Emergent symmetries in atomic nuclei: Probing nuclear dynamics and physics beyond the standard model

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Abstract

Dominant shapes naturally emerge in atomic nuclei from first principles, thereby establishing the shape-preserving symplectic $\mathrm{Sp}(3,\mathbb{R})$ symmetry as remarkably ubiquitous and almost perfect symmetry in nuclei. We discuss the critical role of this emergent symmetry in enabling machine-learning descriptions of heavy nuclei, *ab initio* modeling of α clustering and collectivity, as well as tests of beyond-the-standard-model physics. In addition, the $\mathrm{Sp}(3,\mathbb{R})$ and SU(3) symmetries provide relevant degrees of freedom that underpin the *ab initio* symmetry-adapted no-core shell model with the remarkable capability of reaching nuclei and reaction fragments beyond the lightest and close-to-spherical species.

Contents

1 Introduction

Dominant shapes, often very few in number, naturally emerge in atomic nuclei[1]. This remarkable result has been recently shown by large-scale nuclear simulations from first principles [2]. Indeed, each nuclear shape respects an exact symmetry, namely, the symplectic Sp(3, $\mathbb{R}$) symmetry [3, 4]. Thereby the outcome of these simulations establishes the symplectic Sp(3, $\mathbb{R}$) symmetry as remarkably ubiquitous and almost perfect symmetry in nuclei up through the calcium region (anticipated to hold even stronger in heavy nuclei [5]). This outcome also exposes for the first time the fundamental role of the Sp(3, $\mathbb{R}$) symmetry and suggests that its origin is rooted in the strong nuclear force, in the low-energy regime.

This builds upon a decades-long research, starting with the pivotal work of Draayer [6, 4, 7, 8] and that of Rowe and Rosensteel [3, 9, 5, 10], who have successfully harnessed group theory as a powerful tool for understanding and computing the intricate structure of nuclei. This pioneering work has been instrumental in designing the theory that underpins many highly ordered patterns unveiled amidst the large body of experimental data [11, 12, 13]. In addition, it has explained phenomena observed in energy spectra, $E2$ transitions and deformation, giant resonances (GR), scissor modes and $M1$ transitions, electron scattering form factors, as well as the interplay of pairing with collectivity. The new developments and insights have provided the critical structure raised upon the very foundation laid by Elliott [14, 15, 16] and Hecht [17, 18], and opened the path for large-scale calculations feasible today on supercomputers. And while these earlier algebraic models have been very successful in explaining dominant nuclear patterns, they have assumed symmetry-based approximations and have often neglected symmetry mixing. This establishes Sp(3, $\mathbb{R}$) as an *effective symmetry*[2] for nuclei, which may or may not be badly broken in realistic calculations. It is then imperative to probe if this symmetry naturally arises within an *ab initio* framework, which will, in turn, establish its fundamental role.

Indeed, within an *ab initio* framework without *a priori* symmetry assumptions, the symmetry-adapted no-core shell model (SA-NCSM) [20, 21, 8] with chiral effective field theory (EFT) interactions [22, 23, 24] has recently confirmed the goodness of the symplectic Sp(3, $\mathbb{R}$) symmetry that is only slightly broken. With no parameters to adjust, the SA-NCSM is capable then not only to explain but also to predict the emergence of nuclear shapes and collectivity across nuclei, even in close-to-spherical nuclear states without any recognizable rotational properties.

Within an *ab initio* framework, the emergent symmetries play a critical role, as they can inform relevant degrees of freedom. In particular, a symmetry-adapted many-body basis can be employed, as in the SA-NCSM, thereby providing solutions for drastically reduced sizes of the spaces in which particles reside (referred to as "model spaces"') compared to the corresponding ultra-large model spaces, without compromising the accuracy of results for various nuclear observables. By exploiting symplectic symmetry, *ab initio* descriptions of spherical and deformed nuclei up through the calcium region are now possible without the use of effec-

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[2] A familiar example for an effective symmetry is SU(3). While the Elliott model with a single SU(3) irrep explains ground-state rotational states in deformed nuclei, the SU(3) symmetry is, in general, largely mixed, mainly due to the spin-orbit interaction (nonetheless, SU(3) has been shown to be an excellent quasi-dynamical symmetry, that is, each rotational state has almost the same SU(3) content [19]).

tive charges [21,25,26,8,27]. This allows the SA-NCSM to accommodate even larger model spaces and to reach heavier nuclei, such as ^{20}Ne [2], ^{21}Mg [28], ^{22}Mg [29], ^{28}Mg [30], as well as ^{32}Ne and ^{48}Ti [31].

In this paper, we briefly outline the SU(3) and Sp$(3,\mathbb{R})$ schemes utilized by the *ab initio* SA-NCSM. We overview the critical role of the emergent Sp$(3,\mathbb{R})$ symmetry in enabling machine-learning descriptions of heavy nuclei [32], *ab initio* modeling of α clustering and collectivity, along with tests of beyond-the-standard-model physics [33]. In addition, we show that with the help of the SA-NCSM, which expands *ab initio* applications up to medium-mass nuclei by using the dominant symmetry of nuclear dynamics, one can provide solutions to reaction processes in this region, with a focus on elastic neutron scattering.

2 Emergent symmetries in nuclei: Sp$(3,\mathbb{R})$ and SU(3)

2.1 SU(3) scheme

It is well known that SU(3) [14,34,6,35,18] is the symmetry group of the spherical harmonic oscillator (HO) that underpins the valence-shell model and the valence-shell SU(3) (Elliott) model [14,15,16] (for technical details of SU(3), see Ref. [36]). The Elliott model has been shown to naturally describe rotations of a deformed nucleus without the need for breaking rotational symmetry. But even beyond the valence shell, the SU(3) scheme provides a classification of the complete shell-model space in multiple shells, and is related to the LS-coupling and jj-coupling schemes via a unitary transformation. It divides the space into basis states of definite $(\lambda\,\mu)$ quantum numbers of SU(3) that are linked to the intrinsic quadrupole deformation according to the established mapping [37,38,39]. For example, the simplest cases, $(0\,0)$, $(\lambda\,0)$, and $(0\,\mu)$, describe spherical, prolate, and oblate deformation, respectively[3], while a general nuclear state is typically a superposition of several hundred various triaxially deformed configurations. Note that, in this respect, basis states can have little to no deformation, and, e.g., about 60% of the ground state of the closed-shell ^{16}O is described by a single SU(3) basis state, the spherical $(0\,0)$.

Specifically, in the SU(3) scheme, in place of the spherical quantum numbers $\left|\eta l m_l\right\rangle$, one can consider the single-particle HO basis $\left|\eta_z\eta_x\eta_y\right\rangle$, the HO quanta in the three Cartesian directions, z, x, and y, with $\eta_x+\eta_y+\eta_z=\eta$ ($\eta=0,1,2,\dots$ for s, p, sd, ... shells). For a given HO major shell, the complete shell-model space is then specified by all distinguishable distributions of η_z,η_x and η_y. E.g., for $\eta=2$, there are 6 different distributions, $(\eta_z,\eta_x,\eta_y)=(2,0,0),(1,1,0),(1,0,1),(0,2,0),(0,1,1)$ and $(0,0,2)$. The number of these configurations is $\Omega_\eta=(\eta+1)(\eta+2)/2$ (spatial degeneracy) and the associated symmetry is described by the $U(\Omega_\eta)$ unitary group. Each of these (η_z,η_x,η_y) configurations can be either unoccupied or has maximum of two particles with spins $\uparrow\downarrow$.

As a simple example for an SU(3)-scheme basis state, consider $A=2$ protons in the sd shell ($\eta=2$) with a particle in the $(2,0,0)$ level with spin $\uparrow$ and another in the $(1,1,0)$ level with spin $\uparrow$. The total number of quanta in each direction is $(\eta_z^{\rm tot},\eta_x^{\rm tot},\eta_y^{\rm tot},)=(3,1,0)$, or equivalently, $\eta^{\rm tot}(\lambda\,\mu)=4(2\,1)$, where $\eta^{\rm tot}=\eta_x^{\rm tot}+\eta_y^{\rm tot}+\eta_z^{\rm tot}$, together with $\lambda=\eta_z^{\rm tot}-\eta_x^{\rm tot}$ and $\mu=\eta_x^{\rm tot}-\eta_y^{\rm tot}$ labeling an SU(3) irrep, in addition to the total intrinsic spin and its projection SM_S. For given $(\lambda\,\mu)$, the quantum numbers κ, L and M_L are given by Elliott [14,15], according to the SU(3) $\overset{\kappa}{\supset}$ SO$(3)_L\supset$SO$(2)_{M_L}$, where the label κ distinguishes multiple occurrences of the same orbital angular momentum L in the parent irrep $(\lambda\,\mu)$. For our

[3] Following this mapping, quadrupole moments of $(0\,0)$, $(\lambda\,0)$, and $(0\,\mu)$ configurations – in a simple classical analogy to rotating spherical, prolate, and oblate spheroids in the lab frame [40] – are zero, negative, and positive, respectively.

example, $(\lambda\,\mu)=(2\,1)$ with $\kappa=1$, $L=1,2,3$, and $M_L=-L,-L+1,\ldots,L$. Hence, the set $\{\eta^A(\lambda\,\mu)\kappa(LS)JM\}$ completely labels a 2-proton SU(3)-scheme basis state (with $\eta^{\rm tot}=A\eta$). A basis state in this scheme for a 2-particle system is given by, $\{a^\dagger_{(\eta\,0)st_z}\times a^\dagger_{(\eta'0)s't'_z}\}^{(\lambda\,\mu)\kappa(LS)JM}\,|0\rangle$, which is an SU(3)-coupled product, provided that $a^\dagger$ is a proper SU(3) tensor; incidentally, the SU(3) tensor $a^\dagger$ of rank $(\lambda\,\mu)=(\eta\,0)$ coincides with the familiar particle creation operator, $a^\dagger_{(\eta\,0)lms\sigma t_z}\equiv a^\dagger_{\eta lms\sigma t_z}$, while the particle annihilation SU(3) tensor of rank $(\lambda\,\mu)=(0\,\eta)$ is given as $\tilde{a}_{(0\,\eta)l-ms-\sigma t_z}=(-1)^{\eta+l-m+s-\sigma}a_{\eta lms\sigma t_z}$. Note that for $\eta=\eta'=2$, e.g., there are only a few 2-proton configurations $(\lambda\,\mu)=(4\,0)$ with $L=0,2,4$, $(2\,1)$ with $L=1,2,3$, and $(0\,2)$ with $L=0,2$. Furthermore, these basis states are related to LS-coupled basis states (similarly, to jj-coupled basis states) via a simple unitary transformation,

$$\{a^\dagger_{(\eta\,0)st_z}\times a^\dagger_{(\eta'0)s't'_z}\}^{(\lambda\,\mu)\kappa(LS)JM}\,|0\rangle=\sum_{l,l'}\langle(\eta\,0)l;(\eta'0)l'\|(\lambda\,\mu)\kappa L\rangle\{a^\dagger_{\eta lst_z}\times a^\dagger_{\eta'l's't'_z}\}^{(LS)JM}\,|0\rangle\,, \tag{1}$$

where $\langle\ldots;\ldots\|\ldots\rangle$ is the SU(3) analog of the familiar reduced Clebsch-Gordan coefficient [note that there is no dependence on the particle orbital angular momenta, l and l', in the SU(3)-scheme basis states].

An important feature of the SU(3) scheme is that all possible configurations within a major HO shell η (for protons or neutrons) are not constructed using the tedious procedure of coupling of creation operators referenced above, but are readily available based on the $U(\Omega_\eta)$ unitary group of the many-body three-dimensional HO. In particular, the basis construction is implemented according to the reduction [41]

$$\begin{array}{ccccc} \mathrm{U}(\Omega_\eta) & & \times & \mathrm{SU}(2) & \\ \left[f_1,f_2,\ldots f_{\Omega_\eta}\right] & & & S_\eta & \\ \cup & \alpha_\eta & & & , \\ \mathrm{SU}(3) & & & & \\ (\lambda_\eta\,\mu_\eta) & & & & \end{array} \tag{2}$$

with $\mathrm{SU}(3)_{(\lambda_\eta\,\mu_\eta)}\overset{\kappa_\eta}{\supset}\mathrm{SO}(3)_{L_\eta}\supset\mathrm{SO}(2)_{M_{L_\eta}}$ [14, 15], where a multiplicity index α_η distinguishes multiple occurrences of an SU(3) irrep $(\lambda_\eta\,\mu_\eta)$ in a given $\mathrm{U}(\Omega_\eta)$ irrep labeled by Young tableaux, $[\mathbf{f}]=[f_1,f_2,\ldots,f_{\Omega_\eta}]$, with $f_1\geq f_2\geq\cdots\geq f_{\Omega_\eta}$ and $f_i=0$ (unoccupied), 1 (occupied by a particle), or 2 (occupied by 2 particles of spins $\uparrow\downarrow$). An illustrative example for 4 particles in the pf shell ($\eta=3$) is shown in Table 1.

2.2 $\mathrm{Sp}(3,\mathbb{R})$ scheme

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 [11] makes the quadrupole moment a dominant fundamental property of the nucleus. Hence, the quadrupole moment Q (or deformation) and the monopole moment r^2 (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 $\mathrm{Sp}(3,\mathbb{R})$ symmetry.

Specifically, for A particles in three-dimensional space, the complete basis for the shell model is described by $\mathrm{Sp}(3A,\mathbb{R})\times\mathrm{U}(4)$ [10], where $\mathrm{Sp}(3A,\mathbb{R})$ is the group of all linear canonical transformations of the $3A$-particle phase space and Wigner’s supermultiplet group U(4) describes the complementary spin-isospin space. A complete translationally invariant shell-

Spatial d.o.f.			Spin d.o.f.
U(10)	$\supset$	SU(3)	SU(2)
$[f_1 f_2 \ldots f_{10}]$		$(\lambda\,\mu)$	S
$[2^2]$		$(8\,2),(7\,1),(4\,4)^2,(5\,2),(0\,6),(6\,0),(3\,3)$ $(1\,4),(4\,1),(2\,2)^2,(1\,1)$	$S=0$
$[21^2]$		$(9\,0),(6\,3),(7\,1),(4\,4),(2\,5),(5\,2)^2,(3\,3)^2$ $(1\,4)^2,(4\,1)^2,(2\,2),(0\,3),(3\,0)^2,(1\,1)$	$S=1$
$[1^4]$		$(5\,2),(0\,6),(3\,3),(2\,2),(3\,0)$	$S=2$

Table 1: SU(3)×SU(2)$_S$ configurations for 4 protons (neutrons) in the pf shell ($\eta=3$ with $\Omega_\eta=10$). Note that a spatial symmetry represented by a Young tableau $\left[f_1,\ldots,f_{\Omega_\eta}\right]$ is uniquely determined by its complementary spin symmetry of a given intrinsic spin S_η (conjugate Young tableaux) ensuring the overall antisymmetrization of each $U(\Omega_\eta)\times\mathrm{SU}(2)_{S_\eta}$ configuration with respect to spatial and spin degrees of freedom (d.o.f.) [41].

model basis is classified according to (see, e.g., [5, 10]),

$$\begin{array}{ccc} \mathrm{Sp}(3(A-1),\mathbb{R}) & \times & \mathrm{U}(4) \\ \cup & & \cup \\ \mathrm{Sp}(3,\mathbb{R})\times\mathrm{O}(A-1) & & \mathrm{SU}(2)_S\times\mathrm{SU}(2)_T \end{array} . \tag{3}$$

The Sp(3, $\mathbb{R}$) scheme utilizes the symplectic group Sp(3, $\mathbb{R}$). It consists of all *particle-independent* linear canonical transformations of the single-particle phase-space observables, the positions $\vec{r}_i$ and momenta $\vec{p}_i$ (with particle index $i=1,\ldots,A$ and spacial directions $\alpha,\beta=x,y,z$)

$$r'_{i\alpha} = \sum_\beta A_{\alpha\beta} r_{i\beta} + B_{\alpha\beta} p_{i\beta} \tag{4}$$

$$p'_{i\alpha} = \sum_\beta C_{\alpha\beta} r_{i\beta} + D_{\alpha\beta} p_{i\beta} \tag{5}$$

that preserve the Heisenberg commutation relations $[r_{i\alpha}, p_{j\beta}] = i\hbar\delta_{ij}\delta_{\alpha\beta}$ [5, 42, 8]. Generators of these transformations, symbolically denoted as matrices **A**, **B**, **C**, and **D**, are constructed as "quadratic coordinates" in phase space, $\vec{r}_i$ and $\vec{p}_i$, and, most importantly, sum over all the particles and act on the space orientation. Hence, the generators include physically relevant operators: the total kinetic energy ($\frac{p^2}{2} = \frac{1}{2}\sum_i \vec{p}_i\cdot\vec{p}_i$), the monopole moment ($r^2=\sum_i \vec{r}_i\cdot\vec{r}_i$), the quadrupole moment ($Q_{2M} = \sqrt{16\pi/5}\sum_i r_i^2 Y_{2M}(\hat{r}_i)$), the orbital angular momentum ($\vec{L}=\sum_i \vec{r}_i\times\vec{p}_i$), and the many-body harmonic oscillator Hamiltonian ($H_0=\frac{p^2}{2}+\frac{r^2}{2}$). In addition, other generators describe multi-shell collective vibrations and vorticity degrees of freedom for a description from irrotational to rigid rotor flows.

On the contrary, the generators of the complementary O(A) sum over the three spatial directions and act on the particle index, with a growing complexity with increasing particle number. One can then organize the A-particle model space according to the dual group O($A-1$), with $O(A) \supset$ O($A-1$) $\supset S_A$. The O(A) is the group of orthogonal transformations that act on the "particle-index" space (transformations of nucleon coordinates, $r_{i\alpha} \rightarrow \sum_{j=1}^{A} r_{j\alpha} P_{ji}$, that leave the O(A) scalars $r_\alpha \cdot r_\beta = \sum_{i=1}^{A} r_{i\alpha} r_{i\beta}$ invariant for $\alpha, \beta = x, y, z$). This scheme is reviewed in detail in Refs. [5, 10]. O($A-1$) is the subgroup of O(A) which leaves center-of-mass coordinates invariant (note that center-of-mass coordinates are symmetric with respect to nucleon indices and, therefore, invariant under S_A permutations) and has as a subgroup the permutation group S_A, which permutes the spatial coordinates of a system of A particles.

The Sp(3, $\mathbb{R}$) scheme utilizes an important group reduction to classify many-particle basis states $|\sigma n\rho\omega\kappa LM\rangle$ of a symplectic irrep,

$$\begin{array}{ccccccc} \mathrm{Sp}(3,\mathbb{R}) & \supset & U(3) & \supset & \mathrm{SO}(3) & \supset & SO(2) \\ \sigma & n\rho & \omega & \kappa & L & & M \end{array}, \tag{6}$$

where $\sigma \equiv N_\sigma\,(\lambda_\sigma\,\mu_\sigma)$ labels the Sp(3, $\mathbb{R}$) irrep, $n \equiv N_n\,(\lambda_n\,\mu_n)$, $\omega \equiv N\,(\lambda_\omega\,\mu_\omega)$, and $N = N_\sigma + N_n$ is the total number of HO quanta (ρ and κ are multiplicity labels) [5]. The relation of these symplectic basis states to M-scheme states of the NCSM is provided in Ref. [43]. Importantly, a single-particle Sp(3, $\mathbb{R}$) irrep spans *all* positive-parity (or negative-parity) states for a particle in a three-dimensional spherical or triaxial (deformed) harmonic oscillator.

The translationally invariant (intrinsic) symplectic Sp(3, $\mathbb{R}$) generators can be written as SU(3) tensor operators in terms of the harmonic oscillator raising, $b^{\dagger(10)}_{i\alpha} = \frac{1}{\sqrt{2}}(r_{i\alpha} - ip_{i\alpha})$, and lowering $b^{(01)}$ dimensionless operators (with $\mathbf{r}$ and $\mathbf{p}$ the laboratory-frame position and momentum coordinates and $\alpha = 1, 2, 3$ for the three spatial directions),

$$A^{(20)}_{\mathcal{L}M} = \frac{1}{\sqrt{2}}\sum_{i=1}^{A}\{b^\dagger_i \times b^\dagger_i\}^{(20)}_{\mathcal{L}M} - \frac{1}{\sqrt{2}A}\sum_{s,t=1}^{A}\{b^\dagger_s \times b^\dagger_t\}^{(20)}_{\mathcal{L}M} \tag{7}$$

$$C^{(11)}_{\mathcal{L}M} = \sqrt{2}\sum_{i=1}^{A}\{b^\dagger_i \times b_i\}^{(11)}_{\mathcal{L}M} - \frac{\sqrt{2}}{A}\sum_{s,t=1}^{A}\{b^\dagger_s \times b_t\}^{(11)}_{\mathcal{L}M},$$

$$H^{(00)}_{00} = \sqrt{3}\sum_{i}\{b^\dagger_i \times b_i\}^{(00)}_{00} - \frac{\sqrt{3}}{A}\sum_{s,t}\{b^\dagger_s \times b_t\}^{(00)}_{00} + \frac{3}{2}(A-1), \tag{8}$$

together with $B^{(02)}_{\mathcal{L}M} = (-)^{\mathcal{L}-M}(A^{(20)}_{\mathcal{L}-M})^\dagger$ ($\mathcal{L} = 0, 2$), where the sums run over all A particles of the system. Equivalently, the symplectic generators, being one-body-plus-two-body operators can be expressed in terms of the fermion creation operator $a^\dagger_{(\eta\,0)}$ and its SU(3)-conjugate annihilation operator, $\tilde{a}_{(0\,\eta)}$. This is achieved by using the known matrix elements of the position and momentum operators in a HO basis, and hence, e.g., the first sum of $A^{(20)}_{\mathcal{L}M}$ in Eq. (7) becomes, $\sum_\eta \sqrt{\frac{(\eta+1)(\eta+2)(\eta+3)(\eta+4)}{12}}\left\{a^\dagger_{(\eta+2\,0)} \times \tilde{a}_{(0\,\eta)}\right\}^{(20)}_{\mathcal{L}M}$ [44]. Note that this operator describes excitations of a nucleon from the η shell to the $\eta+2$ shell, which corresponds to creating two single-particle HO excitation quanta, as manifested in the first term of Eq. (7). The eight $0\hbar\Omega$ operators $C^{(11)}_{\mathcal{L},M}$ ($\mathcal{L} = 1, 2$) generate the SU(3) subgroup of Sp(3, $\mathbb{R}$). They realize the angular momentum operator (dimensionless), $L_{1M} = C^{(11)}_{1M}$, and the Elliott "algebraic" quadrupole moment tensor $\mathcal{Q}^a_{2M} = \sqrt{3}C^{(11)}_{2M}$.

The many-body basis states of an Sp(3, $\mathbb{R}$) irrep are built over a bandhead $|\sigma\rangle$ (defined by the usual requirement that the symplectic lowering operators $B^{(02)}_{\mathcal{L}M}$ annihilate it) by $2\hbar\Omega$ 1p-1h monopole or quadrupole excitations, realized by the first term in $A^{(20)}_{\mathcal{L}M}$ of Eq. (7), together with a smaller $2\hbar\Omega$ 2p-2h correction for eliminating the spurious center-of-mass (CM) motion, realized by the second term in $A^{(20)}_{\mathcal{L}M}$:

$$|\sigma n\rho\omega\kappa(LS_\sigma)JM\rangle = \sum_{M_L M_S} \langle LM_L; S_\sigma M_S|JM\rangle \{\{A^{(20)} \times A^{(20)} \cdots \times A^{(20)}\}^n \times \left|\sigma; S_\sigma M_S\right\rangle\}^{\rho\omega}_{\kappa L M_L}. \tag{9}$$

States within a symplectic irrep have the same spin value, which are given by the spin S_σ of the bandhead $\left|\sigma; S_\sigma\right\rangle$. Symplectic basis states span the entire shell-mode space. A complete set of labels includes additional quantum numbers $|\{\alpha\}\sigma\rangle$ that distinguish different bandheads with the same N_σ $(\lambda_\sigma\,\mu_\sigma)$. Remarkably, these $\mathrm{Sp}(3,\mathbb{R})$ basis states are in one-to-one correspondence with a coupled product of the states of the Bohr vibrational model (realized in terms of giant monopole-quadrupole resonance states with irrotational flows), $\{\{A^{(20)} \times A^{(20)} \cdots \times A^{(20)}\}^n \times \left|N_\sigma(0\,0)\right\rangle\}^{(\lambda_n\,\mu_n)}$, and $(\lambda_\sigma\,\mu_\sigma)$ deformed states of an SU(3) model [42].

2.3 *Ab initio* symmetry-adapted no-core shell model

Not surprisingly, the symplectic $\mathrm{Sp}(3,\mathbb{R})$ symmetry, the underlying symmetry of the symplectic rotor model [3,5], has been found to play a key role across the nuclear chart – from the lightest systems [45, 46], through intermediate-mass nuclei [4, 47, 8], up to strongly deformed nuclei of the rare-earth and actinide regions [5, 48, 49, 19]. 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 [11, 29, 50].

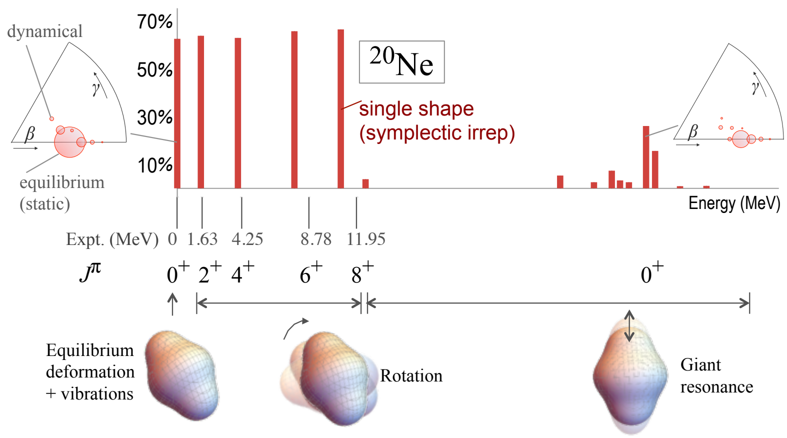

Figure 1: Emergence of almost perfect symplectic $\mathrm{Sp}(3,\mathbb{R})$ symmetry in nuclei from first principles, enabling *ab initio* descriptions of collectivity and clustering. *Source:* Figure from [2] @ APS; reproduced with permission.

The symmetry-adapted no-core shell model [20, 8, 2] capitalizes on these findings and presents solutions in terms of a physically relevant basis of nuclear shapes. It exploits both the SU(3) and $\mathrm{Sp}(3,\mathbb{R})$ schemes. Indeed, since the symplectic symmetry does not mix nuclear shapes, the SA-NCSM provides important insight from first principles into the physics of nuclei and their low-lying excitations as dominated by only a few (typically one or two) collective shapes – equilibrium shapes with their vibrations – that rotate (Fig. 1).

By exploiting this almost perfect symmetry, the SA framework resolves the scale explosion problem in nuclear structure calculations, *i.e.*, the explosive growth in computational resource demands with increasing number of particles and model spaces size. We note that the SA-NCSM uses the complete model space (that is, all possible shapes) as usually done in conventional shell models, but expands, in a prescribed way, only for those deformed configurations with vibrations that lie outside of the complete model space. This is critical for enhanced prolate deformation, since spherical and less deformed or oblate shapes easily develop in comparatively small model-space sizes.

The SA-NCSM, when combined with a high-precision realistic inter-nucleon interaction, provides *ab initio* predictions of nuclear observables. We often adopt the NNLO$_{\text{opt}}$ chiral potential [51] that is used without 3N forces, which have been shown to contribute minimally to the 3- and 4-nucleon binding energy [51]. Chiral potentials are typically parameterized by two-nucleon (and three-nucleon) data, whereas the parameters, called the low-energy constants (LECs), remain unchanged and are not adjusted from one many-body system to another. This ensures a predictive power. At the next-to-next-to-leading order (NNLO), there are 14 LECs that enter into the chiral nucleon-nucleon (NN) potential. Our recent findings reveal the remarkable result that the chiral potential parameterizations have no significant effect on the dominant nuclear features, such as nuclear shape and the associated Sp(3,$\mathbb{R}$) symmetry, along with cluster formation (Fig. 2), but only slightly vary details in the nuclear wave functions, such as the contributions of the equilibrium deformation and its vibrations within the predominant nuclear shape (Fig. 2, left, inset) [52].

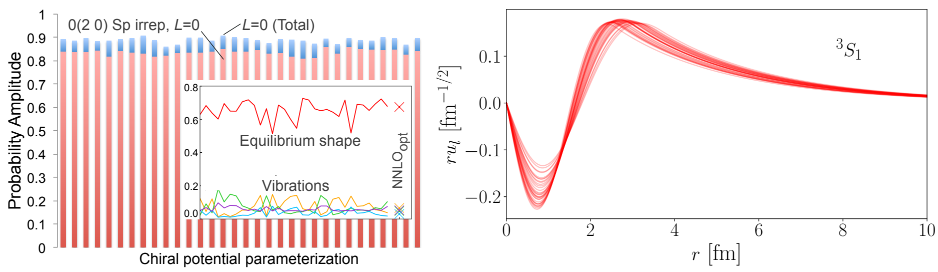

Figure 2: Chiral parameterization independence for nuclear shapes and cluster formation: (Left) Probability amplitude of the predominant Sp(3,$\mathbb{R}$) irrep $N_\sigma(\lambda_\sigma\,\mu_\sigma) = 0(2\,0)$ ($L=0$) in the ^{6}Li 1^+ ground state. Inset: Contributions from the equilibrium shape (symplectic bandhead) and its vibrations (the case for the NNLO$_{\text{opt}}$ is also shown). (Right) $\alpha + d$ $^3S_1$-wave vs. the relative distance r. Calculated from the ^{6}Li 1^+ ground state, computed with the SA-NCSM in the Sp(3,$\mathbb{R}$) scheme with NNLO chiral potential for 10 HO shells and $\hbar\Omega$=15 MeV. The $\pm$10% variation in the LECs of the chiral potential is shown (left) on the horizontal axis and (right) by the spread of the curve. *Source:* Figures adapted/reused from [52] @ Frontiers; reproduced under the terms of its CC BY license.

3 Critical Role of Symmetries for Studies and Predictions of Nuclear Properties

3.1 Machine learning pattern recognition with the SA-NCSM

Machine learning approaches are ideal for pattern recognition, thereby providing a suitable framework to detect and utilize the highly organized patterns in atomic nuclei governed by the symplectic Sp(3,$\mathbb{R}$) symmetry.

Specifically, Ref. [32] introduces a novel machine learning approach to provide further insight into atomic nuclei and to detect orderly patterns amidst a vast data of large-scale calculations. The method utilizes a physics-informed neural network that is trained on *ab initio* results from the SA-NCSM for light nuclei. Indeed, the SA-NCSM, which expands *ab initio* applications up to medium-mass nuclei, can reach even heavier nuclei when coupled with the machine learning approach. In particular, we find that a neural network trained on probability amplitudes for s-and p-shell nuclear wave functions not only predicts dominant configurations for heavier nuclei but in addition, when tested for the ^{20}Ne ground state, it accurately reproduces the probability distribution (Fig. 3).

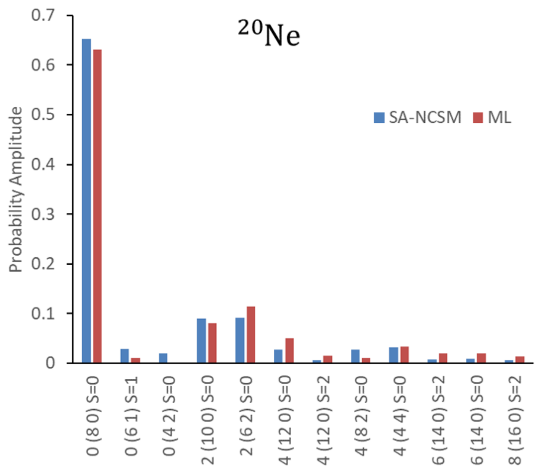

Figure 3: A novel machine learning approach coupled with the *ab initio* SA-NCSM is capable to detect orderly patterns amidst a vast data of large-scale calculations and to describe sd-shell nuclei, such as ^{20}Ne (shown), ^{24}Si, ^{40}Mg, and even the extremely heavy nuclei such as ^{166,168}Er and ^{236}U, by training only on nuclei up to ^{16}O. *Source:* Figure from [32] @ APS; reproduced with permission.

The nonnegligible configurations predicted by the network provide an important input to the SA-NCSM for reducing ultra-large model spaces to manageable sizes that can be, in turn, utilized in SA-NCSM calculations to obtain accurate observables. The neural network is capable of describing nuclear deformation and is used to track the shape evolution along the $^{20-42}$Mg isotopic chain, suggesting a shape-coexistence that is more pronounced toward the very neutron-rich isotopes [32]. Furthermore, the neural network provides first descriptions of the structure and deformation of ^{24}Si and ^{40}Mg of interest to x-ray burst nucleosynthesis, and even of the extremely heavy nuclei such as ^{166,168}Er and ^{236}U, that build upon first principles considerations [32].

3.2 Probing clustering and physics beyond the standard model

The left-handed vector minus axial-vector (V−A) structure of the weak interaction was postulated in late 1950's and early 1960's guided in large part by a series of beta-decay experiments, and later was incorporated in the Standard Model of particle physics. However, in its most general form, the weak interaction can also have scalar, tensor, and pseudoscalar terms as well as right-handed currents. The β decay of ^{8}Li to ^{8}Be, which subsequently breaks up into two α particles, has long been recognized as an excellent testing ground to search for new physics (e.g. see [53]) due to the high decay energy and the ease of detecting the β and two α particles. These experiments have achieved remarkable precision (e.g., see [54,55]) that now requires confronting the systematic uncertainties that stem from the higher-order corrections in nuclear beta decay that are difficult to measure experimentally.

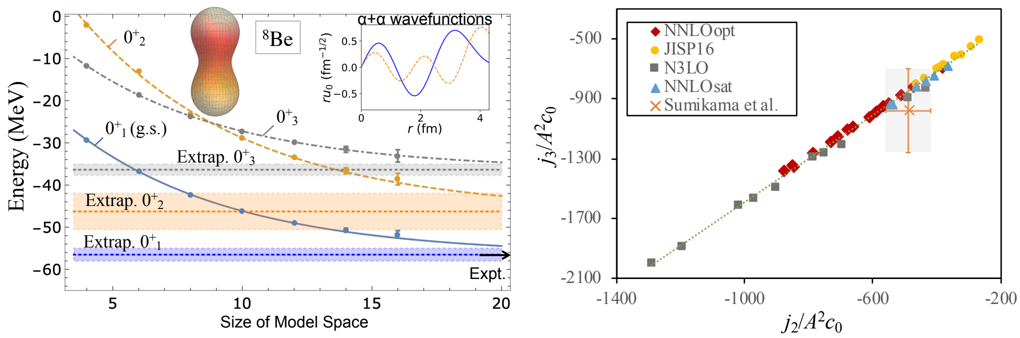

Figure 4: The *ab initio* SA-NCSM places unprecedented constraints on higher-(recoil-) order corrections (j_2/A^2c_0 and j_3/A^2c_0) in the β decay of ^{8}Li→^{8}Be by addressing the challenging $\alpha+\alpha$ structure of ^{8}Be. The results are essential for largely improving the sensitivity of high-precision experiments that probe the weak interaction theory and test physics beyond the Standard Model [55, 33]. Calculations performed on the NERSC and Frontera HPC systems. *Source:* Figures from [33] @ APS; reproduced with permission.

As a remarkable result, the *ab initio* SA-NCSM has recently determined the size of the recoil-order form factors in the β decay of ^{8}Li (Fig. 4). It has shown that states of the $\alpha+\alpha$ system not included in the evaluated ^{8}Be energy spectrum have an important effect on all $j_{2,3}/A^2c_0$, b/Ac_0 and d/Ac_0 recoil-order terms, and can explain the elusive $M_{\rm GT}$ discrepancy in the $A=8$ systems common to all other *ab initio* approaches.

The SA-NCSM outcomes of Ref. [33] reduce – by over 50% – the uncertainty on these recoil-order corrections. These results help improve the sensitivity of high-precision β-decay experiments that probe the V−A structure of the weak interaction in the most stringent limit on tensor current contribution to the weak interaction theory to date, established in Ref. [55]. Furthermore, the SA-NCSM predicted b/Ac_0 and d/Ac_0 values are important for other investigations of the Standard Model symmetries, such as the conserved vector current hypothesis and the existence of second-class currents in the weak interaction.

3.3 Optical potential in the symmetry-adapted framework for nuclear reactions

In recent years there has been a significant interest in describing nuclear reactions from *ab initio* approaches, and especially in constructing from first principles effective inter-cluster interactions, often referred to as optical potentials. *Ab initio* optical potentials for elastic scattering at low energy are of particular interest for experiments at rare isotope beams. To utilize the efficacy of the symmetry-adapted basis, we combine the *ab initio* symmetry-adapted no-core shell model with the Green's function technique (SANCSM/GF) and construct non-local optical potentials rooted in first principles [56,57]. Using the Green's function technique ensures that all relevant cluster partitionings are included in the effective potential between the two reaction fragments (clusters) that are typically in their ground state in the entrance channel. With the view toward studying neutron and proton elastic scattering from deformed and heavy targets, we first examine a target of ^{4}He (Fig. 5a), where the effect of the spurious center-of-mass motion is most evident.

In a complementary symmetry-adapted resonating group method (SA-RGM) framework [58], one starts from an *ab initio* description of all particles involved and derives the effective potential for localized clusters, which are properly normalized and orthogonalized in the

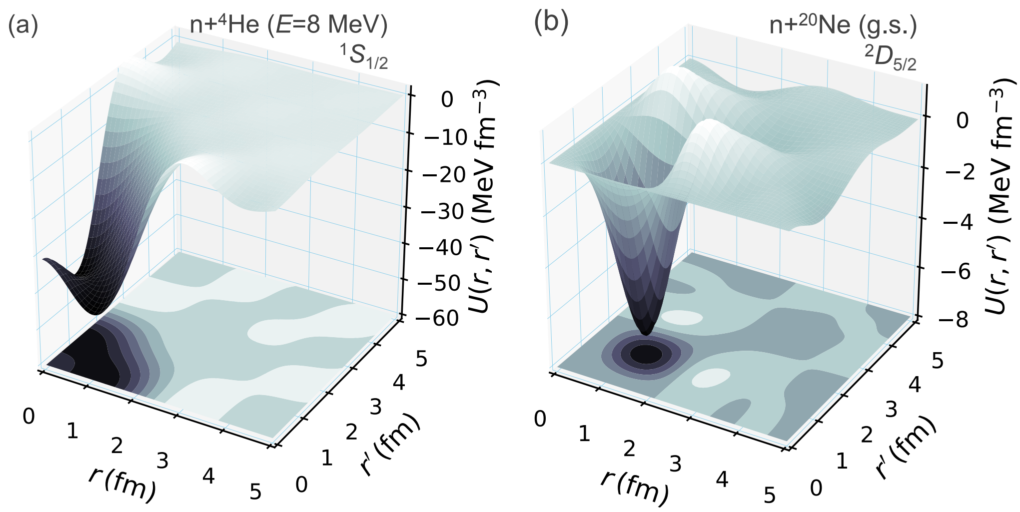

Figure 5: (a) Translationally invariant non-local optical potential for elastic neutron scattering for a ^{4}He target at $E = 8$ MeV center-of-mass energy, calculated in the SA-NCSM with the Green's function technique (10 shells, $\hbar\Omega$=17MeV). Figure from [56]. (b) Effective neutron-nucleus non-local potential (translationally invariant) for the ^{20}Ne ground state, where effects of the target excitations and antisymmetrization involving three nucleons are neglected (based on *ab initio* SA-NCSM calculations of ^{20}Ne with NNLO$_{\rm opt}$ in a model space of 11 shells and $\hbar\Omega$=15 MeV inter-shell distance). *Source:* Figure from [1] @ Annual Reviews; reproduced under the terms of its CC BY license.

particle sector, which yields non-local effective nucleon-nucleus interactions for the cluster partitioning or channel under consideration. For a single channel, if the effects of the target excitations are neglected, the non-local effective nucleon-nucleus interaction can be calculated for each partial wave, as illustrated for n+^{20}Ne($0^+_{\rm g.s.}$) with NNLO$_{\rm opt}$ in 11 shells (Fig. 5b). While these calculations limit the antisymmetrization to two nucleons only, this is a first step toward constructing effective nucleon-nucleus potentials for light and medium-mass nuclei for the astrophysically relevant energies [59, 60].

4 Conclusion

We have discussed the critical role of the emergent Sp(3,$\mathbb{R}$) symmetry in atomic nuclei and the associated subgroup SU(3), which in turn underpin the Sp(3,$\mathbb{R}$) and SU(3) schemes. By exploiting these schemes, the *ab initio* SA-NCSM has enabled machine-learning pattern recognition and descriptions of heavy nuclei, *ab initio* modeling of α clustering and collectivity, along with tests of beyond-the-standard-model physics. In addition, we show that with the help of the SA-NCSM, which expands *ab initio* applications up to medium-mass nuclei by using the dominant symmetry of nuclear dynamics, one can provide solutions to reaction processes in this region, with a focus on elastic neutron scattering.

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