core Shell Model Vary, Navrátil, Barrett, Maris, ... (2000–Present) [1, 46] First-principle descriptions ($A \leq 16$) ◦ No-core shell model ◦ Realistic interactions (local/nonlocal; NN, NNN, ...) ◦ “Horizontal” cutoff ◦ <i>Complementary developments</i>: (2000–Present) GFMC [43], CC method [44], Lattice-EFT [14] (for details, see [45])</p>	<p>Symplectic Sp(3, \mathbb{R})* Model Rowe & Rosensteel (1980s) [4] *Sp(3, \mathbb{R}) is naturally realized in nuclei (see first-principle findings, Fig. 4 & [2]) Successful reproduction of rotational bands & transition rates without effective charges (Fig. 3b [39] and Section 4) ◦ Shell model in Sp(3, \mathbb{R})-adapted basis (fixed-core & no-core, NCSpM) ◦ Schematic and effective interactions, long-range central force ◦ “Vertical” cutoff (by symplectic slices)</p>
<p>Symmetry-Adapted NCSM (SA-NCSM) Dytrych, Draayer, Launey, Maris, Vary, ... (2007–Present) [2] Discovery of emergence of symmetries from first principles (see, e. g., Fig. 4); expanding the reach of <i>ab initio</i> models to lower <i>sd</i>-shell nuclei</p> <ul style="list-style-type: none"> ◦ <i>Ab initio</i> NCSM with SU(3)-adapted basis (any interaction) <ul style="list-style-type: none"> ◦ Manage spurious center-of-mass motion ◦ Fully microscopic & equals NCSM if the complete space is included <ul style="list-style-type: none"> ◦ No effective charges 	

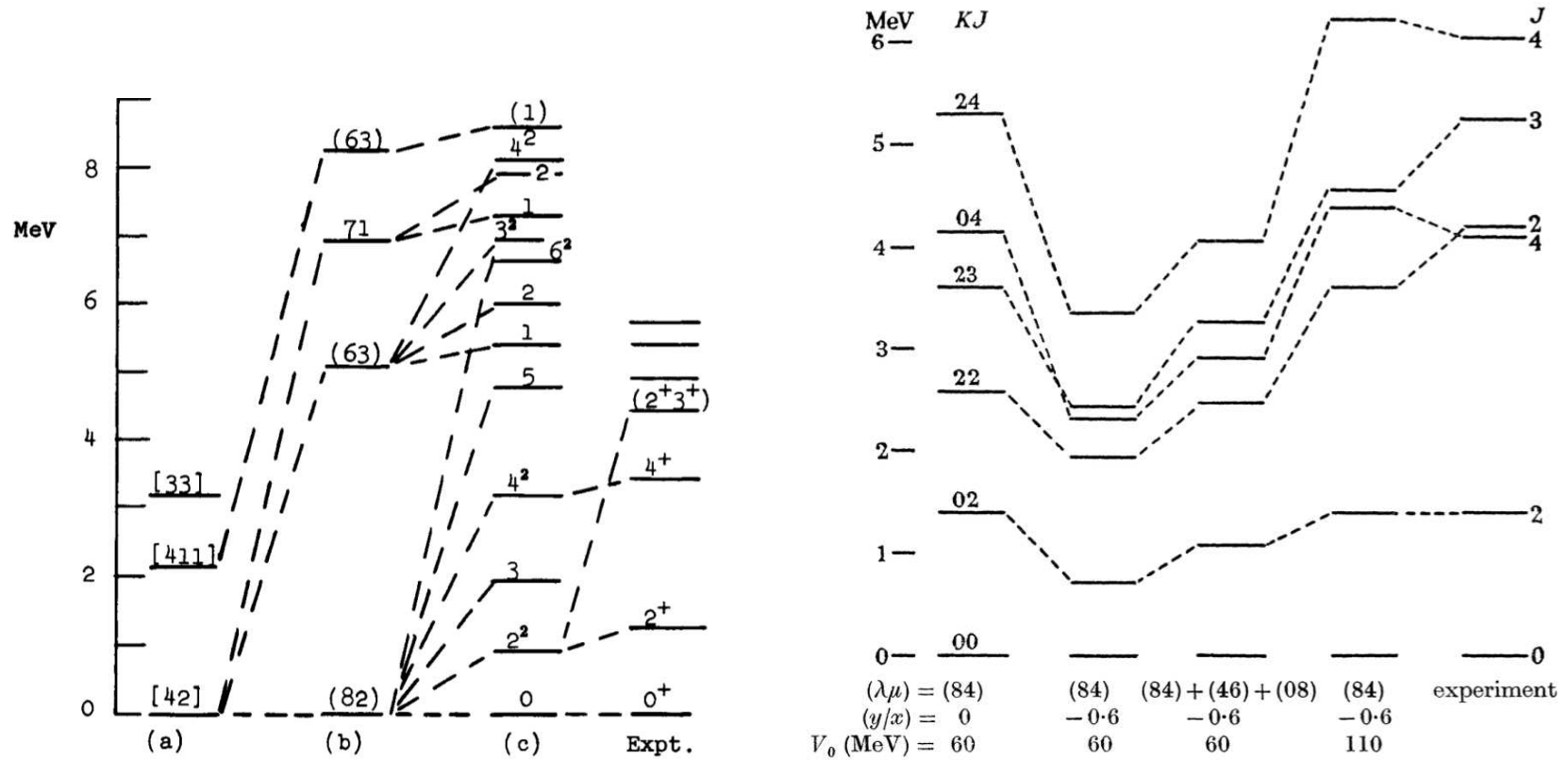


Figure 1: Elliott's SU(3) model applied to sd -shell nuclei. Left panel: Spectrum of ^{22}Ne (or ^{22}Mg) (a) with a Majorana potential, (b) with the addition of the second-order SU(3) Casimir invariant, C_2^{su3} , and (c) with the Majorana potential plus an attractive $Q \cdot Q$ interaction [or (b) with the addition of L^2]. Figure taken from [26]. Right panel: Spectrum of ^{24}Mg with a Gaussian central force. Figure taken from [22]. The vertical axis in both figures represents energy in MeV. Note the importance of the most deformed SU(3) configuration (82) in ^{22}Ne and (84) in ^{24}Mg for reproducing the experimental low-lying states.

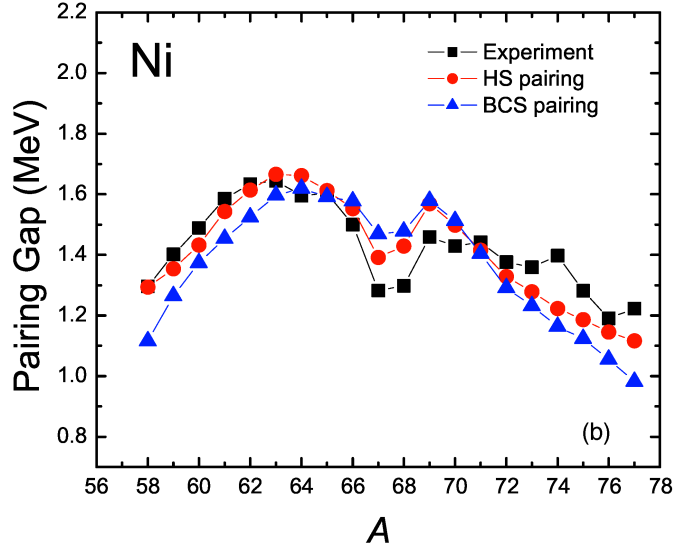


Figure 2: Pairing gaps in MeV as calculated by the exact pairing theory (“HS pairing”) and using the BCS approach (“BCS pairing”), and compared to experiment for Ni isotopes, ^{58}Ni to ^{77}Ni , using four j shells, $f_{5/2}$, $p_{1/2}$, $p_{3/2}$, $g_{9/2}$ and $G = 23/A$ MeV. Figure taken from [32].

With an expanding body of experimental evidence that exposed prominent systematic features of nuclei, such as pairing gaps in energy spectra and enhanced electric quadrupole transitions within collective rotational bands, deformation modes were added to the independent-particle model to yield the Nilsson Model (deformed HO mean field) [28]; pairing correlations were taken into account in various algebraic [29–31] and exact pairing models (e. g., see Fig. 2). For the latter, the pairing Hamiltonian includes non-degenerate single-particle energies plus standard pairing and is exactly solvable, for example, yielding solutions for the ground states of Ca, Ni, and Sn isotopes reproducing experimentally observed pairing gaps [32].

As noted in Table 1, a more complete Density Functional Theory (DFT) is a modern derivative theory of this general type, a self-consistent mean-field theory, that can incorporate correlation effects and can accommodate realistic interactions to achieve better predictive capabilities across most of the Chart of the Nuclides. For example, outcomes using this approach generally yield an excellent accounting of binding energies as well as near ground state phenomena across much of the nuclear landscape [33].

Also noted in the Table 1 on the “Shape Focus” side, are two other complementary models that served to inform us of the importance of deformation and pairing; namely, the Geometric Collective Model (GCM) [34] advanced by Greiner and collaborators, and the intriguing Interacting Boson Model (IBM) of Iachello and associates [35]. The latter has offered a bosonic realization of these phenomena in terms of a common overarching $U(6)$ algebraic structure and its physical subgroups, $U(5)$ for pairing modes, $SU(3) \supset SO(3)$ for rotations and $O(6) \supset SO(3)$ for triaxial systems.

The pairing interaction has been microscopically incorporated into the Elliott Model where it breaks the $SU(3)$ symmetry and mixes different $(\lambda\mu)$ configurations. It has been shown in Ref. [36] (see also Fig. 3a adapted from [36]) that using an $SU(3)$ -symmetric interaction-plus-pairing yields results close to experiment and to the energies obtained using full sd -shell-model calculations [37]. It is remarkable that, even in the presence of pairing, comparable results have been obtained in a truncated model space that includes only about 10 most deformed configurations.

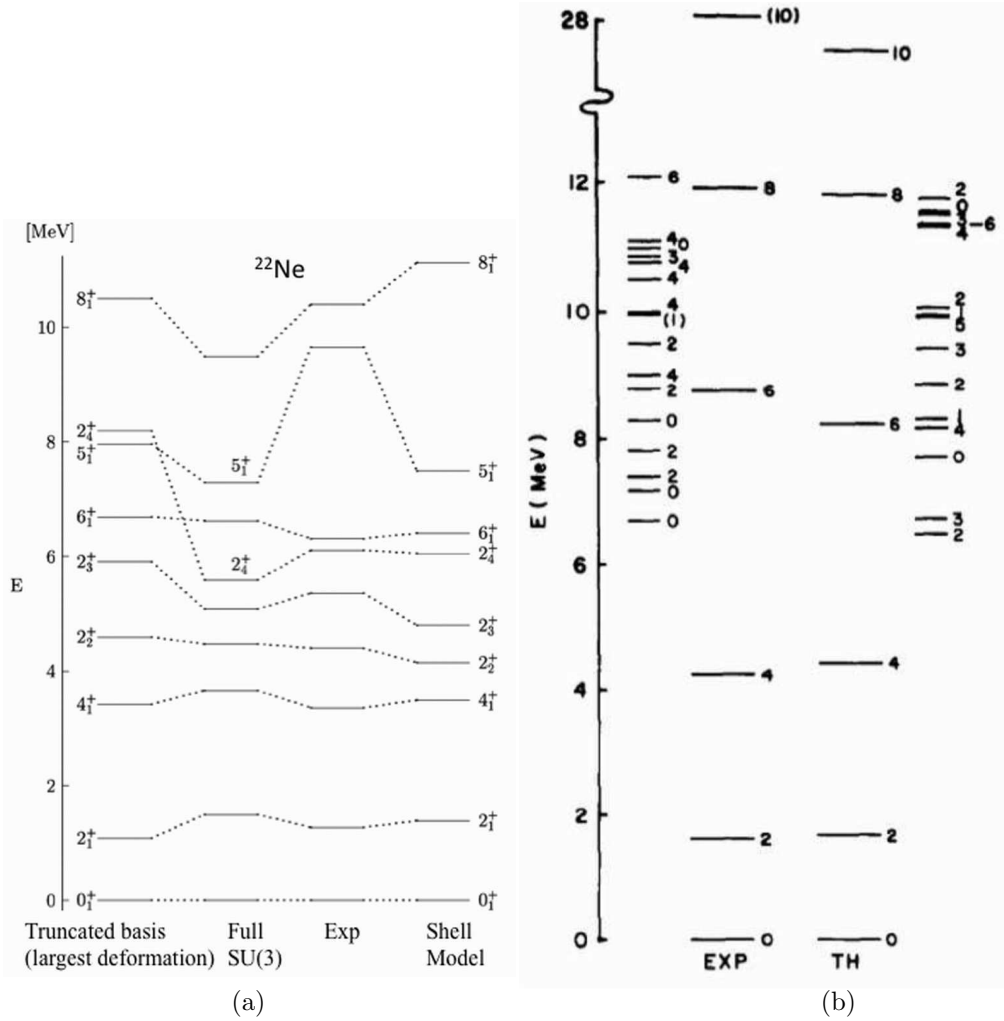


Figure 3: (a) Elliott's model with a $SU(3)$ -preserving interaction + pairing in the sd valence shell for ^{22}Ne . Figure adapted from [36]. (b) Microscopic symplectic model with a set of effective single-particle energies, a $Q \cdot Q$ -type interaction + pairing for ^{20}Ne [calculated $B(E2 \downarrow)$ transition strengths, not shown in the figure, for $J^\pi = 2^+, 4^+, 6^+$, and 8^+ without effective charges fall within the uncertainties of the corresponding experimental measurements]. Figure taken from [39].

Another very significant advance is the microscopic symplectic model [4, 5], developed by Rowe and Rosensteel, which provides a theoretical framework for understanding deformation-dominated collective phenomena in atomic nuclei [6] that involves particle-particle as well as particle-hole excitations across multiple shells. The significance of the symplectic $Sp(3, \mathbb{R})$ symmetry, the embedding symmetry of $SU(3)$ [$Sp(3, \mathbb{R}) \supset SU(3)$], for a microscopic description of a quantum many-body system of interacting particles naturally emerges from the physical relevance of its 21 generators, which are directly related to the particle momentum ($p_{s\alpha}$) and coordinate ($r_{s\alpha}$) operators, with $\alpha = x, y,$ and z for the 3 spatial directions and s labeling an individual nucleon, and realize important observables. Namely, the many-particle kinetic energy $\sum_{s,\alpha} p_{s\alpha}^2/2m$, the HO potential, $\sum_{s,\alpha} m\Omega^2 r_{s\alpha}^2/2$, the mass quadrupole moment $Q_{(2\mathcal{M})} = \sum_s q_{(2\mathcal{M})s} = \sum_s \sqrt{16\pi/5} r_s^2 Y_{(2\mathcal{M})}(\hat{r}_s)$ and angular momentum L operators, together with multi-shell collective vibrations and vorticity degrees of freedom for a description from irrotational to rigid rotor flows are all part of this symmetry. Indeed,

the symplectic $\text{Sp}(3, \mathbb{R})$ symmetry underpins the symplectic shell model that provides a microscopic formulation of the Bohr–Mottelson collective model and is a multiple oscillator shell generalization of the successful Elliott $\text{SU}(3)$ model. The symplectic model with $\text{Sp}(3, \mathbb{R})$ -preserving interactions² have achieved a remarkable reproduction of rotational bands and transition rates without the need for introducing effective charges, while only a single $\text{Sp}(3, \mathbb{R})$ configuration is used [6, 38]. A shell-model study in a symplectic basis that allows for mixing of $\text{Sp}(3, \mathbb{R})$ configurations due to pairing and non-degenerate single-particle energies above a ^{16}O core [39] has found that using only seven $\text{Sp}(3, \mathbb{R})$ configurations is sufficient to achieve a remarkable reproduction of the ^{20}Ne energy spectrum (Fig. 3b) as well as of $E2$ transition rates without effective charges.

I believe one can safely claim that the summit of the particle-hole, shell model climb, with James Vary leading the pack, has been realized with the development of the no-core shell model (NCSM), which, in principle, can straightforwardly accommodate any type of inter-nucleon interaction. Specifically, for a general problem, the NCSM adopts the intrinsic non-relativistic nuclear plus Coulomb interaction Hamiltonian defined as follows:

$$H = T_{\text{rel}} + V_{NN} + V_{NNN} + \dots + V_{\text{Coulomb}}, \quad (1)$$

where the V_{NN} nucleon-nucleon and V_{NNN} 3-nucleon interactions are included along with the Coulomb interaction between the protons. The Hamiltonian may include additional terms such as multi-nucleon interactions among more than three nucleons simultaneously and higher-order electromagnetic interactions such as magnetic dipole-dipole terms. It adopts the HO single-particle basis characterized by the $\hbar\Omega$ oscillator strength and retains many-body basis states of a fixed parity, consistent with the Pauli principle, and limited by a many-body basis cutoff N_{max} . The N_{max} cutoff 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 and is dictated by particle-hole excitations (this is complementary to the microscopic symplectic model, which divides the space in vertical slices selected by collectivity-driven rules). It seeks to obtain the lowest few eigenvalues and eigenfunctions of the Hamiltonian (1). The NCSM has achieved remarkable descriptions of low-lying states from the lightest s -shell nuclei up through ^{12}C , ^{16}O , and ^{14}F , and is further augmented by several techniques, such as NCSM/RGM [40], Importance Truncation NCSM [41] and Monte Carlo NCSM [42]. This supports and complements results of other first-principle approaches, also shown in Table 1, such as Green’s function Monte Carlo (GFMC) [43], Coupled-cluster (CC) method [44], and Lattice Effective Field Theory (EFT) [14] (see also, this proceedings volume [45]). For further details on NCSM, see Vary’s distinguished lecture in this proceedings [46].

We have recently explored a fully microscopic no-core symplectic shell model, NCSpM (for details, see Sec. 4) that utilizes a $\text{Sp}(3, \mathbb{R})$ -preserving $Q \cdot Q$ -type interaction plus a symmetry-breaking $l \cdot s$ interaction. The study has revealed that with a simple interaction and only a few $\text{Sp}(3, \mathbb{R})$ configurations the model can provide a successful description of the ^{12}C Hoyle state and low-lying states in nuclei from Be to Si [10, 11] (including energy spectra, $E2$ transition strengths, quadrupole moments, and matter rms radii). The key to this outcome is the ability of the model to include higher-lying HO shells, thereby making large- N_{max} calculations feasible.

The next-generation *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [2] combines the first-principle concept of the NCSM with symmetry-guided considerations of the collectivity-driven models. The SA-NCSM has revealed the emergence

²An important $\text{Sp}(3, \mathbb{R})$ -preserving interaction is $\frac{1}{2}Q \cdot Q = \frac{1}{2} \sum_s q_s \cdot (\sum_t q_t)$, as this realizes the physically relevant interaction of each particle with the total quadrupole moment of the nuclear system.

of clear symmetry patterns from first principles [2] — such as the $SU(3)$ and the symplectic $Sp(3, \mathbb{R})$ symmetries inherent to nuclei, and in addition, have demonstrated the power of using symmetry-dictated subspaces to reach new domains of nuclear structure currently inaccessible by *ab initio* calculations. The model and its recent findings are described in the next section.

3 *Ab initio* SA-NCSM

The *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [2] 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 (for a review, see [21]). This allows the full model space to be down-selected to the physically relevant space. 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 [3], and a subgroup of the $Sp(3, \mathbb{R})$ symplectic model [4]. The basis states of the SA-NCSM are based on HO single-particle states and for a given N_{\max} , are constructed in the proton-neutron formalism using an efficient construction based on powerful group-theoretical methods. The SA-NCSM basis states are related to the NCSM basis states through a unitary transformation (hence, the SA-NCSM results obtained in a complete N_{\max} space are equivalent to the N_{\max} -NCSM results). They are labeled by the $SU(3) \supset SO(3)$ subgroup chain quantum numbers $(\lambda \mu) \kappa L$, together with proton, neutron, and total intrinsic spins S_p , S_n , 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 $|\tilde{\gamma}(\lambda \mu) \kappa L; (S_p S_n) S; J M_J\rangle$. The label κ distinguishes multiple occurrences of the same L value in the parent irrep $(\lambda \mu)$, and $\tilde{\gamma}$ distinguishes among configurations carrying the same $(\lambda \mu)$ and $(S_p S_n) S$ labels.

3.1 Emergence of a simple structure — 'Bottom Up' considerations

The *ab initio* SA-NCSM results for p -shell nuclei reveal a dominance of configurations of large deformation (typically large $|\lambda - \mu|$) in the $0\hbar\Omega$ subspace. For example, the *ab initio* $N_{\max} = 6$ SA-NCSM results with the bare JISP16 realistic interaction [47] for the 0^+ ground state (g. st.), first 2^+ and first 4^+ states of ^{12}C reveal the dominance of the $0\hbar\Omega$ component with the foremost contribution coming from the leading (04) $S = 0$ irrep (Fig. 4). Furthermore, we find that important $SU(3)$ configurations are then organized into structures with $Sp(3, \mathbb{R})$ symplectic symmetry, that is, the (04) symplectic irrep gives rise to (02) and (24) configurations in the $2\hbar\Omega$ subspace and so on (see Fig. 4, inset), 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 other p -shell nuclei. The outcome points to the fact that the relevant model space can be systematically determined by down-selecting to important spin configurations in lower subspaces while expanded to include a limited set of strongly deformed configurations in the higher N_{\max} regime.

In short, the SA-NCSM advances an extensible microscopic framework for studying nuclear structure and reactions that capitalizes on advances being made in *ab initio* methods while exploiting symmetries — exact and partial, known to dominate the dynamics.

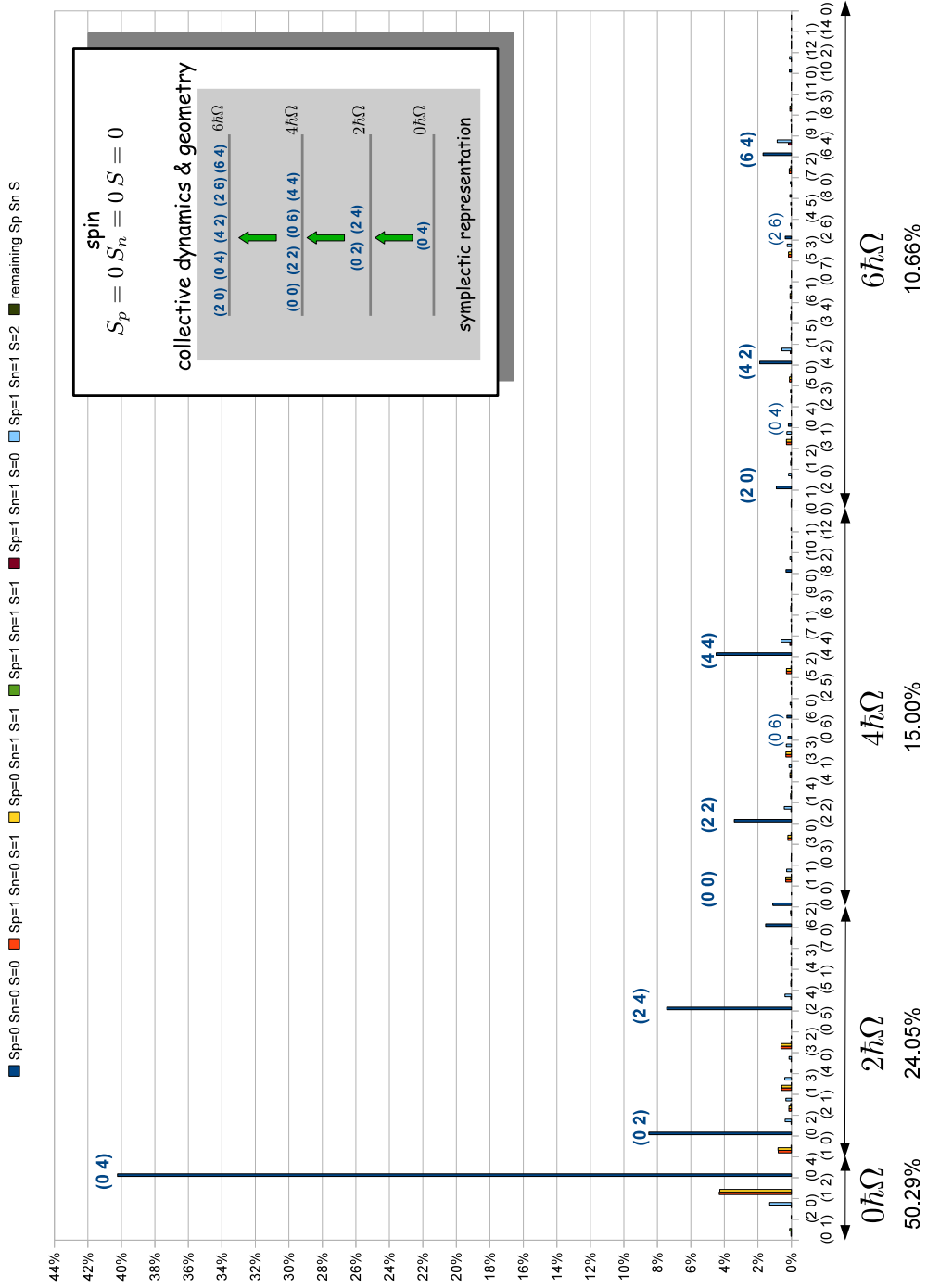


Figure 4: Probability distribution of the lowest calculated 0^+ state for ^{12}C over deformed subspaces labeled by $(\lambda\mu)$ for six of the most important spin components $\{S_p, S_n, S\} = \{0, 0, 0\}, \{1, 0, 1\}, \{0, 1, 1\}, \{1, 1, 1\}, \{1, 1, 0\}$ and $\{1, 1, 2\}$. Labels above the columns denote SU(3) quantum numbers of states that belong to the leading (04) symplectic $\text{Sp}(3, \mathbb{R})$ irrep. The wavefunction was obtained using the $N_{\text{max}} = 6$ SA-NCSM with the JISP16 bare interaction and $\hbar\Omega = 10$ MeV.

3.2 Symmetries in realistic nucleon-nucleon interactions

The nucleon-nucleon interaction itself possesses a clear structure when its $SU(3)$ content is studied. This is observed in the decomposition of the NN interaction into $SU(3) \times SU(2)_S \times SU(2)_T$ tensors (isoscalar interactions will be henceforth considered). This is analogous to the unitary transformation of a V_{2b} two-body interaction represented in a m -scheme harmonic oscillator (HO) basis to a JT -coupled basis, which renders V_{2b} as only one $SU(2)_J \times SU(2)_T$ tensor of rank $J_0 = 0$ and $T_0 = 0$ (a scalar with respect to rotations in coordinate and isospin space). For example, the scalar interaction part of $(\lambda_0 \mu_0) = (00)$ does not mix nuclear deformation in analogy to the isoscalar part of an interaction that does not mix isospin values. In addition, the $(\lambda_0 \mu_0)$ interaction parts with $\lambda_0 = \mu_0$ are almost diagonal, that is, connect configurations within a few shells, while interaction parts with a large difference $|\lambda_0 - \mu_0|$ typically couple low-lying and higher-lying shell-model configurations.

This decomposition organizes the interaction into only a small number of pieces of information that bring forward important physics. In particular, as a measure of the strength or “size” of each interaction tensor, we use its Hilbert–Schmidt norm, which is directly related to the square of the $(\lambda_0 \mu_0)S_0$ reduced matrix elements. For example, we find a dominance of the (00) scalar part followed by the symplectic-like modes of (02) , and equally, the conjugate (20) , and then tensors as (11) , (22) , (33) , and etc., which typically dominate for the pairing interaction or contact term (see Fig. 5 for the bare JISP16, which is used for $N_{\max} = 6$ SA-NCSM calculations in Fig. 4). These results, we find, repeat for various realistic bare and renormalized interactions.

4 NCSpM model — ‘Top Down’ considerations

The no-core symplectic shell model (NCSpM) is a fully microscopic no-core shell model that uses a symplectic $Sp(3, \mathbb{R})$ basis and $Sp(3, \mathbb{R})$ -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. The NCSpM, while selecting the most relevant symplectic configurations, is employed to provide shell model calculations beyond current NCSM limits, namely, up through $N_{\max} = 20$ for ^{12}C , the model spaces we found sufficient for the convergence of results [10].

We employ a very simple Hamiltonian with an effective interaction derived from the long-range expansion of the two-body central nuclear force together with a spin-orbit term,

$$H_{\text{eff}} = H_0 + \frac{\chi}{2} \frac{(e^{-\gamma Q \cdot Q} - 1)}{\gamma} - \kappa \sum_{i=1}^A l_i \cdot s_i. \quad (2)$$

This includes the spherical HO potential, which together with the kinetic energy yields the HO Hamiltonian, $H_0 = \sum_{i=1}^A \left(\frac{\mathbf{p}_i^2}{2m} + \frac{m\Omega^2 \mathbf{r}_i^2}{2} \right)$, and the $Q \cdot Q$ quadrupole-quadrupole interaction not restricted to a single shell. For the latter term, the average contribution, $\langle Q \cdot Q \rangle_n$, of $Q \cdot Q$ within a subspace of n HO excitations is removed [48], that is, the trace of $Q \cdot Q$ divided by the space dimension for a fixed n . Hence, the large monopole contribution of the $Q \cdot Q$ interaction is removed, which, in turn, helps eliminate the considerable renormalization of the zero-point energy, while retaining the $Q \cdot Q$ -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. We take the coupling constant χ to be proportional to $\hbar\Omega$ and,

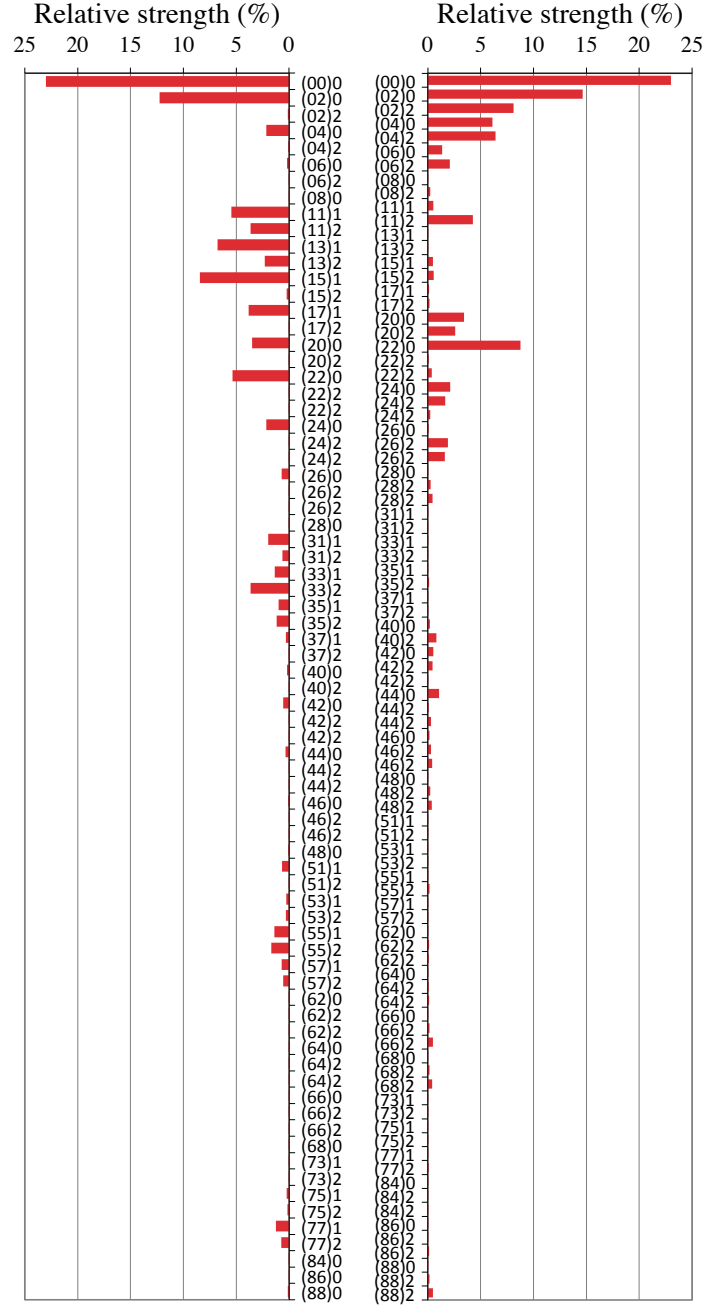


Figure 5: Relative strengths of the $T = 1$ (left) and $T = 0$ (right) bare JISP16 interaction tensors labeled by $(\lambda_0 \mu_0) S_0$ for $\hbar\Omega = 15$ MeV and $N_{\max} = 6$ for p -shell nuclei.

to leading order, to decrease with the total number of HO excitations, as shown by Rowe [49] based on self-consistent arguments.

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 [10]. The low-lying energy spectrum and eigenstates for ^{12}C were calculated using the NCSpM with H of Eq. (2) for $\hbar\Omega = 18$ MeV given by the empirical estimate $\approx 41/A^{1/3} = 17.9$ MeV and for $\kappa \approx 20/A^{2/3} = 3.8$ MeV (see, e. g., [20]). The results are shown for $N_{\max} = 20$, which we found sufficient to yield

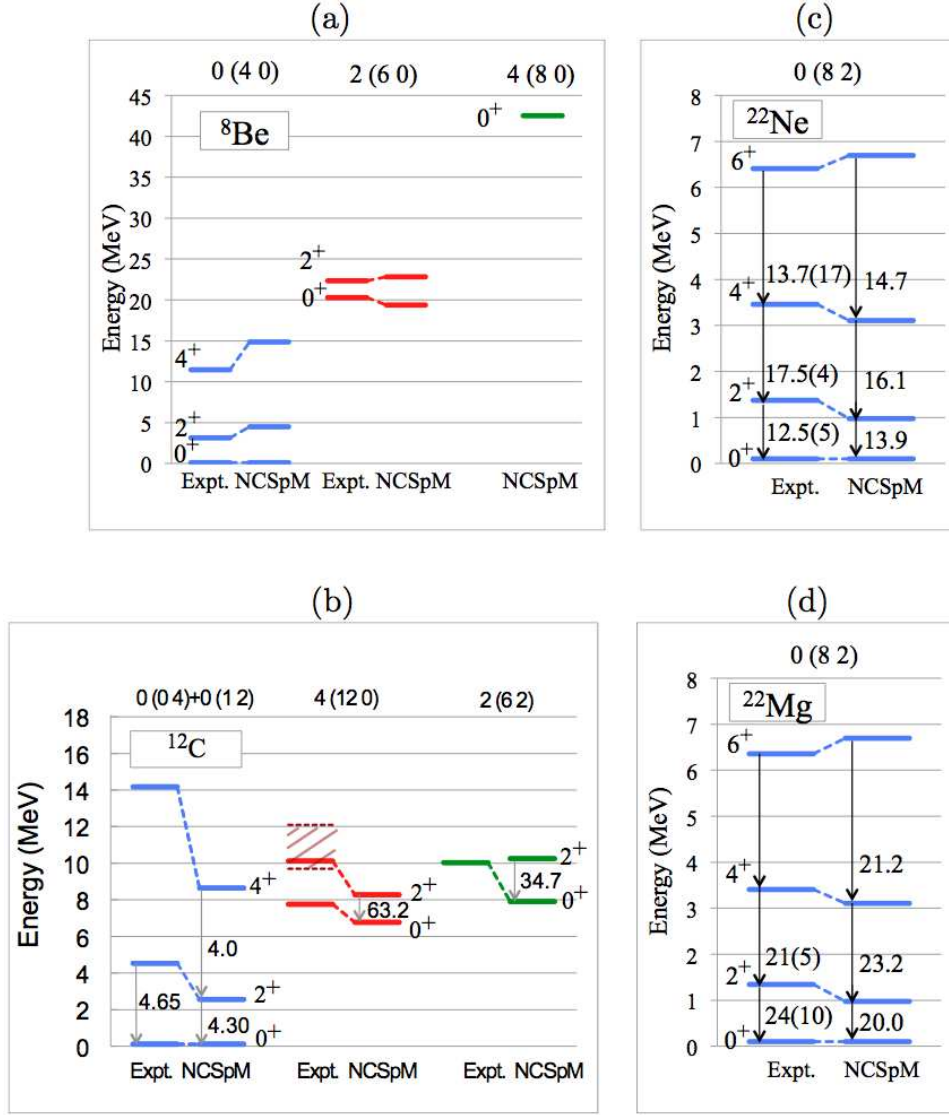


Figure 6: Energy spectra calculated by the NCSpM with $\gamma = -1.71 \times 10^{-4}$ for (a) ^8Be in an $N_{\text{max}} = 24$ model space, (b) ^{12}C in an $N_{\text{max}} = 20$ model space, (c) ^{22}Ne and (d) ^{22}Mg in an $N_{\text{max}} = 12$ model space, and compared to experiment (“Expt.”).

convergence. This N_{max} model space is further reduced by selecting the most relevant symplectic irreps, namely, the spin-zero ($S = 0$) $0\hbar\Omega$ 0p-0h (0 4), $2\hbar\Omega$ 2p-2h (6 2), and $4\hbar\Omega$ 4p-4h (12 0) symplectic bandheads together with the $S = 1$ $0\hbar\Omega$ 0p-0h (1 2) and all multiples thereof up through $N_{\text{max}} = 20$ of total dimensionality of 6.6×10^3 . In comparison to the experimental energy spectrum (Fig. 6b), the outcome reveals that the lowest 0^+ , 2^+ , and 4^+ states of the 0p-0h symplectic slices 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 (12 0) and the $2\hbar\Omega$ 2p-2h (6 2) slices are found to lie close to the Hoyle state and the 10-MeV 0^+ resonance (third 0^+ state), respectively. The model successfully reproduces other observables for ^{12}C that are informative of the state structure, such as mass rms radii, electric quadrupole moments and $B(E2)$ transition strengths (Fig. 6b).

A preponderance of the (0 4) $S = 0$ configuration and also (1 2) $S = 1$ configuration is observed for the ground-state rotational band, thereby indicating an oblate

shape. The Hoyle-state rotational band includes shapes of even larger deformations but prolate, with the largest contribution of (16 0).

While the model includes an adjustable parameter, γ , this parameter only controls the decrease rate of the $Q \cdot Q$ interaction with increasing n . The entire many-body apparatus is fully microscopic and no adjustments are possible. Hence, as γ varies, there is only a small window of possible γ values that, for large enough N_{\max} , closely reproduces the relative positions of the three lowest 0^+ states.

The outcome of the present analysis is not limited to ^{12}C . The model we find is also applicable to the low-lying states of other p -shell nuclei, such as ^8Be , as well as sd -shell nuclei without any adjustable parameters (Fig. 6). In particular, using the same $\gamma = -1.71 \times 10^{-4}$ as determined here for ^{12}C , we describe selected low-lying states in ^8Be in an $N_{\max} = 24$ model space with only 3 spin-zero $0\hbar\Omega$ (4 0), $2\hbar\Omega$ (6 0), and $4\hbar\Omega$ (8 0) symplectic irreps. Furthermore, we have successfully applied the NCSpM without any adjustable parameters to the ground-state rotational band of heavier nuclei, such as ^{20}Ne , $^{22,24}\text{Ne}$, $^{22,26}\text{Mg}$, and $^{24,26}\text{Si}$ (see Fig. 6 for ^{22}Ne and ^{22}Mg). This suggests that the fully microscopic NCSpM model has indeed captured an important part of the physics that governs the low-energy nuclear dynamics.

5 Conclusion

Symmetries in atomic nuclei that have been long recognized have been recently utilized and further understood in the framework of the *ab initio* symmetry-adapted no-core shell model SA-NCSM as well as of the microscopic no-core symplectic model NCSpM that combine the shell-model and collectivity-driven concepts. The findings pointed to a remarkable new insight, namely, understanding the mechanism on how such simple structures emerge from a fundamental level.

Symmetry-adapted, no-core shell-model calculations with SU(3) the underpinning symmetry were presented. We showed that employing symmetry considerations is effective in providing an efficient description of low-lying states. This holds promise to significantly enhance the reach of *ab initio* shell models toward heavier nuclear systems as well as to achieve descriptions of collective and cluster phenomena from underlying quark/gluon considerations. In addition, the NCSpM study with a schematic many-nucleon interaction showed how both collective and cluster-like structures emerge out of a no-core shell-model framework, which extended to and took into account essential high-lying shell-model configurations.

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References

- [1] P. Navrátil, J. P. Vary and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000); Phys. Rev. C **62**, 054311 (2000).

- [2] T. Dytrych, K. D. Launey, J. P. Draayer, P. Maris, J. P. Vary, E. Saule, U. Çatalyürek, M. Sosonkina, D. Langr and M. A. Caprio, LSU Preprint PA/NP2013-0005 (2013).
- [3] J. P. Elliott, Proc. Roy. Soc. A **245**, 128 (1958).
- [4] G. Rosensteel and D. J. Rowe, Phys. Rev. Lett. **38**, 10 (1977).
- [5] G. Rosensteel and D. J. Rowe, Ann. Phys. (NY) **126**, 343 (1980).
- [6] D. J. Rowe, Rep. Progr. Phys. **48**, 1419 (1985).
- [7] P. Maris, A. M. Shirokov and J. P. Vary, Phys. Rev. C **81**, 021301 (R) (2010).
- [8] G. Hagen, T. Papenbrock, D. J. Dean and M. Hjorth-Jensen, Phys. Rev. Lett. **101**, 092502 (2008).
- [9] S. C. Pieper and R. B. Wiringa Ann. Rev. Nucl. Part. Sci. **51**, 53 (2001).
- [10] A. C. Dreyfuss, K. D. Launey, T. Dytrych, J. P. Draayer and C. Bahri, *submitted* (2013); arXiv:1212.2255 [nucl-th] (2012).
- [11] K. D. Launey, T. Dytrych, J. P. Draayer, G. K. Tobin, M. C. Ferriss, D. Langr, A. C. Dreyfuss, P. Maris, J. P. Vary and C. Bahri, in *Proc. 5th Int. Conf. "Fission and properties of neutron-rich nuclei", ICFN5*. World Scientific, to be published, 2013.
- [12] F. Hoyle, Astrophys. J. Suppl. **1**, 121 (1954).
- [13] R. B. Wiringa *et al.*, in *INT Program 12-3 "Light nuclei from first principles"*, 2012.
- [14] E. Epelbaum, H. Krebs, D. Lee and U.-G. Meissner, Phys. Rev. Lett. **106**, 192501 (2011).
- [15] M. Hjorth-Jensen, Physics **4**, 38 (2011).
- [16] M. Chernykh, H. Feldmeier, T. Neff, P. Von Neumann-Cosel and A. Richter, Phys. Rev. Lett. **98**, 032501 (2007).
- [17] B. R. Barrett, P. Navrátil and J. P. Vary, Progr. Part. Nucl. Phys. **69**, 131 (2013).
- [18] J. E. Drut, R. J. Furnstahl and L. Platter, Progr. Part. Nucl. Phys. **64**, 120 (2010).
- [19] O. Haxel, J. H. D. Jensen and H. E. Suess, Phys. Rev. **75**, 1766 (1949); M. G. Mayer, *ibid.* **75**, 1969 (1949); *ibid.* **78**, 16 (1950).
- [20] A. Bohr and B. R. Mottelson, *Nuclear Structure, Vol. 1*. Benjamin, New York, 1969; *Vol. 2. ibid.*, 1974; B. R. Mottelson, *Nobel Lectures, Physics 1971–1980*. World Scientific, Singapore, 1992.
- [21] T. Dytrych, K. D. Sviratcheva, J. P. Draayer, C. Bahri and J. P. Vary, J. Phys. G. **35**, 123101 (2008).
- [22] J. P. Elliott and M. Harvey, Proc. Roy. Soc. A **272**, 557 (1963).
- [23] G. Rosensteel and D. J. Rowe, Ann. Phys. (NY) **104**, 134 (1977).
- [24] Y. Leschber and J. P. Draayer, Phys. Letts. B **190**, 1 (1987).
- [25] O. Castaños, J. P. Draayer and Y. Leschber, Z. Phys **329**, 33 (1988).

- [26] M. Harvey, *Adv. Nucl. Phys.* **1**, 62 (1968).
- [27] J. P. Draayer, C. Bahri and S. Moszkowski, *Phys. Rev. Lett.* **68**, 557 (1992).
- [28] S. G. Nilsson, *Dan. Mat. Fys. Medd.* **29**, No 16 (1955).
- [29] G. Racah, *Phys. Rev.* **62**, 438 (1942); *ibid.* **63**, 367 (1943).
- [30] B. H. Flowers, *Proc. Roy. Soc. (London) A* **212**, 248 (1952).
- [31] A. K. Kerman, *Ann. Phys. (NY)* **12**, 300 (1961).
- [32] X. Guan, K. D. Launey, M. Xie, L. Bao, F. Pan and J. P. Draayer, *Phys. Rev. C* **86**, 024313 (2012).
- [33] UNEDF SciDAC Collaboration, <http://unedf.org/>.
- [34] J. Eisenberg and W. Greiner, *Nuclear Theory I: Nuclear collective Models*. North-Holland, Amsterdam, 1987; G. Gneuss, U. Mosel and W. Greiner, *Phys. Lett. B* **30**, 397 (1969).
- [35] F. Iachello and A. Arima, *The Interacting Boson Model*. Cambridge University Press, Cambridge, 1987; A. Arima and F. Iachello, *Phys. Rev. Lett.* **35**, 1069 (1975).
- [36] C. E. Vargas, J. G. Hirsch and J. P. Draayer, *Nucl. Phys. A* **690**, 409 (2001).
- [37] B. M. Freedom and B. H. Wildenthal, *Phys. Rev. C* **6**, 1633 (1972).
- [38] C. Bahri and D. J. Rowe, *Nucl. Phys. A* **662**, 125 (2000).
- [39] J. P. Draayer, K. J. Weeks and G. Rosensteel, *Nucl. Phys. A* **413**, 215 (1984).
- [40] S. Quaglioni and P. Navrátil, *Phys. Rev. Lett.* **101**, 092501 (2008).
- [41] R. Roth, J. Langhammer, A. Calci, S. Binder and P. Navrátil, *Phys. Rev. Lett.* **107**, 072501 (2011).
- [42] T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno and J. P. Vary, *Phys. Rev. C* **86**, 054301 (2012).
- [43] S. Pieper, K. Varga and R. B. Wiringa, *Phys. Rev. C* **66**, 044310 (2002); S. C. Pieper, *Nucl. Phys. A* **751**, 516c (2005).
- [44] M. Włoch, D. J. Dean, J. R. Gour, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock and P. Piecuch, *Phys. Rev. Lett.* **94**, 212501 (2005); G. Hagen, T. Papenbrock, D. J. Dean and M. Hjorth-Jensen, *Phys. Rev. C* **82**, 034330 (2010).
- [45] *Proc. Int. Conf. Nucl. Theor. Supercomputing Era (NTSE-2013), Ames, IA, USA, May 1-17, 2013*, eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, 2014 (see these Proceedings), <http://www.ntse-2013.khb.ru/Proc/>.
- [46] J. P. Vary, *Computational Nuclear Physics: Key to Discovery Opportunities*, Distinguished Lecture at NTSE-2013, see these Proceedings, p. 15, <http://www.ntse-2013.khb.ru/Proc/JPVary.pdf>.
- [47] A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, *Phys. Lett. B* **644**, 33 (2007).
- [48] G. Rosensteel and J. P. Draayer, *Nucl. Phys. A* **436**, 445 (1985).
- [49] D. J. Rowe, *Phys. Rev.* **162**, 866 (1967).