Physics of nuclei:
Key role of an emergent symmetry

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Exact symmetry and symmetry-breaking phenomena play a key role in providing a better understanding of the physics of many-particle systems, from quarks and atomic nuclei, to molecules and galaxies. In atomic nuclei, exact and dominant symmetries such as rotational invariance, parity, and charge independence have been clearly established. However, even when these symmetries are taken into account, the structure of nuclei remains illusive and only partially understood, with no additional symmetries immediately evident from the underlying nucleon-nucleon interaction. Here, we show through \textit{ab initio} large-scale nuclear structure calculations that the special nature of the strong nuclear force determines additional highly regular patterns in nuclei that can be tied to an emergent approximate symmetry. We find that this symmetry is remarkably ubiquitous, regardless of its particular strong interaction heritage, and mathematically tracks with a symplectic group. Specifically, we show for light to intermediate-mass nuclei that the structure of a nucleus, together with its low-energy excitations, respects symplectic symmetry at about 70-80\% level, unveiling the predominance of only a few equilibrium shapes, deformed or not, with associated vibrations and rotations. This establishes the symplectic symmetry as a remarkably good symmetry of the strong nuclear force, in the low-energy regime. This may have important implications to studies, e.g., in astrophysics and neutrino physics that rely on nuclear structure information, especially where experimental measurements are incomplete or not available. A very important practical advantage is that this new symmetry can be utilized to dramatically reduce computational resources required in \textit{ab initio} large-scale nuclear structure modeling. This, in turn, can be used to pioneer predictions, e.g., for short-lived isotopes along various nucleosynthesis pathways.

I. INTRODUCTION

The nucleus was discovered early in the last century. Yet the nature of its dynamics remains poorly understood. The standard shell model of nuclear physics is based on the premise that atomic nuclei have an underlying spherical harmonic oscillator (HO) shell structure, as in the Mayer-Jensen model \cite{1}, with residual interactions. In fact, with effective interactions and large effective charges, the shell model is successful at explaining many properties of nuclei. However, it has been much less successful at predicting the many surprises that surface, such as the highly collective rotational states that are observed and are described phenomenologically by the successful Bohr-Mottelson collective model \cite{2}, as well as the recognition that the first excited state of the doubly closed shell nucleus of \textit{16}O is the head of a strongly deformed rotational band \cite{3,4}. The coexistence of states of widely differing deformation in many nuclei is now well established \cite{5,6} as an emergent phenomenon and dramatically exposes the limitations of the standard shell model.

To address this and to understand the physics of nuclei without limitations within the interaction and approximations during the many-body nuclear simulations, we use an \textit{ab initio} framework that starts with realistic interactions tied to elementary particle physics considerations and fitted to nucleon-nucleon data. Such calculations are now possible and are able to give converged results for light nuclei by the use of supercomputers. However, in \textit{ab initio} calculations the complexity of the nuclear problem dramatically increases with the number of particles, and when expressed in terms of literally billions of shell-model basis states, the structure of a nuclear state is unrecognizable. But expressing it in a more informative basis, the symmetry-adapted collective basis \cite{10,11}, leads to a major breakthrough: in this article, we report on the very unexpected outcome from first-principle investigations of light to intermediate-mass nuclei (below the calcium region), namely, the incredible simplicity of nuclear low-lying states and the dominance we observe of an associated symmetry of nuclear dynamics, the symplectic Sp(3, \mathbb{R}) symmetry, which together with its slight symmetry breaking is shown here to naturally describe atomic nuclei. This exposes for the first time the fundamental role of the symplectic Sp(3, \mathbb{R}) symmetry and unveils it as a remarkably good symmetry of the strong nuclear force, represented here by interactions derived in the state-of-the-art chiral effective field theory.

It is known that SU(3), a subgroup of Sp(3, \mathbb{R}), is the symmetry group of the spherical harmonic oscillator that
underpins the shell model and the valence-shell SU(3) (Elliott) model. The Elliott model has been shown to naturally describe rotations of a deformed nucleus without the need for breaking rotational symmetry. The key role of deformation in nuclei and the coexistence of low-lying quantum states in a single nucleus characterized by configurations with different quadrupole moments makes the quadrupole moment a dominant fundamental property of the nucleus, and together with the monopole moment or “size” of the nucleus – along with nuclear masses – establishes the energy scale of the nuclear problem. Indeed, the nuclear monopole and quadrupole moments underpin the essence of symplectic Sp(3, \mathbb{R}) symmetry (Fig. 1). Not surprisingly, the symplectic Sp(3, \mathbb{R}) symmetry, the underlying symmetry of the symplectic rotor model, has been found to play a key role across the nuclear chart – from the lightest systems through intermediate-mass nuclei, up to strongly deformed nuclei of the rare-earth and actinide regions. The results agree with experimental evidence that supports formation of enhanced deformation and clusters in nuclei, as well as vibrational and rotational patterns, as suggested by energy spectra, electric monopole and quadrupole transitions, radii and quadrupole moments. And while these studies have assumed symmetry-based approximations, even in close-to-spherical nuclear states without any recognizable rotational properties, the present outcome not only explains but also predicts the emergence of nuclear collectivity.

The ab initio nuclear shell-model theory solves the many-body Schrödinger equation for A particles,

$$H \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = E \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A),$$

with

$$H = T_{\text{rel}} + V_{NN} + V_{3N} + \ldots + V_{\text{Coulomb}},$$

and, in its most general form, is an exact many-body “configuration interaction” method, for which the interaction and basis configurations are as follows.

**Interaction** – The intrinsic non-relativistic nuclear Hamiltonian \( H \) includes the relative kinetic energy \( T_{\text{rel}} = \frac{1}{A} \sum_{i<j} \left( \frac{\vec{p}_i \cdot \vec{p}_j}{2m} \right) \) (\( m \) is the nucleon mass), the nucleon-nucleon (\( NN \)) and, possibly, three-nucleon (\( 3N \)) interactions,
along with the Coulomb interaction between the protons. In our study, we have adopted various realistic interactions without renormalization in nuclear medium (referred to as “bare”), with results illustrated here for up to the next-to-next-to-next-to-leading order (fourth order), namely, for the Entem-Machleidt (EM) \( N^3 \text{LO} \) and \( \text{NNLO}_{\text{opt}} \) chiral potentials. We neglect explicit 3N contributions in \(^3\text{H}\) and \(^{3,4}\text{He} \) as compared to other parameterizations of chiral interactions up to \( N^3 \text{LO} \).

**Basis configurations and symmetry-adapted (SA) basis** – A complete orthonormal basis \( \psi_k \) is adopted, such that the expansion \( \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \sum_k c_k \psi_k(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) \), renders Eq. (1) into a matrix eigenvalue equation with unknowns \( c_k \), \( \sum_k H_{kk'} c_k' = E c_k \), where the many-particle Hamiltonian matrix elements \( H_{kk'} = \langle \psi_k | H | \psi_{k'} \rangle \) are calculated for the given interaction (the solution \( \{c_k\} \) defines a set of probability amplitudes). Here, the basis is a finite set of antisymmetric products of single-particle states of a spherical harmonic oscillator of frequency \( \hbar \Omega \), referred to as a “model space”, that is truncated by the total number of HO quanta \( N_{\text{max}} \). With larger model spaces (higher \( N_{\text{max}} \)), the eigenenergies and nuclear observables become independent of \( \hbar \Omega \) and converge to the exact values. Such a basis allows for preservation of translational invariance of the nuclear self-bound system. Furthermore, the model space can be reorganized via a unitary transformation – without loss of information – to a basis that respects an approximate symmetry of the nuclear system, referred to as a symmetry-adapted basis. This leads to a much faster convergence and to quantum states that can be described by a drastically smaller number of SA basis states.

### III. RESULTS AND DISCUSSIONS

#### A. Nature’s preference

In this article, we report on the remarkable outcome, as unveiled from first-principle calculations of nuclei below the calcium region, that nuclei exhibit relatively simple physics. We now understand that a low-lying nuclear state is predominantly composed of a few equilibrium shapes that vibrate and rotate, with each shape characterized by a single symplectic irreducible representation (irrep).

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**FIG. 2:** (a) Excitation energies (horizontal axis) of the ground-state (gs) rotational band \( J^\pi = 0^+, 2^+, 4^+, 6^+, \text{ and } 8^+ \) and \( 0^+ \) states in \(^{20}\text{Ne} \), shown together with the contribution to each state (vertical axis) of the single shape that dominates the ground state. According to this, states are grouped and schematically illustrated by “classical” shapes, vibrations, and rotations, where the \textit{ab initio} one-body density profile in the body-fixed frame is shown for \( 0^+ \). (b) Deformation distribution of the equilibrium shapes that make up a state with contributions given by the area of the circles, specified by the average deformation \( \beta \) and triaxiality angle \( \gamma \). Results reported for \textit{ab initio} SA-NCSM calculations with the bare \( \text{NNLO}_{\text{opt}} \) \( NN \) for an SU(3)-adapted basis that yields a fast convergence of the gs rms radius (model space of 11 HO shells with 15 MeV inter-shell distance).

To illustrate this, we consider the physics of \(^{20}\text{Ne} \) (Fig. 2) and the contribution of a single symplectic irrep to its low-lying states, Fig. 2(a). Indeed, the physics of a single symplectic irrep can provide insight into the nuclear dynamics: all configurations within a symplectic irrep preserve an equilibrium shape and realize its rotations, vibrations, and spatial orientations, implying that the \(^{20}\text{Ne} \) \textit{ab initio} wave functions for \( J^\pi = 0^+, 2^+, \ldots, 8^+ \) indeed exhibit a predominance of a single equilibrium shape that vibrates and rotates [see also, Fig. 2(b), largest circle].
That a single Sp\((3, \mathbb{R})\) irrep naturally describes the shape dynamics of a deformed nucleus has been earlier shown in an algebraic symplectic model \[13, 14, 20\] and can be illustrated with two simple examples: (1) in the limit of a valence shell, the symplectic basis recovers the SU\((3)\)-adapted basis of the Elliott model that describes shapes (referred to as “equilibrium shapes” or simply “shapes”) and their rotations – note that a shape associated with a given many-body SU\((3)\)-adapted state is specified by the familiar shape parameters, \(\beta\) and \(\gamma\), calculated according to the correspondence of the expectation value of \(Q \cdot Q\) and \(Q \times Q \cdot Q\) to \(\beta^2\) and \(\beta^3 \cos 3\gamma\), respectively \[20\]; and (2) for a single spherical shape, its symplectic excitations (referred to as “dynamical shapes”) realize the microscopic counterpart of the surface vibrations of the Bohr-Mottelson collective model \[27\]. As further shown in the \(\beta-\gamma\) plots of Fig. 2(a), the set of higher-lying \(0^+\) states with nonnegligible contribution of the 1p-1h vibrations of the ground-state shape describes a fragmented giant monopole resonance (breathing mode) with a centroid around 29 MeV and a typical deformation content spread out to higher \(\beta\) values due to vibrations \[28\], as compared to the ground state. Implications of this outcome for understanding the physics of nuclei are discussed next.

![Graphs and plots](Figures/3)

**FIG. 3:** (a)-(c) Symplectic Sp\((3, \mathbb{R})\) irreps that make up the rotational band states of \(^6\text{Li}\), \(^4\text{He}\), and \(^{20}\text{Ne}\) (in a close agreement with the results of Fig. 2): each irrep is specified by its equilibrium shape, labeled by the shape deformation \(\beta\) and the corresponding SU\((3)\) labels \((\lambda \mu)\) together with total intrinsic spin \(S\). Insets: the same irreps but without the predominant contribution, together with the \(\beta-\gamma\) plot for the ground state. (d) Observables for \(^6\text{Li}\) and \(^{20}\text{Ne}\) calculated in the \textit{ab initio} SA-NCSM with Sp\((3, \mathbb{R})\)-adapted basis using only a small number (specified in the \(x\)-axis labels) dominant symplectic irreps including the most dominant one, as compared to experiment (“Expt.”); dimensions of the largest model spaces used are also shown. Energies (with errors \(\sim\) 100 keV) and reduced electromagnetic \(B(E2)\) transition strengths (in W.u.) are reported for extrapolations to infinitely many shells of converging results across variations in the model space size and resolution (see also Fig. 1). Results for nuclear states (a)-(c) and energies [(d), labeled as “All”] are reported for \textit{ab initio} SA-NCSM calculations for an SU\((3)\)-adapted basis that yields a fast convergence of the \(gs\) rms radius: complete (selected) model space of 14 (11) HO major shells for \(^{6}\text{Li}\) and \(^4\text{He}\) \((^{20}\text{Ne})\) with inter-shell distance of (a)-(b) 20 MeV and (c)-(d) 15 MeV.
B. Approximate symplectic symmetry and physics of nuclei

The Sp(3, R)-adapted basis is constructed for various nuclei, pointing to unexpectedly ubiquitous symplectic symmetry, with the illustrative examples for the odd-odd $^6$Li, $^8$He (generally considered to be spherical), and the intermediate-mass $^{20}$Ne shown in Fig. 3. The outcome provides further evidence that nuclei are predominantly comprised – typically in excess of 70-80% – of only a few shapes, often a single shape (a single symplectic irrep) as for, e.g., $^6$Li, $^8$B, $^8$Be, $^{16}$O, and $^{20}$Ne, or two shapes, e.g., for $^8$He and $^{12}$C [see also results in Ref. [11] based on SU(3) analysis]. Hence, e.g., the ground state of $^6$Li and $^{20}$Ne ($^{16}$O) is found to exhibit prolate (spherical) shape deformation, while an oblate shape dominates in the case of $^8$He. Besides the predominant irrep(s), there is a manageable number of symplectic irreps, each of which contributes at a level that is typically at least an order of magnitude smaller, as shown in Fig. 3(a)-(c). Furthermore, the outcome implies that the richness of the low-lying excitation spectra naturally emerges from these shapes through their rotations. Indeed, practically the same symplectic content observed for the low-lying states in $^6$Li, Fig. 3(a), and for those in $^{20}$Ne, Fig. 3(c), is a rigorous signature of rotations of a shape and can be used to identify members of a rotational band. And finally, $E2$ transitions are determined by the quadrupole operator $Q$, an Sp(3, R) generator that does not mix symplectic irreps – the predominance of a single symplectic irrep reveals the remarkable result that the largest fraction of these transitions, and hence nuclear collectivity, necessarily emerges within this symplectic irrep, Fig. 3(d) [similarly for rms radii, since $r^2$ is also an Sp(3, R) generator]. A notable outcome is that even excitation energies calculated in model spaces selected down to a few symplectic irreps closely reproduce the experimental data.

The outcome is neither sensitive to the type of the realistic interaction used (details such as contribution percentages slightly vary, but dominant features retain), nor to the parameters of the basis, $\hbar \Omega$ and $N_{\text{max}}$. It has been shown [29] that these two model parameters can be related to $L_{\text{eff}}$, the infrared IR cutoff, and $a_{\text{eff}}$, the ultraviolet UV cutoff $\Lambda_{\text{eff}} = 1/a_{\text{eff}}$, which can be understood as the effective size of the model space box in which the nucleus resides and its grid size (resolution), respectively. Indeed, the symplectic content of a nucleus is found to be stable against variations in the box size or resolution – Fig. 4 reveals that no new dominant shapes appear for values around the optimal ones for $^6$Li shown in Fig. 3(a), retaining the predominance of the single irrep. This has an important implication: complete SA-NCSM calculations are performed in smaller box sizes and/or low resolution to identify the nonnegligible symplectic irreps, while the model space is then augmented by extending these irreps to high (otherwise inaccessible) HO major shells vital to account for collectivity.

![FIG. 4: Symplectic Sp(3, R) irreps, labeled by ($\lambda \mu$)S, that make up the ground state of $^6$Li, as calculated by the ab initio SA-NCSM with SU(3)-adapted basis with the bare N$^3$LO N$N$ interaction and the effect on the symplectic content (a) as the resolution improves (grid size decreases) for the same box size, and (b) as the box size increases for the same resolution. No new dominant equilibrium shapes are observed as the box size or grid resolution increases.](image)

In short, this work shows that nuclei below the calcium region and their low-energy excitations display relatively simple emergent physics that is collective in nature and tracks with an approximate symplectic symmetry heretofore gone unrecognized in the strong nuclear force.
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