What a wonderful world - Simplicity within complexity

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What a wonderful world –
simplicity within complexity

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Abstract. In this lecture, Louis Armstrong’s transformational Jazz, as exemplified by his signature recital of “What a Wonderful World”, will take us to the ever evolving World of Nuclear Physics. In particular, I will focus on the discovery of simplicities, or symmetry patterns, in complex nuclear systems. And as Jazz is to music, so too Nuclear Physics is a restless endeavor – the dissonance of forlorn flattened notes tracking with the intrigue of symmetry, and its breaking in nuclei. I will also discuss some recent approaches to nuclear structure at this dawn of the 21st century, linking the intrigue of quarks and gluons with the fundamental science of the strong and weak interactions to the emergence of simplicity within complexity unveiled in atomic nuclei.

1. Emerging symmetries within complex nuclear systems
A forefront challenge in nuclear physics is to advance our understanding of atomic nuclei based on the nature of the strong force and how it impacts complex nuclear dynamics, keying on features that are central to nuclear reactions, astrophysics, neutrino and cosmology research, as well as to applied studies of nuclear energy and radioactive isotopes for medicine. Indeed, while the non-perturbative nature of Quantum Chromodynamics (QCD) in the regime of low energies together with the computationally intensive many-body problem place tremendous difficulties on achieving a description of nuclei starting from QCD itself (“ab initio”), establishing a connection from the quark/gluon foundation to nuclear properties with their diverse characteristics is essential for understanding nuclear structure at a fundamental level.

Notwithstanding, complex nuclear systems often display striking simplicities. Furthermore, experimental evidence supports the fact that low-lying nuclear states in light and medium-mass nuclei favor a dominance of low spin and high deformation, which has been also recently demonstrated through our first-principle studies [1, 2]. We have also showed the power of using symmetry-dictated subspaces to reach new domains of nuclear structure currently inaccessible by ab initio calculations. This, in turn, points to a remarkable new insight into the symmetry

1 Public lecture presented at the “Horizons of Innovative Theories, Experiments, and Supercomputing in Nuclear Physics”, HITES, in New Orleans, June 4-7, 2012. The able assistance of Kristina D. Launey in the planning, presentation and publication of the lecture is gratefully acknowledged.

2 Louis Armstrong, whose bigger than life statue with trumpet in hand greets visitors to the New Orleans International Airport, is a favorite son of Louisiana, known for his “... foundational influence in jazz, shifting the music’s focus from collective improvisation to solo performance ... ” (Wikipedia).
patterns observed in atomic nuclei, namely, understanding the mechanism on how such simple structures emerge from the fundamental level of the underlying quark/gluon physics.

The symmetry-guided approach we have developed utilizes symmetry to reduce the dimensionality of the model space through a very structured winnowing of the basis states to physically relevant subspaces. We achieve significantly enhanced reach beyond that of the current no-core shell model (NCSM) by taming the scale explosion problem through the development of a practical, \textit{ab initio} symmetry-adepted no-core shell model (SA-NCSM) framework. This framework exploits our knowledge of dominant symmetries, first of the interaction itself and then of those that emerge as a result of the many-body dynamics, and utilizes the power of the current and unfolding next-generation of high performance computing (HPC) facilities. This combination opens up new regions of the periodic chart, the ‘\textit{sd-shell}’, to investigation with \textit{ab initio} methods. Our approach enables the inclusion of higher-order correlations as required, for example, for understanding excited $0^+$ states – e.g., the elusive Hoyle state – in the lighter nuclei, and sets the stage for advancing the applicability of the current \textit{ab initio} methods to systems beyond (e.g., ‘\textit{fp-shell}’ nuclei, and even beyond to ‘upper \textit{fp-shell}’ and ‘lower \textit{gds-shell}’ as well as rare-earth and actinide species where deformation plays an even more dominant role) that are necessary, for example, for a better understanding of astrophysical processes among higher-mass nuclei.

Furthermore, we find that the results of various symmetry-adepted, no-core shell-model calculations for light and medium-mass nuclei are independent of whether the system Hamiltonian is phenomenological in nature or derived from realistic nucleon-nucleon (\textit{NN}) interactions. They imply that only a small fraction of the full model space is needed for a description of low-lying states in these nuclei, and this in turn points to the importance of using a symmetry-adepted, no-core shell-model framework for describing such nuclei, one based on an \textit{LS} coupling scheme with spatial configurations organized according to deformation.

The outcome confirms the relevance of the pioneering work of early developers of the field, J.P. Elliott and his SU(3) model \cite{3} and M. Moshinsky with his U(3) many-body oscillator work \cite{4}, extended to open, multi-shell environments. Specifically, the results demonstrate the relevance of these algebraic methods in this region, and in particular, how they can be used to quell the combinatorial growth in the dimensionality of the problem with the addition of higher oscillator shells to the model space. Indeed, the results show the utility of a symmetry-adepted, no-core shell-model approach for light nuclei that takes maximum advantage of group-theoretical methods as well as advanced computational techniques.

The theory is applied to a study of the structure of various light nuclei, e.g. $^6\text{Li}$, $^6\text{He}$, $^8\text{Be}$, $^{16}\text{O}$ and presented here for the case of $^{12}\text{C}$, as well as to first studies of \textit{sd-shell} nuclei such as $^{24}\text{Si}$ and $^{22}\text{Mg}$, now rendered feasible due to symmetry-based considerations. Comparisons with results from no-core shell model analyses illustrate the efficacy of the symmetry-adepted framework. In addition, a simple algebraic interaction, which reduces to the Elliott model in its single-shell limit, is shown to reproduce all features of the elusive Hoyle state in $^{12}\text{C}$. While this requires that the no-core underpinning of the model be extended beyond the current reach of the standard no-core shell model to excitations as high as eighteen major oscillator shells, only the most deformed configurations in the extended region are required. This further affirms the importance of exploiting algebraic methods in exploring special correlations in many-particle and multi-shell environments. The latter also suggests a possible path forward for realizing macroscopic theories that target collective degrees of freedom in terms of more microscopic ones that build forward from the \textit{NN} interaction itself.
2. Symmetry-guided framework

2.1. Symmetry patterns revealed in results of ab initio studies and the SA-NCSM model

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)⊃SO(3) subgroup chain. This allows the full model space to be down-selected to the physically relevant space [1, 5]. 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 [6, 7, 8], and a subgroup of the Sp(3, R) symplectic model [9].

The conventional NCSM basis spaces are constructed using harmonic oscillator (HO) single-particle states and are characterized by the $h\Omega$ 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)⊃SO(3) subgroup chain quantum numbers $(\lambda \mu)\kappa L$, together with proton, neutron, and total intrinsic spins $S_z$, $S_\nu$, 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
\[ |\gamma(\lambda \mu)\kappa L; (S_\pi S_\nu) S; JM, J_t \rangle \]. 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 \( \lambda \mu \) and \( (S_\pi S_\nu) S \) labels.

The \textit{ab initio} SA-NCSM results for \( p \)-shell nuclei reveal a dominance of shapes of large deformation (typically large \(|\lambda - \mu|\)) in the \( 0\hbar \Omega \) subspace. For example, the \textit{ab initio} \( N_{\text{max}} = 6 \) SA-NCSM results with the bare JISP16 realistic interaction \cite{10} for the \( 0^+ \) ground state (g.st.), first \( 2^+ \) and first \( 4^+ \) states of \( ^{12}\text{C} \) reveal the dominance of the \( 0\hbar \Omega \) component with the foremost contribution coming from the leading \((04)\ S = 0 \) irrep (Fig. 1). Furthermore, we find that important \( \text{SU}(3) \) configurations are then organized into structures with \( \text{Sp}(3, \mathbb{R}) \) symplectic symmetry, that is, the \((04)\) symplectic irrep gives rise to \((02)\) and \((24)\) configurations in the \( 2\hbar \Omega \) subspace, and 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 \( N_{\text{max}} \) regime.

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

2.2. Symmetry patterns of realistic nucleon-nucleon interactions

The nucleon-nucleon interaction itself possesses a clear structure when its \( \text{SU}(3) \) content is studied. This is observed in the decomposition of the \( NN \) interaction into \( \text{SU}(3) \times \text{SU}(2)_S \times \text{SU}(2)_T \) 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 \( \text{SU}(2)_J \times \text{SU}(2)_T \) 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 shape deformations 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. 2 for the bare JISP16). These results, we find, repeat for various realistic bare and renormalized interactions.

2.3. Symmetry-guided shell-model approach and alpha clustering phenomena: NCSpM model

The no-core symplectic shell model (NCSpM) is a fully microscopic no-core shell model that uses a symplectic \( \text{Sp}(3, \mathbb{R}) \) basis and \( \text{Sp}(3, \mathbb{R}) \)-preserving interactions. The NCSpM employed within a full model space up through a given \( N_{\text{max}} \) coincides 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 \( \text{Sp}(3, \mathbb{R}) \) irreps within the \( N_{\text{max}} \) model space. The NCSpM, while selecting the most relevant symplectic configurations, is employed to provide shell model calculations beyond current NCSM limits.
Relative strength (%)

T=0

T=1

Figure 2. Relative strengths of the \( T = 0 \) and \( T = 1 \) bare JISP16 interaction tensors labeled by \( (\lambda_0 \mu_0) \) and \( S_0 \) for the case shown in Fig. 1, namely, \( \hbar \Omega = 15 \text{ MeV} \) and \( N_{\text{max}} = 6 \) for \( p \)-shell nuclei.

namely, up through \( N_{\text{max}} = 20 \) for \(^{12}\text{C}\), the model spaces we found sufficient for the convergence of results.

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

\[
H_{\text{eff}} = H_0 - \frac{\chi}{2} \frac{1}{\gamma} \left( e^{\gamma (Q.Q - (Q.Q)_n)} - 1 \right),
\]

which 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 [11], 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 [6, 8]. We take the coupling constant \( \chi \) to be proportional to \( \hbar \Omega \) and, to leading order, to decrease with the total number of HO excitations, as shown by Rowe [12] based on self-consistent arguments. It is important to note that such a model Hamiltonian (1) fixes the \( \chi \) 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 \(^{12}\text{C}\) were calculated using the NCSpM with \( H \) of Eq. (1) for \( \hbar \Omega = 18 \text{ MeV} \) given by the empirical estimate \( \approx 41/A^{1/3} = 17.9 \text{ MeV} \). 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 \( (S = 0) \) \( 0\hbar \Omega 0p-0h \ (0\ 4), \ 2\hbar \Omega 2p-2h \ (6\ 2), \) and \( 4\hbar \Omega 4p-4h \ (12\ 0) \) 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 $0\hbar\Omega$ $0p-0h$ (0 4) 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 $4\hbar\Omega$ $4p-4h$ (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. We note that the NCSpM energies given in Fig. 3 are 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. Indeed, the model successfully reproduces other observables for $^{12}\text{C}$ that are informative of the state structure, such as mass rms radii, electric quadrupole moments and $B(E2)$ transition strengths (Fig. 3).

In accordance with the mapping [15] between the shell-model ($\lambda\mu$) SU(3) labels and the shape variables of the Bohr-Mottelson collective model [16], the symplectic basis states bring forward important information about the nuclear shapes and deformation. For example, as shown in Fig. 3, the (0 4) symplectic bandhead of the ground-state rotational band and the (12 0) bandhead of the Hoyle-state rotational band describe oblate and prolate shapes, respectively. While a preponderance of the (0 4) shape (of $\sim 65\%$ probability) is observed for the former band (Fig. 4, red/left bars), the latter band includes shapes of even larger deformations (more prolate) with the largest contribution ($\sim 30\%$) of (16 0).

In addition, a close similarity is observed when the probability distributions for the $g.st.$ rotational band are compared to $ab\ initio$ results when only configurations of zero proton and neutron spins ($S_{\pi,\nu} = 0$) are selected (Fig. 4). In particular, NCSpM eigenstates, which are $h\Omega$-independent, are compared to SA-NCSM calculations with the bare JISP16 realistic interaction for $h\Omega = 20$ MeV (around the minimum of the calculated binding energy for $^{12}\text{C}$) and a $N_{\text{max}} = 8$ model space. This space appears to be sufficient to yield convergent results for the $g.st.$ rotational band for both models. The close agreement points to the fact that the schematic interaction used in NCSpM has effectively captured most of the underlying physics of the realistic interaction important to the low-energy nuclear dynamics.

While the model includes an adjustable parameter, $\gamma$, this parameter only controls the
Figure 4. Probability distribution for $^{12}$C as a function of the $n$ total excitations and SU(3) labels, that is, $n(\lambda \mu)$, of the lowest $0^+$, $2^+$, and $4^+$ states as calculated by the NCSpM (left) and the $N_{\text{max}} = 8$ SA-NCSM using the bare JISP16 for $\hbar \Omega = 20$ MeV (right).

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.

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.

3. Conclusion
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 eigenstates of $^{12}$C, which also holds for various other $p$-shell nuclei. A symmetry-guided framework was suggested based on our recent findings of low-spin and high-deformation dominance in realistic NCSM results. 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 first principles.

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