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TOPICAL REVIEW

Ab initio symplectic no-core shell model

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Abstract

The no-core shell model (NCSM) is a prominent ab initio method that yields a good description of the low-lying states in few-nucleon systems as well as in more complex p-shell nuclei. Nevertheless, its applicability is limited by the rapid growth of the many-body basis with larger model spaces and increasing number of nucleons. The symplectic no-core shell model (Sp-NCSM) aspires to extend the scope of the NCSM beyond the p-shell region by augmenting the conventional spherical harmonic oscillator basis with the physically relevant symplectic Sp(3, R) symmetry-adapted configurations of the symplectic shell model that describe naturally the monopole–quadrupole vibrational and rotational modes, and also partially incorporate α-cluster correlations. In this review, the models underpinning the Sp-NCSM approach, namely, the NCSM, the Elliott SU(3) model and the symplectic shell model, are discussed. Following this, a prescription for constructing translationally invariant symplectic configurations in the spherical harmonic oscillator basis is given. This prescription is utilized to unveil the extent to which symplectic configurations enter into low-lying states in 12C and 16O nuclei calculated within the framework of the NCSM with the JISP16 realistic nucleon–nucleon interaction. The outcomes of this proof-of-principle study are presented in detail.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The long-standing goal of theoretical nuclear physics is to describe properties of nuclei starting from the elementary interactions among the constituent nucleons. A solution to this problem
represents a formidable challenge due to the intricate nature of the strong force that precludes perturbative treatments, and due to the complexities of the strongly interacting quantum many-particle systems that exhibit single-particle as well as collective and clustering correlations. Nevertheless, the last decade has witnessed remarkable progress toward this arduous goal. Recent advances in the construction of realistic internucleon interactions together with a dramatic increase in performance achieved by highly parallel computing systems have resulted in a successful utilization of the ab initio approaches to the investigation of properties of light nuclei.

Besides bridging the gap between quantum chromodynamics (QCD) and measured properties of light nuclei, the ab initio approaches hold promise to have a tremendous impact on advancing the present frontiers in multiple branches of physics. Realistic nuclear wavefunctions are crucial for gaining an understanding of astrophysical processes involving exotic and unstable nuclei, the study of electromagnetic, weak and particle decay modes, as well as for testing fundamental symmetries in nature and probing physics beyond the standard model.

The ab initio no-core shell model (NCSM) [1, 2] has become a prominent tool for studying the microscopic aspects of the structure of light nuclei. It has achieved a good description of the nuclear spectra and observables for few-nucleon systems [3] up through more complex p-shell nuclei [1, 2, 4–6] utilizing modern two- and three-nucleon interactions. It is currently the only ab initio technique capable to solve the Schrödinger equation with nonlocal interactions [7, 8]. The main limitation of this method is inherently coupled with the use of a many-body basis constructed from spherical harmonic oscillator single-particle states (m-scheme basis), whose size, and hence the computational complexity and associated storage requirements, grows combinatorially with the number of nucleons and with the number of allowed single-particle states. The NCSM is therefore currently not capable of modeling sd-shell nuclei, and often falls short of accurately reproducing characteristic features and physical observables in p-shell nuclei, as, for example, enhanced B(E2) transitions strengths or states dominated by multiple-particle–multiple-hole configurations.

The symplectic no-core shell-model (Sp-NCSM) approach [9] can extend the many-body basis of the NCSM beyond its current limits through symplectic Sp(3, R) symmetry-adapted basis of the symplectic shell model [10–12]. Symplectic basis states describe naturally monopole and quadrupole vibrational and rotational modes, and also partially incorporate α-cluster correlations, and hence allows one to account for nuclear collective correlations beyond the current computational limits, extensions that are required to realize experimentally measured B(E2) values without an effective charge and to accommodate highly deformed spatial configurations. The Sp-NCSM is based on recognition that the choice of coordinates is often crucial in quantum-mechanical calculations, and that in order to reduce the size of a model space, an appropriate choice of a basis should reflect symmetries inherent to the system under study.

The present review is organized in the following way. In section 2, a brief review of modern two- and three-nucleon realistic interactions is given. In section 3, an overview of the ab initio NCSM framework is presented. The Elliott SU(3) model of nuclear rotations and its multi-shell extension, the symplectic shell model, are introduced in sections 4 and 5. In section 6, a method for the construction of the translationally invariant symplectic Sp(3, R) symmetry-adapted configurations in m-scheme basis is detailed. This method was utilized to analyze symplectic symmetry structure within eigenstates obtained with the NCSM using the JISP16 realistic nucleon–nucleon interaction, and outcomes of that study are presented in sections 7–11. Section 12 summarizes our findings.
2. The nuclear realistic interaction

The success of the \textit{ab initio} methods in the nuclear structure physics would not be possible without improvement in the construction of realistic internucleon interactions. An internucleon interaction is considered realistic if it describes the nucleon–nucleon scattering Nijmegen dataset \cite{13} with a $\chi^2$ per datum very close to one, and, at the same time, reproduces the properties of the deuteron perfectly. Such a condition is not rigorous \cite{14}, e.g. it does not guarantee agreement with experimental data for $A \geq 3$ nuclear system. There exists, however, a ‘zoo’ of modern realistic nuclear potential models that reproduce a wide range of physical observables in more complex nuclei containing up to $A = 16$ nucleons. They can be divided into three main types: phenomenological meson-exchange potentials, potentials derived at a fundamental level from the low-energy regime of the quantum chromodynamics (QCD), and nucleon–nucleon potentials that use unitary transformations to partially absorb effects of multi-nucleon forces.

The family of phenomenological meson-exchange nuclear interactions includes the Nijmegen potentials \cite{15}, the Argonne V18 potential \cite{16} and the CD-Bonn potential \cite{17, 18}. All of these potentials are charge dependent and use about 45 parameters to describe the nucleon–nucleon scattering at energies up to 350 MeV with an unprecedented precision. Their common theoretical background is based upon the meson-exchange model augmented by the electromagnetic interaction and a (more or less) phenomenological short-range interaction. The long-range part of the interaction is generally the one-pion-exchange potential. The CD-Bonn potential uses the full, original, nonlocal Feynman amplitude for one-pion-exchange \cite{18}, while all other potentials apply local approximations. In spite of some seemingly significant differences, all of these phenomenological meson-exchange potential models are about equally successful in reproducing the properties of the deuteron. On the other hand, calculations of the binding energies of $A \geq 3$ nuclei yield values that are consistently less than the corresponding experimental values by about 5–10% \cite{19}. The phenomenological nucleon–nucleon interaction models also fail to describe the nucleon–deuteron elastic scattering data, especially at higher energies \cite{20}. These drawbacks are traditionally overcome by the inclusion of three-nucleon forces whose presence is a direct consequence of the quark substructure of the nucleons. The three-nucleon phenomenological interactions are constructed primarily as two-pion-exchange potentials. The best known of these models are the Tuscon-Melbourne \cite{21, 22} and the Brazil \cite{23} potentials. Other three-nucleon interaction models are the Illinois potential \cite{24}, incorporating three-pion-exchange term, and the Urbana potential \cite{25}, based on the mechanism of two-pion-exchange with the excitation of intermediate $\Delta$ resonance. The parameters of three-nucleon potentials are determined by fitting to the three-nucleon scattering data as well as experimental binding energies and the first excited states of $A \geq 3$ nuclei. The process of finding a consistent combination of phenomenological two- and three-nucleon potentials, accomplished through the fitting to various properties of $A \geq 3$ nuclear system, lacks a solid theoretical foundation. There exist several parameterizations for each three-nucleon force model depending on the nucleon–nucleon potential chosen. The resulting nuclear potentials do not take the chiral symmetry and its breaking pattern systematically into account. Furthermore, even if the particular combination of forces predicts the $^3$H and $^4$He binding energies precisely, it may fail for p-shell nuclei \cite{24}. Clearly, there is a need for a systematic theory of nuclear interactions that would treat two- and many-body forces on an equal footing, and at the same time would be consistent with the symmetries of the low-energy QCD.

The fundamental theory of strong interactions, QCD, is non-perturbative in the low-energy regime characteristic of nuclear physics and hence derivation of the nuclear forces from the
fundamental theory of strongly coupled quarks and gluons is an incredibly complicated task. A promising advance in the theory of nuclear forces emerged when the concept of an effective field theory [26] was applied to low-energy QCD giving rise to chiral perturbation theory [27, 28]. This approach represents a best up-to-date bridge between QCD and the nuclear structure. It is based on the recognition that at energies below 1 GeV, the appropriate degrees of freedom are not quarks and gluons, but pions and nucleons interacting via a force governed by spontaneously broken approximate chiral symmetry. Broken chiral symmetry is a crucial constraint that generates and controls low-energy dynamics of QCD and allows the relevant dynamical features of QCD to be properly incorporated into the nuclear force problem. The explicit and spontaneous breaking of chiral symmetry facilitates a derivation of internucleon interaction from an effective chiral Lagrangian using a perturbation expansion in powers of \(Q/\Lambda_{\chi}\), where \(Q\) denotes a momentum or pion mass and \(\Lambda_{\chi}\) is the chiral symmetry breaking scale of the order of 1 GeV. The resulting power series generates two-, three- and four-nucleon forces on an equal footing, and furthermore, naturally explains the empirically known hierarchy of nuclear forces, i.e. \(V_{2N} \gg V_{3N} \gg V_{4N}\). The nucleon–nucleon interaction based on the chiral perturbation theory was constructed including all the terms appearing in the chiral perturbation expansion up to order \(Q^4\) [29]. The accuracy of the resulting potential is comparable with the high-precision nucleon–nucleon phenomenological potentials. The leading three-nucleon interaction that appears at order \(Q^3\) was also constructed [30]. The first calculations with the two- and three-nucleon chiral potentials have been performed in the NCSM framework for the p-shell nuclei [8, 7]. These results are in reasonably good agreement with the data, especially given the fewer number of parameters in the theory than in the case of the phenomenological meson-exchange interactions.

The computational complexity induced by the inclusion of a three-nucleon potential in the many-body quantum problem has triggered development of the nucleon–nucleon potential models that minimize the role of the three-nucleon interaction. The key principle underlying this approach is provided by the seminal work of Polyzou and Glöckle [14] who demonstrated that the three-body force effect can be, to a certain extent, reproduced by the phase-equivalent unitary nonlocal transformation of the two-body interaction. The nuclear potentials exploiting the residual freedoms of a realistic nucleon–nucleon interaction include the inside-nonlocal–outside Yukawa (INOY) interaction [31], the similarity renormalization group (SRG) transformed interactions [32–34], the unitary correlation operator method (UCOM) interactions [35, 36] and the \(J\)-matrix inverse scattering potential (JISP) [37, 38]. An interaction based on the JISP potential was used to generate the NCSM results presented in this study. The JISP potentials are constructed in two steps. The nucleon–nucleon interaction is first derived from the \(J\)-matrix inverse scattering approach [39], and consequently altered by a unitary phase-equivalent transformation in order to give an improved description of deuteron quadrupole moment, and to obtain excellent fits to the spectra of stable p-shell nuclei. The resulting interaction, JISP6 [37], yields a very good description of the spectra of \(A < 10\) nuclei while providing a rapid convergence of the NCSM calculations. Results are competitive with those obtained with nucleon–nucleon and three-nucleon forces. Nevertheless, the JISP6 interaction overbinds nuclei with \(A \geq 10\). The newer JISP16 [38] potential, obtained from JISP6 by fitting to the excitation energies of \(^6\)Li and binding energies of \(^6\)Li and \(^{16}\)O, eliminates this deficiency.

3. \textit{Ab initio} no-core shell model

The \textit{ab initio} NCSM targets solving the Schrödinger equation for a system of \(A\) point-like non-relativistic strongly interacting nucleons. The general translationally invariant Hamiltonian
for this problem reads

\[ H_A = \frac{1}{A} \sum_{i<j=1}^{A} \frac{(p_i - p_j)^2}{2m} + \sum_{i<j=1}^{A} V_{ij}, \]  

(1)

where the first term is the relative kinetic energy operator and \( V_{ij} \) denotes a realistic nucleon–nucleon interaction.

In principle, three- and even four-body interactions should be included in a realistic nuclear Hamiltonian. As noted in section 2, these higher-order many-body forces are a direct consequence of the quark substructure of the nucleons. They appear naturally in nuclear potentials that are derived from the low-energy limit of the QCD using the chiral perturbation theory [26–28] or the quark–meson coupling model [40]. For simplicity, however, here we limit the discussion to just two-body interactions.

To facilitate finding a solution, the Hamiltonian (1) can be modified by adding a center-of-mass (c.m.) harmonic oscillator (HO) Hamiltonian,

\[ H_{c.m.} = \frac{P^2}{2mA} + \frac{1}{2} Am\Omega^2 R^2, \]  

(2)

where \( \Omega \) is the HO frequency, \( P = \sum_{i=1}^{A} p_i \) and \( R = 1/A \sum_{i=1}^{A} r_i \). The modified Hamiltonian (1) can then be recast as

\[ H_A^{\Omega} = \sum_{i=1}^{A} \left[ \frac{p_i^2}{2m} + \frac{1}{2} m\Omega^2 r_i^2 \right] + \sum_{i<j=1}^{A} \left[ V_{ij} - \frac{m\Omega^2}{2A} (r_i - r_j)^2 \right], \]  

(3)

where the first term is just a sum of one-particle harmonic oscillators that is diagonal in the oscillator basis. This Hamiltonian, \( H_A^{\Omega} \), can be schematically written as

\[ H_A^{\Omega} = \sum_{i=1}^{A} h_i + \sum_{i<j=1}^{A} V_{ij}^{A,\Omega}. \]  

(4)

Although the addition of \( H_{c.m.} \) introduces a pseudo-dependence upon the harmonic oscillator frequency \( \Omega \), it does not affect the final results. This can be readily seen from the fact that the intrinsic eigenstates of the Hamiltonian \( H_A \), which are \( \Omega \) independent, are simultaneously eigenstates of the Hamiltonian \( H_A^{\Omega} \). The addition of the \( H_{c.m.} \) merely increases the energy of the intrinsic eigenstates by an overall constant \( \frac{3}{2}\hbar/\Omega \), which is subtracted in the final stage of the NCSM calculation.

The Hamiltonian \( H_A^{\Omega} \) is not translationally invariant, and hence it yields spurious eigenstates with excited c.m. motion. It is necessary to choose from among the eigenstates of \( H_A^{\Omega} \) only intrinsic ones, that is, those with the c.m. in its ground state. This is done by projecting spurious eigenstates upward in the energy spectrum by addition of the Lawson projection term

\[ \lambda \left( H_{c.m.} - \frac{3}{2}\hbar/\Omega \right), \]  

(5)

into the Hamiltonian \( H_A^{\Omega} \). The Lawson projection term shifts eigenstates with excited c.m. motion up to high energies for sufficiently large value of \( \lambda \), while leaving the energies of the intrinsic states unaltered.

To obtain numerical solutions of the \( A \)-body Schrödinger equation, it is necessary to truncate the full infinite Hilbert space to a finite and computationally tractable model space. The model space is comprised of all many-body states with up to \( N_{\text{max}} \hbar/\Omega \) harmonic oscillator excitations above the valence space configurations. The bare Hamiltonian \( H_A^{\Omega} \) would yield unreasonable results in a finite model space unless the effect of the excluded configurations
is taken into account. As a consequence, $H^A_0$ must be replaced by a model space-dependent effective Hamiltonian $H_{\text{eff}}$ that reproduces the low-lying spectrum of the bare Hamiltonian, and whose eigenstates are the model space components of the true eigenstates of $H^A_0$. Similarly, operators associated with physical observables, such as electromagnetic transitions, should also be replaced by the effective operators tailored to the given model space.

3.1. Lee–Suzuki similarity transformation method

The effective operators in the NCSM scheme are constructed by means of the Lee–Suzuki similarity transformation method [41, 42]. The Lee–Suzuki method considers a bare Hamiltonian of form $H = H_0 + V$, where $H_0$ is the unperturbed Hamiltonian and $V$ is a potential. In the case of the bare nuclear Hamiltonian $H^A_0$, we have $H_0 = \sum_{i=1}^{A} h_i$ and $V = \sum_{i<j}^{A} V_{ij}^{A,\Omega}$. The first step is to divide the full Hilbert space into a finite-dimensional model space which is referred to as the $P$ space, and whose dimension is denoted $d_P$. Complementary to the model space is the space of excluded configurations, the $Q$ space. The basis states of the $P$ and $Q$ spaces are denoted as $|\alpha_P\rangle$ and $|\alpha_Q\rangle$, respectively. Associated with the model space and the excluded space are the projection operators $P$ and $Q$. In addition to the standard properties, e.g. $PQ = QP = 0$, $P^2 = P$, $P^\dagger = P$, the operators $P$ and $Q$ are eigenprojectors of $H_0$, that is

$$[H_0, P] = [H_0, Q] = 0, \quad QH_0P = PH_0Q = 0.$$ (6)

The non-Hermitian form of the Lee–Suzuki method introduces a similarity transformation induced by a transformation operator $\omega$:

$$H \rightarrow e^{-\omega}H e^{\omega}, \quad |\psi\rangle \rightarrow e^{-\omega} |\psi\rangle.$$ (7)

The transformation operator $\omega$ satisfies

$$\omega = Q\omega P,$$ (8)

which implies that $\omega^n = 0$ for $n \geq 2$. This greatly simplifies evaluation of the similarity transformation as

$$e^{\pm \omega} = 1 \pm Q\omega P.$$ (9)

In addition to condition (8), the transformation operator $\omega$ has also to satisfy the decoupling condition

$$Qe^{-\omega}H e^{\omega}P = 0.$$ (10)

This provides the necessary and sufficient condition for determination of the effective Hamiltonian

$$H_{\text{eff}} = P e^{\omega}H e^{-\omega}P = PH_0P + V_{\text{eff}},$$ (11)

where $V_{\text{eff}}$ denotes the effective interaction. The rigorous proof of this statement can be found in [43].

The matrix elements of the transformation operator $\omega$ are needed for the evaluation of the effective Hamiltonian. From (8), it immediately follows that

$$\langle \alpha_P | \omega | \alpha_P \rangle = \langle \alpha_Q | \omega | \alpha_Q \rangle = \langle \alpha_P | \omega | \alpha_Q \rangle = 0.$$ (12)
The non-vanishing matrix elements of the transformation operator \( \omega \) are given by [2]

\[
\langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{|\psi_i\rangle \in \mathcal{K}} \langle \alpha_Q | \psi_k \rangle \langle \psi_k | \alpha_P \rangle,
\]

where \( \mathcal{K} \) denotes a selected set of \( d_P \) eigenstates of the bare Hamiltonian \( H \), and \( \langle \psi_k | \alpha_P \rangle \) is the matrix element of the inverse \( d_P \times d_P \) overlap matrix \( \langle \alpha_P | \psi_k \rangle \), that is, \( \sum_{\alpha_P} \langle \psi_k | \alpha_P \rangle \langle \alpha_P | \psi_k \rangle = \delta_{kk} \) and \( \sum_{\alpha_P} \langle \alpha_P | \psi_k \rangle \langle \psi_k | \alpha_P \rangle = \delta_{\alpha_P \alpha_P} \). The biorthogonal states \( \langle \psi_i | \rangle \) satisfy \( \langle \psi_i | \psi_j \rangle = \delta_{ij} \).

Note that in order to solve for \( \omega \) one needs to find a set of \( d_P \) eigenstates \( |\psi_k\rangle \in \mathcal{K} \) of the bare Hamiltonian \( H \). That is, however, equivalent to solving the eigenproblem in the full Hilbert space.

The similarity transformation (7) produces a non-Hermitian effective Hamiltonian. The Hermitian effective Hamiltonian is constructed through the unitary similarity transformation

\[
H_{\text{eff}} = (P \ e^{\omega})^* H \ e^{\omega} P = P \ e^{\omega} H \ e^{\omega} P - \frac{1}{4},
\]

where \( \omega \) is the transformation operator introduced above and \( \omega^\dagger \) denotes its Hermitian conjugate. Since the above transformation is unitary, it can be rewritten as

\[
H_{\text{eff}} = P \ e^{-\omega} H \ e^{\omega} P,
\]

where the transformation operator \( S \) is anti-Hermitian, \( S^\dagger = -S \). \( S \) can be expressed in terms of \( \omega \) and \( \omega^\dagger \) as [42]

\[
S = \text{arctanh}(\omega - \omega^\dagger).
\]

The operator \( S \) also satisfies the decoupling condition \( Q \ e^{-\omega} H \ e^{\omega} P = P \ e^{-\omega} H \ e^{\omega} Q = 0 \) and the restrictive condition \( PSP = QSQ = 0 \). A compact expression for the matrix elements of the effective Hamiltonian reads [44]

\[
\langle \alpha_P | H_{\text{eff}} | \alpha_P' \rangle = \sum_{|\psi_i\rangle \in \mathcal{K}} \sum_{|\psi_j\rangle \in \mathcal{K}} \sum_{|\psi_k\rangle \in \mathcal{K}} \langle \alpha_P | (1 + \omega^\dagger \omega)^{-1/2} | \alpha_P'' \rangle \langle \alpha_P'' | \psi_k \rangle \langle \psi_k | \alpha_P' \rangle \times \omega_{\alpha_P' \alpha_P''},
\]

where \( H |\psi_k\rangle = E_k |\psi_k\rangle \) and the computation of \( \langle \alpha_P | (1 + \omega^\dagger \omega)^{-1/2} | \alpha_P'' \rangle \) is facilitated by the following expression:

\[
\langle \alpha_P | (1 + \omega^\dagger \omega)^{-1} | \alpha_P' \rangle = \sum_{|\psi_i\rangle \in \mathcal{K}} \langle \alpha_P | \psi_i \rangle \langle \psi_i | \alpha_P' \rangle.
\]

In principle, relation (17) can be utilized to find an effective interaction for a given model space \( P \) such that the lowest-lying eigenspectrum of the effective Hamiltonian \( H_{\text{eff}} \) reproduces exactly the lowest-lying eigenspectrum of the bare Hamiltonian. The eigenstates \( |\xi_k\rangle \) of \( H_{\text{eff}} \) are related to the eigenstates of the bare Hamiltonian as

\[
|\psi_k\rangle = (1 + \omega)(P(1 + \omega^\dagger \omega)P)^{-1/2} |\xi_k\rangle.
\]

Note that until now, no approximations have been employed. In practice, however, an effective Hamiltonian is an \( A \)-body operator whose construction requires finding a set \( \mathcal{K} \) of \( d_P \) lowest-lying eigenstates of a bare Hamiltonian. This makes the straightforward application of the Lee–Suzuki method for \( A > 3 \) nuclei impractical unless one resorts to an approximation.

3.2. Cluster approximation to an effective interaction

An effective interaction is an \( A \)-body operator even if a bare potential consists of two-nucleon interactions only. To construct such an effective interaction is equal to finding the eigensolution of a full-space bare Hamiltonian. For this reason, the Lee–Suzuki method is performed at an
a-body level for which it is feasible to calculate the accurate eigensolution of the full problem. The resultant a-body effective interaction is used as an approximation to the exact A-body effective interaction. This method, known as the cluster approximation method [2, 45–47], does not yield the effective Hamiltonian reproducing exactly a subset of the eigenspectrum of the bare Hamiltonian. The eigensolution, nevertheless, possesses a very important feature: it converges rapidly to the exact solution with increasing model space size or increasing level of clustering.

In the cluster approximation, an A-body effective interaction $V_{\text{eff}}$ is replaced by a superposition of a-body effective interactions

$$V_{\text{eff}} \simeq \sum_{i_1 < i_2 < \cdots < i_a = 1}^{A} V_{i_1 i_2 \cdots i_a \text{eff}}.$$ \hfill (20)

The a-body effective interaction is constructed through the Lee–Suzuki transformation method as

$$V_{i_1 i_2 \cdots i_a \text{eff}} = P_a (e^{-S_{a}^\Omega} H_{a}^\Omega e^{S_{a}^\Omega}) P_a - P_a \left( \sum_{i=1}^{a} h_i \right) P_a,$$ \hfill (21)

where $S_{a}^\Omega$ is an a-body transformation operator, $P_a$ is an a-body model space projection operator and the a-nucleon bare Hamiltonian $H_{a}^\Omega$ is given as

$$H_{a}^\Omega = \sum_{i=1}^{a} h_i + \sum_{i<j}^{a} V_{ij}^{a,\Omega}.$$ \hfill (22)

Once the matrix elements of the a-particle effective interaction $V_{i_1 i_2 \cdots i_a \text{eff}}$ are calculated, the resultant effective Hamiltonian

$$H_{\text{eff}}^{(a)} = \sum_{i=1}^{A} h_i + \sum_{i<j}^{A} V_{ij}^{A,\Omega}$$ \hfill (23)

can be utilized in the NCSM calculations. Note that in order to obtain the matrix elements of the a-body effective interaction $V_{i_1 i_2 \cdots i_a \text{eff}}$ through (17), one first needs to find the full space solution to the a-body Schrödinger equation (22). Such a task is computationally very involved even for the $a = 2$ case. In practice, therefore, one performs the Lee–Suzuki method at the two- and three-body levels only.

In the two-body cluster approximation, $V_{\text{eff}}$ is replaced by a sum of two-body effective interactions $V_{ij \text{eff}}$.

$$V_{\text{eff}} \simeq \sum_{i<j=1}^{A} V_{ij \text{eff}}.$$ \hfill (24)

The two-body matrix elements of $V_{ij \text{eff}}$ are derived from the bare two-body Hamiltonian

$$H_{i_2}^{\Omega} = h_1 + h_2 + V_{i_1 i_2}^{\Omega}.$$ \hfill (25)

in the following manner [48]:

(i) The two-body problem (25) is solved with high-precision in the relative harmonic oscillator basis for a maximal computationally tractable space, so that the resultant eigenstates and eigenvalues can be regarded as the eigensolution to the full two-body problem.
(ii) A set of \( d_p \) lowest-lying eigenstates and corresponding eigenvalues is then utilized to calculate the matrix elements of \( V_{ij}^{A,\Omega} \) through the prescription (17), where the size of the two-body model space \( P_2 \) is determined from the size of the given \( A \)-particle model space \( P \).

The resulting effective Hamiltonian reads

\[
\tilde{H}_{\text{eff}}^{(a=2)} = \sum_{i=1}^{A} h_i + \sum_{i<j}^{A} V_{ij}^{A,\Omega}_{\text{eff}},
\]

and can be utilized in the NCSM calculations for the given model space \( P \). The important property of the two-body cluster approximation is that the two-body interaction \( V_{ij}^{A,\Omega}_{\text{eff}} \) approaches the bare interaction \( V_{ij}^{A,\Omega} \) when \( P_2 \to 1 \). It readily follows from the fact that the transforming operator \( \omega \to 0 \) with \( P_2 \to 1 \). As a consequence, \( \tilde{H}_{\text{eff}}^{(a=2)} \to H_A^{\Omega} \) when \( N_{\text{max}} \to \infty \), which is the essential property required for the effective Hamiltonian. As a result, the deviations of the two-body cluster approximation from the exact effective interaction can be minimized by increasing the size of the model space as much as possible. Furthermore, it has been shown that the short-range operators are renormalized well in the two-body cluster approximation [49, 50], whereas the long-range operators, such as the quadrupole transition operator, are renormalized only weakly.

Because of the cluster approximation, relation (19) between the effective and the bare eigenstates no longer holds. However, it has been shown that even the simplest, i.e. \( a = 2 \), cluster approximation is a very good approximation to the exact effective Hamiltonian in the large model space limit, and that the eigenstates of the Hamiltonian \( H_{\text{eff}}^{(a=2)} \) are good approximations to the model space components of the bare Hamiltonian eigenstates [51].

It can be readily seen from (21) that if \( a \to A \), the approximation becomes exact. Therefore, an improved convergence can be achieved by performing the Lee–Suzuki unitary transformation at a higher-cluster level [52]. The addition of three-body effective interactions becomes imperative when genuine three-nucleon forces are included in a bare Hamiltonian. Such state-of-the-art calculations have been performed for p-shell nuclei [6, 8, 47].

3.3. Scale explosion problem

The applicability of the \textit{ab initio} NCSM approach is severely limited due to the scale explosion problem. The term scale explosion describes the fact that the dimensionality of the basis grows combinatorially with increasing nucleon number and increasing cutoff \( N_{\text{max}} \) (as can be seen in figure 1 where results for an \( m \)-scheme basis, defined ahead, are shown). And even worse, the computational complexity and associated storage requirements typically growing as the square of the growth in the size of the basis. Hence even with the most powerful supercomputers currently available, the \textit{ab initio} NCSM is neither able to model sd-shell nuclei, nor properly describe various important features of p-shell nuclei, including the enhanced E2 transition strengths or low-lying intruder \( \alpha \)-cluster states.

Furthermore, the nuclear Hamiltonian matrices are no longer sparse once the three-nucleon force is introduced, and hence one cannot use specialized algorithms and data structures that take advantage of the sparse structure of the matrix. As a result, the model space must be significantly reduced once three-nucleon interactions are included.

In order to extend the scope of the NCSM approach to heavier nuclei and larger model spaces, we propose augmenting the model space with configurations that are essential for a description of the most dominant modes of the nuclear collective dynamics. Our approach is based on the classification of nuclear many-body states according to their transformation
properties with respect to physically relevant subgroups of the symplectic $\text{Sp}(3, \mathbb{R})$ symmetry group which underpins a microscopic description of the nuclear collective motion. The proposed \textit{ab initio} symplectic no-core shell model framework extends the NCSM concept by recognizing that the choice of coordinates is crucial and should reflect the symmetries inherent to nuclear systems.

4. Elliott SU(3) model of nuclear rotations

In this section, we review the Elliott SU(3) model of nuclear rotations [53–56] which underpins the symplectic shell model. The Elliott SU(3) model is an algebraic model that attempts to describe nuclear rotational states in the p- and sd-shell nuclei by making use of the symmetry group SU(3) for the classification of the many-nucleon states, and, in the simplest case, by using SU(3) generators for the construction of effective inter-nucleon interactions. Such a symmetry-based approach simplifies calculations while providing valuable physical insight into the structure of nuclear wavefunctions. The Elliott model approximates the nuclear mean field by a harmonic oscillator potential and hence is embedded in a microscopic shell model framework.

4.1. $U(3)$ and SU(3) symmetry groups

A microscopic realization of infinitesimal generators of the group $U(3)$ for a system of $A$ particles can conveniently be written as

$$C_{ij} = \frac{1}{2} \sum_{n=1}^{A} (b_{ni}^\dagger b_{nj} + b_{nj}^\dagger b_{ni}), \quad i, j = x, y \quad \text{or} \quad z, \quad (27)$$
where \( b_n^+ \) and \( b_n \) are the harmonic oscillator raising and lowering operators for the \( n \)th particle

\[
b_n^+ = \sqrt{\frac{m \Omega}{2 \hbar}} \left( x_n - \frac{i}{m \Omega} p_n \right),
\]

\[
b_n = \sqrt{\frac{m \Omega}{2 \hbar}} \left( x_n + \frac{i}{m \Omega} p_n \right).
\]

Utilizing the commutation relations for the harmonic oscillator ladder operators,

\[
[b_n^+, b_m^+] = [b_n, b_m] = 0,
\]

\[
[b_n, b_m^+] = \delta_{nm} b_{n+m},
\]

one can show that all nine operators \( C_{ij} \) obey the commutation rules for the Lie algebra \( u(3) \) (we use lowercase letters for algebras and capital letters for groups),

\[
[C_{ij}, C_{kl}] = \delta_{jk} C_{il} - \delta_{il} C_{kj}.
\]

It is convenient to transform the \( C_{ij} \) operators into spherical \( SO(3) \) tensors of rank zero, one and two, respectively:

\[
H_0 = C_{11} + C_{22} + C_{33},
\]

\[
L_{10} = -i(C_{12} - C_{21}),
\]

\[
L_{1\pm 1} = \frac{1}{\sqrt{2}}((C_{13} - C_{31}) \pm i(C_{23} - C_{32})),
\]

\[
Q^{q}_{20} = 2C_{33} - C_{11} - C_{22},
\]

\[
Q^{q}_{2\pm 1} = \mp \sqrt{\frac{3}{2}} ((C_{13} + C_{31}) \pm i(C_{23} + C_{32})),
\]

\[
Q^{q}_{2\pm 2} = \sqrt{\frac{3}{2}} ((C_{11} - C_{22}) \pm i(C_{21} + C_{12})).
\]

The operator \( H_0 \) is the three-dimensional harmonic oscillator Hamiltonian, \( L_{1q} \) \( (q = 0, \pm 1) \) are the orbital angular momentum operators,

\[
L_{1q} = \sum_{n=1}^{A} (x_n \times p_n)_{q},
\]

and the operators \( Q^{q}_{2q} \) \( (q = 0, \pm 1, \pm 2) \) form the five components of the algebraic quadrupole tensor, and can be written in terms of coordinate and momentum observables as

\[
Q^{q}_{2q} = \sqrt{\frac{4\pi}{5}} \sum_{n=1}^{A} \left( \frac{x_n^2}{b^2} Y_{2q}(x_n) + b^2 p_n^2 Y_{2q}(p_n) \right),
\]

where the oscillator length is given by \( b = \sqrt{\hbar/m \Omega} \). The commutation relations for the spherical tensors can be deduced from (30) to be

\[
[L_{1q}, L_{1q'}] = -\sqrt{5}(1q'; 1q' | 1q + q') L_{1q+q'},
\]

\[
[Q^{q}_{2q}, L_{1q'}] = -\sqrt{6}(2q; 1q' | 2q + q') Q^{q}_{2q+q'},
\]

\[
[Q^{q}_{2q}, Q^{q'}_{2q'}] = \sqrt{60}(2q; 2q' | 1q + q') L_{1q+q'},
\]

with \( H_0 \) commuting with all \( U(3) \) generators. Here, \( (l_1m_1; l_2m_2|l_3m_3) \) is the usual notation for a Clebsch–Gordan coefficient. The operator \( H_0 \) is associated with the group \( U(1) \). The unitary transformations \( \exp(i\alpha H_0) \) \( \in U(1) \) simply introduce an overall change of phase for arbitrary real coefficient \( \alpha \), and hence are of no physical interest. The subset of eight operators \( L_{1q} \) and \( Q^{q}_{2q} \) satisfy commutation relations for the infinitesimal generators of the \( SU(3) \) group.
4.2. Labeling scheme

The irreducible representations of the group U(3) are labeled by a set of three non-negative integers \( f_1 \geq f_2 \geq f_3 \) corresponding to the length of rows in the Young tableau. The group SU(3) is obtained from U(3) by removing those transformations, which simply introduce an overall change of phase. As a consequence only two numbers \((\lambda, \mu)\), defined as

\[
\lambda = f_1 - f_2, \\
\mu = f_2 - f_3
\]

are needed to label a SU(3) irreducible representation (irrep). An obvious subgroup of SU(3) is the rotational group SO(3), generated by the orbital angular momentum operators \( L \). This means that we can classify the many-body configurations according to their transformation properties with respect to the physical group reduction chain \( SU(3) \supset SO(3) \). In addition, by coupling the orbital angular momentum \( L \) to the complementary many-particle spin degree-of-freedom \( S \), one can achieve a classification scheme with good total angular momentum \( J \):

\[
SU(3) \supset SO(3) \supset SU(2) \supset U(1)
\]

The multiplicity label \( \kappa \) reflects the fact that multiple occurrences of \( L \) are possible within a generic irrep \((\lambda, \mu)\) of SU(3). Here \( M_J \) is the projection of \( J \) along the \( z \)-axis of the laboratory frame. It is important to note that one can choose an alternative, and from a mathematical point of view more natural labeling scheme that reduces SU(3) canonically; that is, with respect to its SU(2) \( \otimes \) U(1) subgroup chain, SU(3) \( \supset \) SU(2) \( \otimes \) U(1). Nevertheless, most applications of SU(3), including the symplectic shell model, utilizes its reduction with respect to its physical subgroup chain, SU(3) \( \supset \) SO(3).

4.3. SU(3) model Hamiltonians

The quadrupole–quadrupole interaction is a very important ingredient of the long-range part of the internucleon interaction. It plays a particularly significant role in explaining a microscopic origin of nuclear rotations. It is important to emphasize that the mass quadrupole operator differs from \( Q^a_q \). Within a major oscillator shell the matrix elements of \( Q^c_q \) and \( Q^a_q \) are identical, but \( Q^c_q \) couple states spanning the \( \eta \)th shell with those of the \( \eta' \)th shell, \( \eta' = \eta \pm 2 \), whereas the matrix elements of \( Q^a_q \) between states belonging to different shells vanish.

In order to show the way in which rotational spectra arise in the shell model, Elliott considered the effective Hamiltonian

\[
H = H_0 - \frac{1}{2} \chi Q^a \cdot Q^a,
\]

where \( H_0 \) is the three-dimensional harmonic oscillator Hamiltonian. The advantage of using the algebraic quadrupole operator instead of the mass quadrupole operator lies in the fact that \( Q^a \cdot Q^a \) can be expressed in terms of Casimir operators of \( su(3) \) and \( so(3) \) Lie algebras as

\[
Q^a \cdot Q^a = 6\hat{C}_2 - 3\hat{L}^2
\]

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and hence it is diagonal in a $SU(3) \supset SO(3)$ symmetry-adapted basis. It is clear that, within a single $SU(3)$ irrep, the Hamiltonian (44) is equivalent to the quantum rotor Hamiltonian

$$H = H_0 + \frac{1}{2} \chi \hat{I}^2 + \text{const}, \quad (46)$$

and hence gives rise to a rotational band with excitation energies proportional to $L(L + 1)$.

The eigenvalues of the Hamiltonian (44) are given by

$$E(\lambda\mu) = N_\Omega \hbar / \Omega - \frac{1}{2} \chi [6C_2(\lambda, \mu) - 3L(L + 1)], \quad (47)$$

where $N_\Omega \hbar / \Omega$ is the harmonic oscillator energy, $L$ is the orbital angular momentum and $C_2(\lambda, \mu)$ denotes the expectation value of the second-degree Casimir operator of $su(3)$ given by

$$C_2(\lambda, \mu) = \frac{1}{2} (\lambda^2 + 3\lambda + 3\mu + \lambda\mu + \mu^2). \quad (48)$$

If the model space incorporates multiple $SU(3)$ irreps, then the Hamiltonian (44) has a spectrum which is composed of multiple rotational bands lying at relative excitation energies determined by the factor $-3\chi C_2(\lambda, \mu)$. Each rotational band corresponds to a single $SU(3)$ irrep. Such a structure of eigenstates does not reproduce all features of realistic low-lying rotational spectra such as the $K$-band splitting and the inter-band $E2$ transitions. The inclusion of a special minimal set of $SO(3)$ scalars, the so-called $SU(3) \rightarrow SO(3)$ integrity basis, allows one to reproduce these properties [57, 58] as well.

In the simplest version, the Elliott model takes into account only the ‘leading’ $SU(3)$ irrep, that is, the irrep with the largest value $C_2(\lambda, \mu)$. Such a choice gives rise to the rotational band with the lowest energy, which is evident from (47). More sophisticated calculations allowing mixing of $SU(3)$ configurations within a single shell were performed to study the combined effects of the quadrupole–quadrupole, pairing and spin–orbit interactions [59–61].

Generally, spaces restricted to $\hbar / \Omega \, SU(3)$ irreps are inadequate for modeling the low-lying highly deformed states with a dominant multi-particle–multi-hole structure that are found in nuclei throughout the periodic table. Clearly, one needs to include $SU(3)$ irreps that span higher-$\hbar / \Omega$ subspaces and which incorporate core excited configurations. The number of possible $SU(3)$ configurations grows combinatorially with increasing number of active oscillator shells. It is thus imperative to select only those $SU(3)$ symmetry-adapted configurations that are relevant for the description of the nuclear deformed geometry and nuclear collective dynamics. The selection scheme is underpinned by a geometric interpretation of the $SU(3)$ states that is based on the relation between $SU(3)$ and the rigid rotor symmetry groups, and by the symplectic shell model, which enables to relate $SU(3)$ irreps with the nuclear collective motion.

### 4.4. Geometrical interpretation of $SU(3)$ states

A very important property of the $SU(3)$ model is its relation to the microscopic rigid rotor model [62] whose algebra is associated with the rotational limit of the geometric collective (Bohr–Mottelson–Frankfurt) model [63–65]. This in turn allows an interpretation of the microscopic quantum labels $\lambda$ and $\mu$ in terms of the collective shape variables $\beta$ and $\gamma$ of the geometric collective model describing deformation of the nucleus with respect to the principal axis frame.

The relation between the rigid rotor and the Elliott SU(3) model can be derived from the relationship between their Lie algebras. The basic assumption of the rigid rotor model is that the inertia tensor in the model Hamiltonian

$$H_{\text{ROT}} = \sum_{i=1}^{3} \frac{1}{2I_i} \hat{I}_i^2 \quad (49)$$

is
is a function of the mass quadrupole moments $Q_c^2$. The Lie algebra of the rigid rotor is thus spanned by the five commuting mass quadrupole moment operators and the three components of the angular momentum, $\mathfrak{rot}(3) = \{Q_{2q}, L_{1q}\}$, whereas the $\mathfrak{su}(3)$ is spanned by $\{Q_c^2, L_{1q}\}$ (39). Both Lie algebras satisfy the following commutation relations:

$$[L_{1q}, L_{1q'}] = -\sqrt{2}(1q; 1q' q + q')L_{1q+q'},$$  \hspace{1cm} (50)$$

$$[Q_{2q}, L_{1q}] = -\sqrt{6}(2q; 1q' q + q')Q_{2q+q'},$$  \hspace{1cm} (51)$$

where $Q$ denotes $Q^\alpha$ and $Q^c$ in the case of $\mathfrak{su}(3)$ and $\mathfrak{rot}(3)$, respectively. The difference between the two algebras lies in the commutators for their quadrupole operators:

$$[Q_{2q}, Q_{2q'}] = 3\sqrt{10}(2q; 2q' q + q')L_{1q+q'} \times \begin{cases} 0 & \text{for } \mathfrak{rot}(3), \\ +1 & \text{for } \mathfrak{su}(3). \end{cases}$$  \hspace{1cm} (52)$$

To demonstrate the contraction $\mathfrak{su}(3) \rightarrow \mathfrak{rot}(3)$ one can introduce a rescaled quadrupole operator, $Q' = Q^c\hat{C}_2^{-1/2}$, where $\hat{C}_2$ is the second-order Casimir invariant of $\mathfrak{su}(3)$. The commutation relations (50) and (51) remain the same for the new set of generators, but the third one becomes

$$[Q'_{2q}, Q'_{2q'}] = 3\sqrt{10}(2q; 2q' q + q')\hat{C}_2^{-1/2}L_{1q+q'}. \hspace{1cm} (53)$$

This implies that $[Q'_{2q}, Q'_{2q'}] \approx 0$ for $L \ll \hat{C}_2(\lambda, \mu)$ and thus in this contraction limit the operators $\{Q'_{2q}, L_{1q}\}$ span the $\mathfrak{rot}(3)$ Lie algebra. This argument also unveils a difference; namely, since the $\mathfrak{su}(3)$ algebra is compact the angular momentum $L$ is bound (by $\lambda + \mu$ in a $(\lambda, \mu)$ irrep), whereas the non-compact rotor algebra $\mathfrak{rot}(3)$ supports unbound $L$ values.

An alternative way of relating $\mathfrak{su}(3)$ and $\mathfrak{rot}(3)$ algebras is to explore relations between their Casimir invariants. This approach is based on the rationale that the invariant measures of two models used to describe the same quantum phenomena must be related to each other. The relation between two invariants of the rigid rotor algebra, the traces of the square and cube of the mass quadrupole moment matrix $\text{Tr}[(Q^c)^2]$ and $\text{Tr}[(Q^c)^3]$, and the second- and third-order Casimir invariants of $\mathfrak{su}(3)$, $\hat{C}_2$ and $\hat{C}_3$, was derived [66] by invoking a linear mapping between the eigenvalues of these invariant operators

$$\langle \text{Tr}[(Q^c)^2] \rangle = \frac{1}{2}k^2\beta^2 \leftrightarrow C_2(\lambda, \mu) = \frac{1}{2}(\lambda^2 + 3\lambda + 3\mu + \lambda\mu + \mu^2),$$

$$\langle \text{Tr}[(Q^c)^3] \rangle = \frac{1}{2}k^3\beta^3 \cos 3\gamma \leftrightarrow C_3(\lambda, \mu) = \frac{1}{2}(\lambda - \mu)(\lambda + 2\mu + 3)(2\lambda + \mu + 3).$$

Here the constant $k = \sqrt{\frac{5}{9\pi}A<r^2>$, where $A$ is the number of nucleons and $<r^2>$ is the nuclear mean square radius. The exact relation between the microscopic quantum numbers $\lambda$ and $\mu$ and the shape variables $\beta$ and $\gamma$ reads [66]

$$\beta^2 = \left(\frac{4\pi}{5A^2<r^2>^2}\right)(\lambda^2 + \lambda\mu + \mu^2 + 3\lambda + 3\mu + 3),$$  \hspace{1cm} (54)$$

$$\gamma = \tan^{-1}\left[\frac{\sqrt{3}(\mu + 1)}{2\lambda + \mu + 3}\right]. \hspace{1cm} (55)$$

This implies that each $\mathfrak{su}(3)$ irrep $(\lambda, \mu)$ corresponds to a unique shape parameterized by deformation parameters $(\beta \gamma)$. The variables $\beta$ and $\gamma$ can vary continuously, whereas the quantum labels $(\lambda, \mu)$ are discrete and a set of their possible values is limited due to the fermionic nature of the nucleons, a feature that is not included in the collective model. This is illustrated in figure 2 with the help of a grid which is superposed on the $(\beta \gamma)$-plane of the geometric collective model. Note, in particular, that $\mathfrak{su}(3)$ irreps with $\mu = 0$ correspond to
Figure 2. A traditional $(\beta \gamma)$ plot, where $\beta$ ($\beta \geq 0$) is the radius vector and $\gamma$ ($0 \leq \gamma \leq \pi/3$) is the azimuthal angle, demonstrates the relationship between the collective model shape variables $(\beta \gamma)$ and the SU(3) irrep labels $(\lambda \mu)$. A prolate shape, irreps with $\lambda = 0$ correspond to an oblate geometry, and irreps with $\lambda = \mu$ describe a maximally asymmetric shape. A spherical nucleus is described by the $(00)$ irrep.

In short, the SU(3) classification of many-body states allows for a geometrical analysis of the eigenstates of a nuclear system via relations (54) and (55) and hence gives insight into phenomena associated with nuclear deformation.

5. Symplectic shell model

The symplectic model [10–12] is a microscopic algebraic model of nuclear collective motion that includes monopole and quadrupole collective vibrations as well as vorticity degrees of freedom for a description of rotational dynamics in a continuous range from irrotational to rigid rotor flows. It can be regarded as both a microscopic realization of the successful phenomenological Bohr–Mottelson–Frankfurt collective model and a multi-$\hbar\Omega$ extension of the Elliott SU(3) model.

While the NCSM divides the many-nucleon Hilbert space into ‘horizontal’ layers of $N\hbar\Omega$ subspaces, the symplectic model divides it into ‘vertical’ slices of $\text{Sp}(3, \mathbb{R})$ irreducible representations, which is schematically illustrated in figure 4. The symplectic model thus allows one to restrict a model space to vertical slices that admit the most important modes of nuclear collective dynamics.

The symplectic model is based on the 21-dimensional algebra $\text{sp}(3, \mathbb{R})$ and has a very rich group structure (see figure 3). In particular, there are two important subgroup chains that unveil the physical content of the symplectic model: the shell model subgroup chain associated with the Elliott SU(3) group and the collective model chain related to the general collective motion GCM(3) group. The intersection of these chains is the group of rotations $\text{SO}(3)$.

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Figure 3. The symplectic group $\text{Sp}(3, \mathbb{R})$ contains two physically important subgroup chains: the collective model chain, $\text{Sp}(3, \mathbb{R}) \supset \text{GCM}(3) \supset \text{ROT}(3) \supset \text{SO}(3)$ and the shell model chain, $\text{Sp}(3, \mathbb{R}) \supset \text{SU}(3) \supset \text{SO}(3)$.

5.1. Collective model chain

The significance of the symplectic $\text{Sp}(3, \mathbb{R})$ symmetry for a microscopic description of a quantum many-body system of interacting particles emerges from the physical relevance of its 21 infinitesimal generators. The symplectic $\mathfrak{sp}(3, \mathbb{R})$ algebra has realization in terms of well-defined microscopic shell model one-body Hermitian operators. The generators of $\text{Sp}(3, \mathbb{R})$ can be constructed as bilinear products of canonical coordinates:

$$Q_{ij} = \sum_n x_{in} x_{nj},$$

$$S_{ij} = \sum_n (x_{in} p_{nj} + p_{in} x_{nj}),$$

$$L_{ij} = \sum_n (x_{in} p_{aj} - x_{aj} p_{ni}),$$

$$K_{ij} = \sum_n p_{ni} p_{nj},$$

where $x_{ni}$ and $p_{ni}$ denote the $i$th Cartesian component of the position and the momentum of the $n$th nucleon.

The six monopole and quadrupole moments $Q_{ij}$, the six generators of monopole and quadrupole deformations $S_{ij}$, the three generators of rotations $L_{ij}$, and the six generators of quadrupole flow tensor $K_{ij}$, constitute the 21-dimensional Lie algebra $\mathfrak{sp}(3, \mathbb{R})$, which is the smallest Lie algebra that contains both the mass quadrupole moments as well as the many-nucleon kinetic energy.

Several algebraic models of nuclear collective motion that give rise to rotational spectra are associated with subgroups of the $\text{Sp}(3, \mathbb{R})$ symmetry in the collective model chain,

$$\text{Sp}(3, \mathbb{R}) \supset \text{GCM}(3) \supset \text{ROT}(3) \supset \text{SO}(3).$$
The general collective motion group GCM(3) is generated by a 15-dimensional non-compact algebra spanned by the operators \{Q_{ij}, L_{ij}, S_{ij}\}. It is the symmetry group of the microscopic collective model [67, 68]. This model represents a fully microscopic extension of the Bohr–Mottelson–Frankfurt model. While the latter can describe monopole–quadrupole vibrations and either the rigid rotor or the irrotational flow characteristics of rotational motion, the collective dynamics embraced by the GCM(3) structure includes a vorticity degree of freedom and thus describes a continuous range of rotational dynamics from the rigid rotor to the irrotational flow. Note that in the classical limit, \(\text{Sp}(3, \mathbb{R})\) and GCM(3) symmetries are important for stellar dynamics as they underpin symmetry of rotating stars and galaxies [69].

The algebra rot(3) associated with a rigid rotor is also a subalgebra of \(\text{sp}(3, \mathbb{R})\). States of a rigid rotor do not have square-integrable wavefunctions in the many-nucleon Hilbert space [70]. Therefore one cannot utilize the basis of the collective model chain in microscopic nuclear structure calculations.

Due to the presence of the quadrupole flow tensor \(K_{ij}\) among the generators of \(\text{Sp}(3, \mathbb{R})\), the many-body three-dimensional harmonic oscillator Hamiltonian is an element of the symplectic \(\text{sp}(3, \mathbb{R})\) algebra. The symplectic model thus unifies the Bohr–Mottelson–Frankfurt model and the shell model associated with the U(3) group. This also means that we can construct a basis of the Hilbert space according to a classification scheme that reduces another alternative subgroup chain of \(\text{Sp}(3, \mathbb{R})\); namely, the shell model subgroup chain.

5.2. Shell model chain

The shell model subgroup chain, \(\text{Sp}(3, \mathbb{R}) \supset \text{SU}(3) \supset \text{SO}(3)\), is directly responsible for the computational tractability of the symplectic model. It transcends the Elliott SU(3) group and as a consequence bridges between the microscopic shell model and the nuclear collective dynamics. The shell model structure of the \(\text{Sp}(3, \mathbb{R})\) generators is elucidated if the symplectic algebra is realized in terms of bilinear products in the harmonic oscillator raising and lowering operators:

\[
A_{ij} = \sum_{n=1}^{A} b_{n}^{\dagger} b_{n}^{\dagger},
\]

\[
B_{ij} = \sum_{n=1}^{A} b_{n},
\]

\[
C_{ij} = \frac{1}{2} \sum_{n=1}^{A} (b_{n}^{\dagger} b_{n} + b_{n} b_{n}^{\dagger}).
\]

The operators \(C_{ij}\) act only within a major harmonic oscillator shell, while the six operators \(A_{ij}\) are \(2\hbar\Omega\) raising operators and their adjoint \(B_{ij}\) are \(2\hbar\Omega\) lowering operators.

The Cartesian components of the monopole and quadrupole moment operators \(Q_{ij}\) can be expressed in terms of the symplectic generators as

\[
Q_{ij} = \frac{1}{2}(A_{ij} + B_{ij} + C_{ij} + C_{ji}),
\]

and thus they connect not only states within a single major oscillator shell, but also states differing in oscillator energy by \(\pm 2\hbar\Omega\).

To construct \(\text{Sp}(3, \mathbb{R})\) irreducible representations in the basis of the shell model subgroup chain, it is advantageous to express the symplectic generators as SU(3) tensor operators. The
harmonic oscillator raising and lowering operators can be written as three-dimensional SU(3) tensor operators transforming according to the (10) and (01) irreps, respectively [71]:

\[
b_{i=1}^{(10)} = \pm \frac{1}{\sqrt{2}} (b_1 \pm i b_2), \quad b_{10}^{(10)} = b_3,
\]

and

\[
b_{i=1}^{(01)} = \pm \frac{1}{\sqrt{2}} (b_1 \pm i b_2), \quad b_{10}^{(01)} = b_3,
\]

with \(b_{10}^{(01)} = (-1)^q \langle b_{i=1}^{(01)} \rangle^\dagger\). Since the harmonic oscillator ladder operators are SU(3) tensors, they can be coupled to form new SU(3) tensors. In this way, the symplectic generators can be written as SU(3) tensor operators,

\[
A_{L,M}^{(20)} = \frac{1}{\sqrt{2}} \sum_{n=1}^{A} [b_n^{(10)} \times b_n^{(10)}]_{L,M}^{(20)},
\]

\[
B_{L,M}^{(02)} = \frac{1}{\sqrt{2}} \sum_{n=1}^{A} [b_n^{(01)} \times b_n^{(01)}]_{L,M}^{(02)},
\]

\[
C_{L,M}^{(11)} = \sqrt{2} \sum_{n=1}^{A} [b_n^{(10)} \times b_n^{(01)}]_{L,M}^{(11)},
\]

\[
H_{00}^{(00)} = \sqrt{3} \sum_{n=1}^{A} [b_n^{(10)} \times b_n^{(01)}]_{00}^{(00)} + \frac{3}{2} A.
\]

The eight operators \(C_{L,M}^{(11)}\) generate the SU(3) subgroup of Sp(3, \(\mathbb{R}\)) and are related to the angular momentum operator \(L_{1q}\) and the Elliott algebraic quadrupole moment tensor \(Q_{a2q}\) as follows,

\[
C_{L,M}^{(11)} = L_{1q}, \quad q = 0, \pm 1,
\]

\[
C_{L,M}^{(11)} = \frac{1}{\sqrt{3}} Q_{a2q}, \quad q = 0, \pm 1, \pm 2.
\]

The mass quadrupole operator \(Q_{c2q}\) can be expressed as a linear combination of \(L = 2\) components of SU(3) tensors:

\[
Q_{c2q} = \sqrt{3} [A_{2q}^{(20)} + B_{2q}^{(02)} + C_{2q}^{(11)}].
\]

The lowering tensor \(B_{L,M}^{(02)}\) is the adjoint of \(A_{L,M}^{(20)}\) tensor and their spherical components are related as

\[
B_{L,M}^{(02)} = (-)^{L-M} (A_{L,-M}^{(20)})^\dagger.
\]

### 5.3. Translationally invariant form of symplectic generators

The symplectic generators introduced in the preceding sections are not translationally invariant and hence give rise to irreducible representations that are contaminated with spurious center-of-mass excitations. One way to overcome this problem is to construct the Sp(3, \(\mathbb{R}\)) generators in terms of intrinsic coordinates, namely, \(x'_n = x_n - X_l\) and \(p'_n = p_n - P_l\), defined with respect to the center-of-mass momentum \(P_l = \sum_{n=1}^{A} p_n\) and position \(X_l = (1/A) \sum_{n=1}^{A} x_n\).
Figure 4. The schematic plot illustrating decomposition of the shell model space as direct sum of the symplectic $Sp(3, \mathbb{R})$ irreps. Each ellipsoid in the figure corresponds to a definite deformation of the nucleus as given by the SU(3) quantum numbers $(\lambda\omega\mu\nu)$ via relations (54) and (55). The action of the symplectic raising and lowering operators $A^{(20)}_{LM}$ and $B^{(02)}_{LM}$ within a $Sp(3, \mathbb{R})$ irrep is also schematically depicted.

[72]. The translationally invariant $Sp(3, \mathbb{R})$ generators can then be written in SU(3)-coupled form as

$$A^{(20)}_{LM} = \frac{1}{\sqrt{2}} \sum_{n=1}^{A} [b^{(10)}_{n} \times b^{(10)}_{n}]^{(20)}_{LM} - \frac{1}{\sqrt{2}A} \sum_{s,t=1}^{A} [b^{(10)}_{s} \times b^{(10)}_{t}]^{(20)}_{LM},$$

(72)

$$B^{(02)}_{LM} = \frac{1}{\sqrt{2}} \sum_{n=1}^{A} [b^{(01)}_{n} \times b^{(01)}_{n}]^{(02)}_{LM} - \frac{1}{\sqrt{2}A} \sum_{s,t=1}^{A} [b^{(01)}_{s} \times b^{(01)}_{t}]^{(02)}_{LM},$$

(73)

$$C^{(11)}_{LM} = \frac{\sqrt{2}}{A} \sum_{n=1}^{A} [b^{(10)}_{n} \times b^{(01)}_{n}]^{(11)}_{LM} - \frac{\sqrt{2}}{A} \sum_{s,t=1}^{A} [b^{(10)}_{s} \times b^{(01)}_{t}]^{(11)}_{LM},$$

(74)

$$H^{(00)}_{00} = \sqrt{3} \sum_{n=1}^{A} [b^{(10)}_{n} \times b^{(01)}_{n}]^{(00)}_{00} - \sqrt{3} \sum_{s,t=1}^{A} [b^{(10)}_{s} \times b^{(01)}_{t}]^{(00)}_{00} + \frac{3}{2}(A-1).$$

(75)

This form of the intrinsic $Sp(3, \mathbb{R})$ generators can also be obtained from the translationally non-invariant $Sp(3, \mathbb{R})$ generators (64)–(67) after the subtraction of the center-of-mass realization of the $sp(3, \mathbb{R})$ algebra, which is spanned by the two-body operators:

$$A^{(20)}_{LM}^{\text{c.m.}} = \frac{1}{\sqrt{2}}[\mathcal{B}^{1} \times \mathcal{B}^{1}]^{(20)}_{LM},$$

$$B^{(02)}_{LM}^{\text{c.m.}} = \frac{1}{\sqrt{2}}[\mathcal{B} \times \mathcal{B}]^{(02)}_{LM},$$

$$C^{(11)}_{LM}^{\text{c.m.}} = \frac{\sqrt{2}}{A}[\mathcal{B}^{1} \times \mathcal{B}^{1}]^{(11)}_{LM},$$

$$H^{(00)}_{00}^{\text{c.m.}} = \sqrt{3}[\mathcal{B}^{1} \times \mathcal{B}^{1}]^{(00)}_{00} + \frac{3}{2}. $$

(76)
These operators are expressed by means of the c.m. harmonic oscillator ladder operators

\[ \mathcal{B}_i^j = \frac{1}{\sqrt{A}} \sum_{n=1}^{A} b_{ni} \]  

(77)

\[ \mathcal{B}_i = \frac{1}{\sqrt{A}} \sum_{n=1}^{A} b_{ni} \]  

(78)

The translationally invariant symplectic raising operators (72) are utilized to generate basis states of \( \text{Sp}(3, \mathbb{R}) \) irreps and hence it is instructive to examine their action on \( A \)-nucleon configurations. The first term in (72) raises a single nucleon by two shells, that is, it induces \( 2\hbar/\Omega \) one-particle–one-hole \((1p-1h)\) monopole \((L = 0)\) or quadrupole \((L = 2)\) excitations. The second term eliminates the spurious c.m. excitations in the symplectic states by evoking small \((\sim 1/A) 2\hbar/\Omega \) two-particle–two-hole \((2p-2h)\) corrections (two particles raised by one shell each). This is schematically illustrated in figure 5.

5.4. Symplectic basis states

The symplectic states are labeled (in standard notation [10, 12]) in the shell model chain as

\[ \text{Sp}(3, \mathbb{R}) \supset \text{SU}(3) \supset \text{SO}(3) \supset \text{SU}(2) \supset U(1) \]

(79)

\[ \sigma \quad n \rho \quad \omega \quad \kappa \quad (LS_{\pi}) \quad J \quad M_J. \]

Note that the elements of the \( \mathfrak{sp}(3, \mathbb{R}) \) algebra act merely on nucleon spatial coordinates leaving the spin part unaffected. Each symplectic irrep thus carries a definite value of the total intrinsic spin \( S_{\pi} \), which can be coupled with the total orbital angular momentum \( L \) to produce the total angular momentum \( J \) and its projection \( M_J \).
A basis of a symplectic irrep is constructed by acting with symmetrically coupled polynomials in the symplectic raising operators, \( A^{(20)} \), on a set of basis states of a symplectic bandhead, \( |\sigma; S_\sigma\rangle \), which is a \( \text{Sp}(3, \mathbb{R}) \) lowest-weight state,

\[
|\sigma \rho \omega \kappa (L S_\sigma J M_J) \rangle = [A^{(20)} \times A^{(20)} \times \cdots \times A^{(20)}]^n \times |\sigma; S_\sigma\rangle^\rho \omega \kappa (L S_\sigma J M_J),
\]

where \( \sigma \equiv N_\sigma (\lambda_\sigma \mu_\sigma) \) labels \( \text{Sp}(3, \mathbb{R}) \) irreps, \( n \equiv N_n (\lambda_n \mu_n) \) and \( \omega \equiv N_\omega (\lambda_\omega \mu_\omega) \). The quantum number \( N_\omega = N_\sigma + N_n \) is the total number of oscillator quanta related to the eigenvalue, \( N_\Omega \), of a three-dimensional harmonic oscillator Hamiltonian that excludes the c.m. spurious modes.

The quantum numbers \((\lambda_n \mu_n)\) specify the overall SU(3) symmetry of \( N_n/2 \) coupled symplectic raising operators. A multiple coupling of \((20)\) irrep always produces a set of unique irreps and thus there is no need to introduce an additional multiplicity label. As the raising operators \( A^{(20)} \) commute, only the symmetrically coupled raising operators are non-vanishing \([11]\). It can be shown that all possible \((\lambda_n \mu_n)\) quantum numbers are enumerated by \( \Omega^n \) defined as

\[
\Omega^n = \{(\lambda_n \mu_n) | n_1 + n_2 + n_3 = N_n, \lambda_n = n_1 - n_2, \mu_n = n_2 - n_3, n_1 \geq n_2 \geq n_3\},
\]

where \( n_1, n_2, n_3 \) range over all even non-negative integers.

The \( \rho \omega \kappa \equiv \rho N_\omega (\lambda_\omega \mu_\omega) \) quantum labels specify the SU(3) symmetry of the symplectic state. The symbol \( \rho \) denotes a multiplicity label which is needed to distinguish between multiple occurrences of the \((\lambda_\omega \mu_\omega)\) irrep within the direct product \((\lambda_n \mu_n) \times (\lambda_\sigma \mu_\sigma)\). In accordance with the mapping between the microscopic \((\lambda \mu)\) SU(3) labels and the shape variables of the Bohr–Mottelson collective model \((\beta\gamma)\), the symplectic basis states bring forward important information about the nuclear shapes and deformation, which is schematically depicted in figure 4.

The basis states, \(|\sigma \kappa_0 (L_0 S_\sigma) J_0 M_0\rangle\), of the symplectic bandhead \( \sigma \) are the starting state configurations upon which a \( \text{Sp}(3, \mathbb{R}) \) irrep is built according to (80). A symplectic bandhead is a \( \text{Sp}(3, \mathbb{R}) \) lowest-weight state and, consequently, it is annihilated upon the action of the \( B_{\text{CM}}^{(02)} \) symplectic lowering operators,

\[
B_{\text{CM}}^{(20)} |N_\sigma (\lambda_\sigma \mu_\sigma) \kappa_0 (L_0 S_\sigma) J_0 M_0\rangle = 0.
\]

Trivially, all the SU(3) irreps that span the \( 0\hbar \Omega \) and \( 1\hbar \Omega \) subspaces satisfy the above condition. However, a general SU(3) irrep belonging to a higher-\( \hbar \Omega \) subspace is not guaranteed to be a symplectic bandhead, and thus one has to test explicitly whether it is annihilated by the symplectic lowering operators. Note that if one were to include all possible symplectic bandheads and allowed symplectic excitations thereof, one would span the entire shell model Hilbert space.

It is important to note that the construction formula (80) does not produce an orthogonal basis. Specifically, the symplectic states with identical \( N_\omega (\lambda_\omega \mu_\omega) \) labels but different \( \rho \) and \( n \) quantum numbers are generally not orthogonal. In order to find a unitary transformation that gives rise to an orthonormal basis it is necessary to evaluate inner products between overlapping symplectic states. This is done by making use of the \( K \)-matrix theory \([73–75]\).

### 5.5. Relation between \( \alpha \)-cluster and symplectic states

\( \alpha \)-Cluster modes manifest themselves most obviously in low-lying spectra of \( A = 4n \), \( N = Z \) nuclei, e.g., the low-lying highly deformed 0+ intruder states in \(^{12}\text{C}\) and \(^{16}\text{O}\), which have been successfully described by various \( \alpha \)-cluster models \([76–82]\). For example, the first
excited 0+ state in 16O together with the isospin zero states below 15 MeV were remarkably well reproduced by Suzuki’s microscopic cluster model [78, 83] using phenomenological interactions. This model describes the states of 16O by exciting the relative motion degree of freedom of an α-particle and the 12C nucleus. Suzuki and Hecht established a relation [84, 85] between the cluster model wavefunctions basis and the symplectic Sp(3, ℝ) basis states. We emphasize that even though such a cluster model basis is suitable for a description of α-cluster dynamics, the cluster model results are strongly influenced by the effective interaction used. Hence, such a relation between both bases is informative but not conclusive.

The translationally invariant states of the microscopic cluster model for a nucleus made up of fragments of mass number $f$ and $A - f$ can be written in the SU(3)-coupled form as

\[ |(\lambda_0, \mu_0) \times (Q 0)\rangle = \mathcal{A} \left[ \left( |\varphi_f^{(\lambda_0\mu_0)} \times \varphi_{A-f}^{(\lambda_0\mu_0)}\rangle \right) \times \chi^{(Q 0)}(R) \right] (\lambda_0\mu_0)\alpha_\omega, \]

where $\mathcal{A}$ is the antisymmetrization operator. The properly antisymmetrized internal wavefunctions $\varphi_f^{(\lambda_0\mu_0)}$ and $\varphi_{A-f}^{(\lambda_0\mu_0)}$ of the two fragments are assumed to be the lowest possible Pauli-allowed states with SU(3) symmetry $(\lambda_0, \mu_0)$ and $(\lambda_{A-f}, \mu_{A-f})$, and they are coupled to a final SU(3) irrep $(\lambda_0, \mu_0)$. The relative motion wavefunction $\chi$ is a harmonic oscillator function in the relative distance vector $R$ between the two fragments. It carries $Q$ oscillator quanta and hence it spans the SU(3) irrep $(Q 0)$. The minimum value of $Q$ is uniquely determined by the Pauli principle. The SU(3) symmetry of the total wavefunction is the resultant of the coupling $(\lambda_0, \mu_0) \times (Q 0)$ and denoted $(\lambda_0\mu_0)\alpha_\omega$.

The overlaps between a cluster wavefunction and a stretched symplectic wavefunction can be readily calculated using the recursive formula [84]:

\[
\langle \sigma (N_\alpha, 0) | (\lambda_0\mu_0)\alpha_\omega, (\lambda_0, \mu_0) \times (Q 0)\rangle = \sqrt{\frac{1}{2}} (Q + 1)(Q + 2) \times U[(\lambda_\alpha, \mu_\alpha)(Q 0)(\lambda_\omega\mu_\omega)(2, 0); (\lambda_0\mu_0)\alpha_\omega][(Q 2, 0) 11]
\]

\[
\times \langle \sigma (N_\alpha, 0) | (\lambda_0\mu_0)\alpha_\omega, (\lambda_0, \mu_0) \times (Q 0); (\lambda_0\mu_0)\alpha_\omega\rangle,
\]

(82)

where $U[(\lambda_\alpha, \mu_\alpha)(Q 0)(\lambda_\omega\mu_\omega)(20); (\lambda_0\mu_0)\alpha_\omega][(Q 2, 0) 11]$ is an SU(3)–Racah (unitary recoupling) coefficient. The symplectic stretched states are those states with $\mu_\omega = \mu_\sigma$ and maximum value of $\lambda_\omega = \lambda_\sigma + N_\alpha$ for $N_\alpha h\Omega_2$ excitations above the symplectic bandhead, and hence in the above equation $(\lambda_\omega\mu_\omega) = (\lambda_\sigma + N_\alpha + 2, \mu_\sigma)$ and $(\lambda_0\mu_0)\alpha_\omega = (\lambda_\sigma + N_\alpha, \mu_\sigma)$.

In the case of $\alpha + 12C$, the internal wavefunctions of the $\alpha$ and $12C$ clusters are restricted to the lowest Pauli-allowed states with SU(3) symmetry (00) and (04), respectively. The possible SU(3) symmetries $(\lambda_0\mu_0)\alpha_\omega$ of the cluster wavefunctions are

(0, 4) × (Q, 0) = (Q − 4, 0) ⊕ (Q − 3, 1) ⊕ (Q − 2, 2) ⊕ (Q − 1, 3) ⊕ (Q, 4).

All cluster states with $Q < 4$ are forbidden due to the Pauli principle. Only the (00) state is Pauli allowed for $Q = 4$, two states with (10) and (21) are allowed for $Q = 5$, three states with (20), (31) and (42) for $Q = 6$, four states with (30), (41), (52) and (63) for $Q = 7$. For $Q \geq 8$, all five cluster wavefunctions are Pauli allowed.

Furthermore, it turns out that the cluster wavefunctions with SU(3) symmetry (00), (21), (42), (63) and (84), are identical with the most deformed $n$-particle–$n$-hole ($np−nh$) Sp(3, ℝ) bandheads, with $n = 0, 1, \ldots, 4$. The overlaps between the cluster configurations and the stretched symplectic states spanning the leading $np−nh$ Sp(3, ℝ) irreps were calculated [84, 85] using the recursive formula (82). The results, which are summarized in Table 1, indicate that these states display a high degree of overlap, particularly for the first few symplectic excitations above the bandheads and for irreps built over strongly deformed intrinsic bandheads. Qualitatively similar results were obtained for $20$ Ne and $24$ Mg systems [84]. In summary, certain prominent features of the $\alpha$-cluster dynamics are reflected
Table 1. Overlaps of stretched symplectic basis states \((\lambda_\sigma + n, \mu_\sigma)\), \(n = 0, 2, \ldots, 12\), built over different \(^{16}\text{O} (\lambda_\sigma \mu_\sigma)\) bandheads to the \(\alpha + ^{12}\text{C}\) cluster basis states of the same \((\lambda_\sigma + n, \mu_\sigma)\) SU(3) symmetry, according to formula (82) [84]. Each overlap is calculated at a given \(\bar{\hbar}/\Omega_1\) level, e.g., the overlaps for the 4p−4h (84) symplectic irrep is given for 4\(\bar{\hbar}/\Omega_1\) (second column) up to 16\(\bar{\hbar}/\Omega_1\) (last column).

<table>
<thead>
<tr>
<th>(^{16}\text{O} ) symplectic bandhead ((\lambda_\sigma \mu_\sigma))</th>
<th>(\lambda_\sigma)</th>
<th>(\lambda_\sigma + 2)</th>
<th>(\lambda_\sigma + 4)</th>
<th>(\lambda_\sigma + 6)</th>
<th>(\lambda_\sigma + 8)</th>
<th>(\lambda_\sigma + 10)</th>
<th>(\lambda_\sigma + 12)</th>
</tr>
</thead>
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<tr>
<td>(00)</td>
<td>1.00</td>
<td>0.808</td>
<td>0.558</td>
<td>0.376</td>
<td>0.263</td>
<td>0.191</td>
<td>0.143</td>
</tr>
<tr>
<td>(21)</td>
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<td>0.816</td>
<td>0.581</td>
<td>0.405</td>
<td>0.290</td>
<td>0.213</td>
<td>0.161</td>
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<tr>
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<td>0.602</td>
<td>0.437</td>
<td>0.322</td>
<td>0.242</td>
<td>0.185</td>
</tr>
<tr>
<td>(63)</td>
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<td>0.476</td>
<td>0.364</td>
<td>0.281</td>
<td>0.220</td>
</tr>
<tr>
<td>(84)</td>
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<td>0.832</td>
<td>0.668</td>
<td>0.531</td>
<td>0.421</td>
<td>0.335</td>
<td>0.267</td>
</tr>
</tbody>
</table>

in the symplectic Sp(3, \(\mathbb{R}\)) basis states, including symplectic configurations beyond the 0p-0h irreps.

6. Expansion of symplectic states in \(m\)-scheme basis

To facilitate identification of the most important Sp(3, \(\mathbb{R}\)) symmetry-adapted components within NCSM realistic wavefunctions, we expanded the symplectic basis states in the \(m\)-scheme basis [87, 88] that is currently being utilized in the NCSM. Therefore, our task was to find an expansion of a translationally invariant symplectic bandhead in terms of Slater determinants constructed from the harmonic oscillator wavefunctions, upon which we apply the symplectic Sp(3, \(\mathbb{R}\)) basis construction formula (80) using proton–neutron second-quantized formalism.

6.1. Construction of symplectic bandheads

A symplectic bandhead is a SU(3) irrep satisfying condition (81). Therefore, our task was to find the expansion of a general \(N\hbar\Omega\ \hbar p–\hbar k\) SU(3) irrep in terms of \(m\)-scheme configurations and then verify whether it represents a Sp(3, \(\mathbb{R}\)) lowest-weight state [87, 88]. The resultant set of symmetry-adapted states must be free of spurious c.m. excitations and span a basis that is reduced with respect to the physical group chain (42). The method we used for this relies on the fact that the creation operators for fermions in the spherical harmonic oscillator basis are irreducible tensors with respect to the spatial SU(3) and the intrinsic spin SU(2) symmetries with tensor characters \((\eta|0\rangle\) and \(\frac{1}{2}|\eta\rangle\) [89, 90], respectively,

\[
a^\dagger_\eta\big((\frac{l}{2}, \frac{j}{2})_{m_j}\big) \mapsto a^\dagger_{\eta\frac{1}{2}}(\big((\frac{l}{2})_{m_j}\big) \mapsto a^\dagger_{\eta\frac{1}{2}}(\frac{l}{2}, \frac{j}{2})_{m_j}. \tag{83}
\]

Here, the principal quantum number \(\eta = 0, 1, 2, \ldots\) labels a harmonic oscillator shell; \(l, \frac{j}{2}\) and \(m_j\) label the orbital angular momentum, the intrinsic spin, the total angular momentum and its projection, respectively.

An SU(3) symmetry-adapted state of \(N\) fermions is thus created by acting with an SU(3)-coupled product of \(N\) fermion creation operators on the vacuum state,

\[
|f(\lambda, \mu)\kappa(\ell S)JM_J]\rangle = \left[a^\dagger_{\eta\frac{1}{2}}(\frac{l}{2}, \frac{j}{2})_{m_j}\right]^{(\lambda, \mu)}\kappa(\ell S)JM_J |\rangle = \left[a^\dagger_{\eta\frac{1}{2}}(\frac{l}{2}, \frac{j}{2})_{m_j}\right]^{(\lambda, \mu)}\kappa(\ell S)JM_J |\rangle = \left[a^\dagger_{\eta\frac{1}{2}}(\frac{l}{2}, \frac{j}{2})_{m_j}\right]^{(\lambda, \mu)}\kappa(\ell S)JM_J |\rangle. \tag{84}
\]
where \( f = \{ \eta_1, \ldots, \eta_N \} \). Now, let us consider a system of \( A \) nucleons composed by \( Z \) protons and \( N \) neutrons. A distribution of the nucleons over the harmonic oscillator shells is given by two sets of the principal quantum numbers, \( f_p = \{ \eta_1, \ldots, \eta_Z \} \) for protons and \( f_n = \{ \eta_1', \ldots, \eta_N' \} \) for neutrons. Let us further suppose that proton and neutron creation operators can be coupled to tensor operators with \((\lambda_{\pi}, \mu_{\pi})_S\pi, (\lambda_{\nu}, \mu_{\nu})_{S\nu}\) characters, respectively. The construction formula for an SU(3) basis state, \( |\xi(\rho_0(\lambda_0\mu_0)\kappa_0(L_0S_0)J_0M_0)\rangle \), in the proton–neutron formalism is given as

\[
|\xi(\rho_0(\lambda_0\mu_0)\kappa_0(L_0S_0)J_0M_0)\rangle = \left[ \mathcal{P}_{\tau,\Sigma}^{(\lambda_{\pi}, \mu_{\pi})}(a_{\pi}^\dagger) \times \mathcal{P}_{\tau,\Sigma}^{(\lambda_{\nu}, \mu_{\nu})}(a_{\nu}^\dagger) \right] |\kappa_0(0S_0)J_0M_0\rangle \quad \text{(85)}
\]

The label \( \xi = \{ f_\pi, (\lambda_{\pi}, \mu_{\pi})_S\pi, f_\nu, (\lambda_{\nu}, \mu_{\nu})_{S\nu}\} \) schematically denotes additional quantum numbers included to distinguish different distributions of nucleons over the harmonic oscillator shells and different symmetry coupling of protons and neutrons, \( \rho_0 \) gives the multiplicity of \((\lambda_0\mu_0)\) for a given \( \xi \) set of quantum numbers (hereafter, \( \xi \) and \( \rho_0 \) will be omitted from the labeling), and \( \mathcal{P}_{\tau,\Sigma}^{(\lambda_{\pi}, \mu_{\pi})} \) and \( \mathcal{P}_{\tau,\Sigma}^{(\lambda_{\nu}, \mu_{\nu})} \) denote irreducible tensor operators constructed as coupled products of \( Z \) proton \((a_{\pi}^\dagger)\) and \( N \) neutron \((a_{\nu}^\dagger)\) creation operators,

\[
\mathcal{P}_{\tau,\Sigma}^{(\lambda_{\pi}, \mu_{\pi})}(a_{\pi}^\dagger) = \left[ a_{\pi}^{(1(0)0)}_{\frac{1}{2}} \times \cdots \times a_{\pi}^{(1(0)0)}_{\frac{1}{2}} \right]_{S\pi}^{(\lambda_{\pi}, \mu_{\pi})}, \quad \text{(86)}
\]

\[
\mathcal{P}_{\tau,\Sigma}^{(\lambda_{\nu}, \mu_{\nu})}(a_{\nu}^\dagger) = \left[ a_{\nu}^{(1(0)0)}_{\frac{1}{2}} \times \cdots \times a_{\nu}^{(1(0)0)}_{\frac{1}{2}} \right]_{S\nu}^{(\lambda_{\nu}, \mu_{\nu})}. \quad \text{(87)}
\]

Upon a complete uncoupling of the irreducible tensors in formulae (85)–(87), we obtain expansion in terms of products of \( A \) creation operators. When applied on the vacuum state, each term in the expansion generates an \( A \)-nucleon \( m \)-scheme state with the probability amplitude given by the corresponding coefficient in the expansion. In order to construct properly antisymmetrized symmetry-adapted states, special care must be taken to accurately accommodate the anticommutation relation for fermion creation operators, \( \{ a_{\pi}, a_{\nu}\} = 0 \). We implemented the construction formula (85) as a recursive algorithm, by making use of the formula for uncoupling SU(3) \( \supset \) SO(3) \( \supset \) SU(2) tensor operators

\[
\left[ X_{S_1}^{(\lambda_1, \mu_1)} \times Y_{S_2}^{(\lambda_2, \mu_2)} \right]_{\kappa (L, S, J, M)} = \sqrt{(2S + 1)(2L + 1)} \sum_{l_1, l_2} ((\lambda_1 \mu_1) \kappa_1 l_1 \mid (\lambda_2 \mu_2) \kappa_2 l_2 \mid (\lambda \mu) \kappa L)_{\rho} \times \sum_{m_{l_1} m_{l_2}} C_{JM}^{L} \left[ j_1 m_{l_1}, j_2 m_{l_2} \right] \sqrt{(2j_2 + 1)(2j_1 + 1)} \left[ S_1 J_1 S_2 J_2 \right] \times X_{S_1}^{(\lambda_1, \mu_1)} Y_{S_2}^{(\lambda_2, \mu_2)}. \quad \text{(88)}
\]

The symmetry-adapted states generated by the procedure described above are not translationally invariant, with the exception of those constructed within the \( 0\Omega \) model space [91]. Therefore, the symplectic handband construction procedure has to be supplemented by a method eliminating the spurious c.m. excitations.

Techniques for identification and elimination of spurious c.m. excitations in the shell model configurations using the SU(3) classification scheme and the group theoretical methods were initially proposed by Verhaar [92] and Hecht [93], respectively. The method of Verhaar relies on diagonalization of the c.m. harmonic oscillator Hamiltonian, \( \mathcal{H}_{cm} = (\mathcal{B}^1 \cdot \mathcal{B} + 3/2) \hbar \Omega \), in a space spanned by SU(3) irreps of the same rank. The eigenstates of \( \mathcal{H}_{cm} \) corresponding to an eigenvalue of \( 3/2 \hbar \Omega \) do not contain any spurious c.m. excitations and hence compose the subspace of translationally invariant irreps.
We use an alternative and simpler approach based on U(3) symmetry-preserving c.m. projection operators [88]. The method was briefly outlined by Hecht [93] but never utilized for eliminating the c.m. spuriosity from SU(3) or Sp(3, R) symmetry-adapted configurations. The projection technique is based on the fact that a general SU(3) symmetry-adapted A-particle state of \( n_{\text{max}} h \Omega \) excitations above the lowest energy configuration can be written in an SU(3)-coupled form as

\[
| (\lambda \mu) \kappa L M \rangle = \sum_{n=0}^{n_{\text{max}}} \sum_{(\lambda \mu)_{\text{intr}}} c_n^{(\lambda \mu)_{\text{intr}}} | (n0) \times (\lambda \mu)_{\text{intr}}; (\lambda \mu) \kappa L M \rangle,
\]

where \( c_n^{(\lambda \mu)_{\text{intr}}} \) denotes a probability amplitude. The SU(3) quantum numbers, \( (\lambda \mu)_{\text{intr}} \), label the intrinsic wavefunctions of \( (n_{\text{max}} - n) \bar{h}/\Omega \) excitations that are coupled with the c.m. SU(3) irreps \( (n0) \) of \( n\bar{h}/\Omega \) excitations into the final SU(3) symmetry \( (\lambda \mu) \kappa L M \). Note that for the non-spurious part of the state, \( n = 0 \), the quantum numbers \( (\lambda \mu)_{\text{intr}} \) coincide with \( (\lambda \mu) \).

In order to eliminate the c.m. spuriosity from A-particle SU(3)-symmetric states one needs to project out all the \( n \geq 1 \) terms on the right-hand side of the expansion (89) as they describe excited c.m. motion. This is done by employing the simplest U(3) Casimir invariant, namely, the c.m. number operator,

\[
\hat{N}_{c,m} = \mathfrak{B}^\dagger \cdot \mathfrak{B},
\]

in a U(3) symmetry-preserving projecting operator,

\[
\hat{P}(n_{\text{max}}) = \prod_{k=1}^{n_{\text{max}}} \left( 1 - \frac{\hat{N}_{c,m}}{k_0} \right),
\]

The \( | (n0) \times (\lambda \mu)_{\text{intr}}; (\lambda \mu) \kappa L M \rangle \) states (89) are eigenstates of \( \hat{N}_{c,m} \) with eigenvalues \( n \). Therefore, they are also eigenstates of the \( \hat{P}(n_{\text{max}}) \) operator with eigenvalues equal to 0 for excitations \( n = 1, \ldots, n_{\text{max}} \) and 1 when \( n = 0 \), which corresponds to a non-spurious state. Therefore, the c.m. spurious excitations vanish under the action of \( \hat{P}(n_{\text{max}}) \), while a non-spurious state (or the spurious-free part of a state) remains unaltered. The non-spurious states, which are obtained after the projection, are properly orthonormalized and then utilized in the calculations.

The projection operator \( \hat{P}(n_{\text{max}}) \) is a scalar with respect to SU(3) and SUS(2), and hence it preserves \( (\lambda_0 \mu_0)_{\text{intr}}; (L_0 S_0) J_0 M_0 \) quantum labels. However, it mixes the additional quantum numbers, denoted in the construction formula (85) as \( \xi \), which are included to distinguish between a different construction for protons and neutrons.

### 6.2. Symplectic basis construction formula

Although one is tempted to implement the construction formula (80) straightforwardly as the action of polynomials in the \( A_{LM}^{(20)} \) raising operators on a symplectic bandhead, such an approach is not advisable as it becomes computationally cumbersome for higher-\( \bar{h}/\Omega \) subspaces. There are two main reasons for this. First, a \( k \)th-degree polynomial in \( A_{LM}^{(20)} \) represents a \( 2k \)-body operator, which leads to highly complex calculations for \( k \gg 1 \). The second reason is that each symplectic state belonging to a \( N\bar{h}/\Omega \) subspace is a linear combination of nearly all \( N\bar{h}/\Omega \) \( m \)-scheme states, and besides elaborate polynomial operators, as a consequence we, too, would be faced with the scale explosion problem.

An alternative approach is to transform the symplectic construction formula into a recursive relation [71, 86] that allows one to construct a symplectic state of excitation \( N_{\bar{h}}/\Omega \)
by the action of the $A^{(20)}_{LM}$ raising operators on a special linear combination of symplectic states of excitation $(N_\omega - 2)\hbar \Omega$:

$$\langle \sigma \rho \omega \kappa | (L, S_\sigma); J M J \rangle = (-1)^{S_\sigma \sqrt{2L+1}} \sum_{L' M'} U[(20)\ell' \omega \sigma; n1 \rho; \omega' \rho'] \times \sum_{L' M'} C^{(20)}_{LM} \sum_{\omega' k' L'} \langle (20)\ell' \omega \sigma \rightarrow \omega' k' L' \rangle \times \sum_{L' M'} \langle L' S_\sigma | J M J \rangle \times \sum_{M'} C^{M'}_{J M J \ell' \omega} \langle \sigma n' \rho' \omega' k' | (L' S_{\sigma}); J M J \rangle.$$ (92)

Such a recursive scheme makes a parallel implementation rather straightforward and, at the same time, it is computationally less expensive as it enables one to utilize results obtained in the previous step. The starting case is the $m$-scheme expansion of a symplectic bandhead, $\langle \sigma \kappa_0 | (L_0 S_{\sigma}); J_0 M_0 \rangle$, upon which we apply formula (92) to obtain symplectic states of excitation $(N_\omega + 2)\hbar \Omega$. The foregoing procedure is then repeated until all symplectic basis states of a given $\text{Sp}(3, \mathbb{R})$ irrep up to excitation $N_{\text{max}}\hbar \Omega$ are expanded.

For given $n, \rho, \omega, \kappa$ and $L$, the construction formula (92) can be schematically written as

$$\langle \sigma \rho \omega \kappa | (L, S_\sigma); J M J \rangle = (-1)^{S_\sigma \sqrt{2L+1}} \sum_{L' M'} U[(20)\ell' \omega \sigma; n1 \rho; \omega' \rho'] \times \sum_{L' M'} C^{(20)}_{LM} \sum_{\omega' k' L'} \langle (20)\ell' \omega \sigma \rightarrow \omega' k' L' \rangle \times \sum_{M'} C^{M'}_{J M J \ell' \omega} \langle \sigma n' \rho' \omega' k' | (L' S_{\sigma}); J M J \rangle.$$ (93)

where $\langle \sigma S_{\sigma}; J M J \rangle_{LM}$ denotes a special combination of symplectic states of excitation $N_{\text{max}}\hbar \Omega$ spanning a given $\text{Sp}(3, \mathbb{R})$ irrep $\sigma$ and carrying the total intrinsic spin $S_{\sigma}$. This state is obtained as

$$\langle \sigma S_{\sigma}; J M J \rangle_{LM} = \sum_{\omega' k' L'} U[(20)\ell' \omega \sigma; n1 \rho; \omega' \rho'] \times \sum_{L' M'} \langle (20)\ell' \omega \sigma \rightarrow \omega' k' L' \rangle \times \sum_{M'} C^{M'}_{J M J \ell' \omega} \langle \sigma n' \rho' \omega' k' | (L' S_{\sigma}); J M J \rangle.$$ (94)

The construction algorithm is notably simple. For each value of $L$ and $M$ we construct $\langle \sigma S_{\sigma}; J M J \rangle_{LM}$ according to the prescription (94), and then apply the symplectic raising operator $A^{(20)}_{LM}$. In this way we produce five states of excitation $(N_\omega + 2)\hbar \Omega$ spanning the irrep $\sigma S_{\sigma}$. These states are added and multiplied by the phase factor $(-1)^{S_\sigma \sqrt{2L+1}}$ yielding the resulting symplectic state $\langle \sigma \rho \omega \kappa | (L, S_{\sigma}); J M J \rangle$.

The parallel implementation of this procedure is schematically depicted in figure 6. At the beginning, each process is assigned with a particular set of $N_{\text{max}}\hbar \Omega$-scheme states, so that $\langle \sigma S_{\sigma}; J M J \rangle_{LM}$ is split evenly among collaborating processes. In the next step, every process applies the $A^{(20)}_{LM}$ operator on the part of $\langle \sigma S_{\sigma}; J M J \rangle_{LM}$ it maintains (step 1 in figure 6), and obtains a certain linear combination of $(N_\omega + 2)\hbar \Omega$ $m$-scheme states. Some of the resulting $m$-scheme configurations, as indicated in figure 6, occur simultaneously in other processes’ results. In the last step, these ‘overlapping’ $m$-scheme states are redistributed so that at the end each process retains a linear combination of unique configurations (step 2 in figure 6). This represents the most time consuming part of the algorithm due to a large amount of data to be interchanged.
7. Structure of the lowest-lying states of $^{12}$C and $^{16}$O nuclei

In this section, we briefly discuss the structure of the lowest-lying states in $^{12}$C and $^{16}$O as determined by previous theoretical investigations.

The investigations of $^{12}$C and $^{16}$O nuclei structures are relevant for a wide range of physical processes. The latter include parity violating electron scattering from light nuclei \([94–97]\) where targets like $^{12}$C are of particular interest. Accurate microscopic wavefunctions obtained through the \textit{ab initio} NCSM can also provide valuable input for neutrino studies as $^{12}$C is an ingredient of liquid scintillator detectors \([98]\) and $^{16}$O is the main component of water Čerenkov detectors. Light nuclei with equal numbers of protons and neutrons ($N = Z$) and total particle numbers that are multiples of four ($4n\rangle$ display a complex pattern in their low-lying energy spectra with certain states continuing to remain a challenge for \textit{ab initio} techniques. An important example of such a configuration is the first excited 0$^+$ state in $^{12}$C, the Hoyle state, which is essential for a key reaction of stellar nucleosynthesis: the production of $^{12}$C nucleus through the triple-$\alpha$ reaction mechanism \([99, 100]\). Another is the highly deformed first excited 0$^+$ state of $^{16}$O.

The \textit{ab initio} NCSM calculations of $^{12}$C nucleus with the CD-Bonn and JISP16 interactions in the $4\hbar/O$ \([1, 2]\) and the $6\hbar/O$ \([4]\) model spaces have achieved reasonable convergence of the states dominated by $0\hbar/O$ configurations, e.g. the $J = 0^+_0$ and the lowest $J = 2^+(\equiv 2^+_1)$ and $J = 4^+(\equiv 4^+_1)$ states of the ground-state rotational band, as seen in figure 7. In addition, calculated binding energies and other observables such as ground-state proton root-mean-square (rms) radii and the $2^+_1$ quadrupole moment all lie reasonably close to the measured values (see table 2). The electromagnetic transition strengths, $B(E2; 2^+_0 \rightarrow 0^+_0)$, $B(E2; 2^+_1 \rightarrow 0^+_0)$, and $B(M1; 1^+_1 \rightarrow 0^+_0)$, are still underestimated, yielding just over 60% of the corresponding experimental strengths. Note that these physical observables were obtained using bare operators. The additional contributions are expected to arise from excluded, high-$\hbar/O$ basis states, which produce more complete formation of the exponential tails of the wavefunctions to which these observables are sensitive.

In contrast, the low-lying $\alpha$-clustering states, such as the Hoyle state, cannot be reproduced by the NCSM. The structure of the Hoyle state is crucial for accurate prediction of the
Figure 7. Experimental and calculated low-lying spectra of $^{12}\text{C}$ for increasing size of the model space. The NCSM results were obtained using the effective interactions derived from the JISP16 nucleon–nucleon potential with $\hbar/\Omega = 15$ MeV.

Table 2. Comparison of the experimental data of $^{12}\text{C}$ with the results obtained by the NCSM calculation in the $N_{\text{max}} = 6$ model space using the effective interaction derived from the JISP16 with $\hbar/\Omega = 12.5$ MeV and $\hbar/\Omega = 15$ MeV. Non-converged states are labeled ‘N/C’.

<table>
<thead>
<tr>
<th></th>
<th>Exp</th>
<th>$\hbar/\Omega = 12.5$</th>
<th>$\hbar/\Omega = 15$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>E_{gs}</td>
<td>$ (MeV)</td>
<td>92.162</td>
</tr>
<tr>
<td>$r_p$ (fm)</td>
<td>2.35(2)</td>
<td>2.334</td>
<td>2.183</td>
</tr>
<tr>
<td>$Q_{2+}$ (e fm$^2$)</td>
<td>+6(3)</td>
<td>5.213</td>
<td>4.478</td>
</tr>
<tr>
<td>$E_x(0^+0)$ (MeV)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$E_x(2^+0)$ (MeV)</td>
<td>4.439</td>
<td>3.790</td>
<td>4.029</td>
</tr>
<tr>
<td>$E_x(0^+0)$ (MeV)</td>
<td>7.654</td>
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<td>N/C</td>
</tr>
<tr>
<td>$E_x(2^+0)$ (MeV)</td>
<td>11.160</td>
<td>N/C</td>
<td>N/C</td>
</tr>
<tr>
<td>$E_x(1^+0)$ (MeV)</td>
<td>12.710</td>
<td>13.807</td>
<td>13.921</td>
</tr>
<tr>
<td>$E_x(4^+0)$ (MeV)</td>
<td>14.083</td>
<td>13.467</td>
<td>14.490</td>
</tr>
<tr>
<td>$E_x(1^+1)$ (MeV)</td>
<td>15.110</td>
<td>15.927</td>
<td>17.124</td>
</tr>
<tr>
<td>$E_x(2^+1)$ (MeV)</td>
<td>16.106</td>
<td>17.893</td>
<td>19.947</td>
</tr>
<tr>
<td>$B(E2;2^+0 \rightarrow 0^+0)$</td>
<td>7.59(42)</td>
<td>6.213</td>
<td>4.631</td>
</tr>
<tr>
<td>$B(M1;1^+0 \rightarrow 0^+0)$</td>
<td>0.0145(21)</td>
<td>0.005</td>
<td>0.007</td>
</tr>
<tr>
<td>$B(M1;1^+1 \rightarrow 0^+0)$</td>
<td>0.951(20)</td>
<td>0.385</td>
<td>0.588</td>
</tr>
<tr>
<td>$B(E2;2^+1 \rightarrow 0^+0)$</td>
<td>0.65(13)</td>
<td>0.364</td>
<td>0.393</td>
</tr>
</tbody>
</table>

triple-$\alpha$ reaction rate [99]. The $\alpha$–cluster models and the fermionic molecular dynamics model have been more successful in reproducing the properties of this state [76, 79, 80, 101–103]. However, they have not produced results accurate enough to yield the triple-$\alpha$ reaction rate with sufficient precision [104], and thus the structure of the Hoyle state still represents an ultimate challenge for nuclear structure physics.
The $0\hbar \Omega$ configurations of $^{12}$C have four protons and four neutrons distributed over the valence p-shell. Such configurations of valence nucleons give rise to the leading $(04)$ SU(3) irrep describing an oblate deformed nuclear shape. The Elliott SU(3) model of nuclear rotations describes the states of the ground-state rotational band of $^{12}$C solely in terms of the leading $(04)$ SU(3) irrep basis states, and studies performed within the framework of the symplectic shell model reflect this assumption. Symplectic algebraic approaches with the model space restricted to the single $Sp(3, \mathbb{R})$ irrep built over the leading $(04)$ bandhead have achieved a good reproduction of the ground-state rotational band energies and B(E2) values using phenomenological interactions [105] or truncated symplectic basis with simplistic (semi-)microscopic interactions [106–108].

In contrast to $^{12}$C, where several calculated results are found to reproduce the experimental data quite well, $6\hbar \Omega$ NCSM calculations for $^{16}$O with the JISP16 and CD-Bonn interactions only yield reasonable results for the ground-state binding energy [4, 5].

Unlike the ground state, the excited $0^+$ states of the double-magic nuclei are usually strongly deformed [109] which can be attributed to a superposition of low-lying, strongly favored multiple-particle–multiple-hole configurations [110–112]. Perhaps the simplest example is the highly deformed first excited $0^+_2$ state of $^{16}$O where $4p^-4h$ configurations were recognized to be prominent in [111]. Later theoretical investigations suggested a dominant $4p^-4h$ character, albeit with some admixture of $0p-0h$ and $2p-2h$ configurations [113–119]. Very large model spaces, well beyond the current computational limits, are needed for an accurate description of low-lying deformed $0^+$ states. The current ab initio methods such as the $6\hbar \Omega$ NCSM [4, 5] or coupled cluster calculations [120] fail to reproduce the observed excitation energies of the low-lying exited $0^+$ states of $^{16}$O.

At the same time, it is also well established that the first and the second excited $0^+$ states in $^{16}$O have a pronounced $\alpha$-cluster structure [82, 81]. Both states are well described by the microscopic $\alpha$-$^{12}$C cluster model [78, 83] whose wavefunctions were found to overlap at a significant level with the basis states of the leading $4\hbar \Omega$ $4p^-4h$ \((\lambda, \mu) = (84)\) and $2\hbar \Omega$ $2p^-2h$ \((\lambda, \mu) = (42)\) $Sp(3, \mathbb{R})$ irreps [85, 121, 84]. Recently, the coupled-SU(3) algebraic model [122] calculations confirm the significant role of these two leading symplectic irreps [123].

8. Dominant role of $0p-0h$ symplectic irreps

In this section, the role of $0p-0h$ symplectic $Sp(3, \mathbb{R})$ irreps in the lowest-lying states of $^{16}$O and the ground-state rotational band of $^{12}$C is considered [87]. The lowest-lying eigenstates of $^{12}$C and $^{16}$O nuclei were calculated using the $ab$ initio NCSM as implemented through the many-fermion dynamics (MFD) code [124, 125] with an effective interaction derived from the realistic JISP16 nucleon–nucleon potential [38] for different $\hbar \Omega$ oscillator strengths, and also using the bare JISP16 interaction; that is, without taking into account effects of the excluded configurations. In our analysis, we are particularly interested in the $J = 0^+_g$ and the lowest $J = 2^+ (\equiv 2^+_7)$ and $J = 4^+ (\equiv 4^+_5)$ states of the ground-state rotational band of $^{12}$C, and also the ground state of $^{16}$O, which all appear to be relatively well converged in the $N_{\text{max}} = 6$ model space. These states are projected onto translationally invariant basis states of $0p-0h$ $Sp(3, \mathbb{R})$ irreps.

8.1. Ground-state rotational band in $^{12}$C nucleus

For $^{12}$C there are 13 distinct $SU(3) \otimes SU_6(2)$ irreps at the $0\hbar \Omega$ space, listed in table 3, which form the symplectic bandheads with $N_\sigma = 24.5$. For each bandhead we generated $Sp(3, \mathbb{R})$
irrep basis states with the total angular momentum $J = 0, 2$ and $4$ up to $6\hbar\Omega$ space and expanded these symplectic states in the $m$-scheme basis. We then projected the NCSM eigenstates of the ground-state rotational band onto the symplectic model space.

Analysis of overlaps of the symplectic states with the NCSM eigenstates for the $0^+_g$, and the lowest $2^+$ and $4^+$ states reveals non-negligible overlaps for only 3 out of the 13 $0p-0h$ Sp(3, $\mathbb{R}$) ($N_\sigma = 24.5$) irreps. Specifically, the leading (most deformed) representation $(\lambda_\sigma \mu_\sigma)_{S_\sigma} = (04)$ carrying spin $S_\sigma = 0$ together with the two irreps of identical labels $(\lambda_\sigma \mu_\sigma)_{S_\sigma} = (12)$ and spin $S_\sigma = 1$ with different bandhead constructions for protons and neutrons as indicated in table 3. Had we adopted the isospin formalism, we would have obtained two $(12)S_\sigma = 1$ irreps, one with isospin $T = 0$ and the other with $T = 1$. In this case, only one of the two $S_\sigma = 1(12)$ irreps is expected to significantly contribute ($T = 0$), while the other state of definite isospin may only slightly mix because of the presence of the Coulomb interaction.

The overlaps of the most dominant symplectic states with the NCSM eigenstates for the $0^+_g$, $2^+_1$ and $4^+_1$ states in the $0, 2, 4$ and $6\hbar\Omega$ subspaces are given for $\hbar\Omega = 12$ MeV (table 4) and $\hbar\Omega = 15$ MeV (table 5). In order to speed up the calculations, we retained only the largest amplitudes of the NCSM states, those sufficient to account for at least 98\% of the norm which is also quoted in the tables. The results show that typically more than 80\% of

| Table 3. 0p-0h Sp(3, $\mathbb{R}$) irreps in $^{12}$C, $N_\sigma = 24.5$. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $(\lambda_\sigma \mu_\sigma)_{S_\sigma}$ ⊗ $(\lambda_\mu_\nu)_{S_\nu}$ → $(\lambda_\mu_\nu)_{S_\sigma}$ |
| $0^+_g$       | $0^+_g$         | $0^+_g$         | $0^+_g$         |
| $(02)S_\sigma = 0$ | $(02)S_\sigma = 0$ | $(04)(12)(20)$ | 0               |
| $(02)S_\sigma = 0$ | $(10)S_\sigma = 1$ | $(01)(12)$     | 1               |
| $(10)S_\sigma = 1$ | $(02)S_\sigma = 0$ | $(01)(12)$     | 1               |
| $(10)S_\sigma = 1$ | $(10)S_\sigma = 1$ | $(01)(20)$     | 0, 1, 2         |

| Table 4. Probability distribution of NCSM eigenstates for $^{12}$C across the dominant 3 0p-0h Sp(3, $\mathbb{R}$) irreps, $\hbar\Omega = 12$ MeV. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
|                | $0\hbar\Omega$ | $2\hbar\Omega$ | $4\hbar\Omega$ | $6\hbar\Omega$ |
| $J = 0$         |                 |                 |                 |                 |
| $(04)S_\sigma = 0$ | 41.39           | 19.66           | 8.73            | 3.14            | 72.92          |
| $(12)S_\sigma = 1$ | 2.24            | 1.49            | 0.80            | 0.41            | 4.94           |
| $(12)S_\sigma = 1$ | 2.19            | 1.46            | 0.78            | 0.41            | 4.84           |
| Total           | 45.82           | 22.61           | 10.31           | 3.96            | 82.70          |
| NCSM            | 45.90           | 27.41           | 15.89           | 9.03            | 98.23          |
| $J = 2$         |                 |                 |                 |                 |
| $(04)S_\sigma = 0$ | 41.20           | 19.34           | 8.44            | 3.06            | 72.04          |
| $(12)S_\sigma = 1$ | 2.50            | 1.51            | 0.77            | 0.38            | 5.16           |
| $(12)S_\sigma = 1$ | 2.42            | 1.47            | 0.75            | 0.37            | 5.01           |
| Total           | 46.12           | 22.32           | 9.96            | 3.81            | 82.21          |
| NCSM            | 46.19           | 27.10           | 15.76           | 9.25            | 98.30          |
| $J = 4$         |                 |                 |                 |                 |
| $(04)S_\sigma = 0$ | 44.21           | 19.23           | 8.01            | 2.91            | 74.36          |
| $(12)S_\sigma = 1$ | 1.69            | 0.90            | 0.44            | 0.21            | 3.24           |
| $(12)S_\sigma = 1$ | 1.68            | 0.89            | 0.43            | 0.21            | 3.21           |
| Total           | 47.59           | 21.02           | 8.88            | 3.33            | 80.81          |
| NCSM            | 47.59           | 25.87           | 15.24           | 9.46            | 98.16          |
The most deformed irrep \((04)S_\sigma = 0\) is clearly dominant. Its overlap with all three NCSM eigenstates ranges from about 65\% for \(h\Omega = 18\) MeV to 75\% for \(h\Omega = 11\) MeV. This reveals the significance of the \((04)S_\sigma = 0\) irrep, which in the framework of the symplectic shell model gives rise to a prominent \(J = 0, 2\) and 4 rotational structure and hence suitable for a microscopic description of the ground-state rotational band in \(_{12}\)C \([105]\). Clearly, the restriction of the early symplectic shell model calculations upon the single \((04)\) leading Sp(3, \(R\)) irrep turns to be a reasonable approximation. The outcome also demonstrates that the dominance of the three symplectic irreps is consistent throughout the band. The mixing of the two \((12)S_\sigma = 1\) irreps is comparatively much smaller for all the three \(0^+_g, 2^+_l\) and \(4^+_l\) states, yet it may affect electric quadrupole transitions from higher-lying \(J = 0, 2\) and 4 states toward the ground-state band.

Examination of the role of the model space truncation specified by \(N_{\text{max}}\) reveals that the general features of all outcomes are retained as the space is expanded from \(2h\Omega\) to \(6h\Omega\) (see, e.g., figure 8 for the \(0^+_g\)). This includes a strong dominance of the most deformed \((04)S_\sigma = 0\) irrep as well as the continued importance of the next most important \((12)S_\sigma = 1\) \(0\Omega\) irreps. In particular, the same three Sp(3, \(R\)) irreps dominate for all \(N_{\text{max}}\) values with the large overlaps of the NCSM eigenstates with the leading symplectic irreps preserved, albeit distributed outward across higher \(h\Omega\) excitations as the number of active shells increases. The \(0^+_g\) and \(2^+_l\) states, constructed in terms of the three Sp(3, \(R\)) irreps with probability amplitudes defined by the overlaps with the \(_{12}\)C NCSM wavefunctions, were also used to determine \(B(E2)\) transition rates. These quantities are typically less accurately reproduced by \textit{ab initio} methods with realistic interactions. The Sp(3, \(R\)) \(B(E2 : 2^+_l \rightarrow 0^+_g)\) values clearly reproduce the NCSM results, namely they slightly increase from 101\% to 107\% of the corresponding NCSM numbers with

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### Table 5. Probability distribution of NCSM eigenstates for \(_{12}\)C across the dominant 3 0p-0h Sp(3, \(R\)) irreps, \(h\Omega = 15\) MeV.

<table>
<thead>
<tr>
<th>(J)</th>
<th>(0\Omega)</th>
<th>(2\Omega)</th>
<th>(4\Omega)</th>
<th>(6\Omega)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>(J = 0)</td>
<td>((04)S_\sigma = 0)</td>
<td>46.26</td>
<td>12.58</td>
<td>4.76</td>
<td>1.24</td>
</tr>
<tr>
<td></td>
<td>((12)S_\sigma = 1)</td>
<td>4.80</td>
<td>2.02</td>
<td>0.92</td>
<td>0.38</td>
</tr>
<tr>
<td></td>
<td>((12)S_\sigma = 1)</td>
<td>4.72</td>
<td>1.99</td>
<td>0.91</td>
<td>0.37</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>55.78</td>
<td>16.59</td>
<td>6.59</td>
<td>1.99</td>
</tr>
<tr>
<td>NCSM</td>
<td></td>
<td>56.18</td>
<td>22.40</td>
<td>12.81</td>
<td>7.00</td>
</tr>
<tr>
<td>(J = 2)</td>
<td>((04)S_\sigma = 0)</td>
<td>46.80</td>
<td>12.41</td>
<td>4.55</td>
<td>1.19</td>
</tr>
<tr>
<td></td>
<td>((12)S_\sigma = 1)</td>
<td>4.84</td>
<td>1.77</td>
<td>0.78</td>
<td>0.30</td>
</tr>
<tr>
<td></td>
<td>((12)S_\sigma = 1)</td>
<td>4.69</td>
<td>1.72</td>
<td>0.76</td>
<td>0.30</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>56.33</td>
<td>15.90</td>
<td>6.09</td>
<td>1.79</td>
</tr>
<tr>
<td>NCSM</td>
<td></td>
<td>56.63</td>
<td>21.79</td>
<td>12.73</td>
<td>7.28</td>
</tr>
<tr>
<td>(J = 4)</td>
<td>((04)S_\sigma = 0)</td>
<td>51.45</td>
<td>12.11</td>
<td>4.18</td>
<td>1.04</td>
</tr>
<tr>
<td></td>
<td>((12)S_\sigma = 1)</td>
<td>3.04</td>
<td>0.95</td>
<td>0.40</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td>((12)S_\sigma = 1)</td>
<td>3.01</td>
<td>0.94</td>
<td>0.39</td>
<td>0.15</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>57.50</td>
<td>14.00</td>
<td>4.97</td>
<td>1.34</td>
</tr>
<tr>
<td>NCSM</td>
<td></td>
<td>57.64</td>
<td>20.34</td>
<td>12.59</td>
<td>7.66</td>
</tr>
</tbody>
</table>
increasing $\hbar \Omega$ (figure 9). Both theoretical estimates for $\hbar \Omega = 11$ MeV agree, at the 2% level, with the measured value of 7.59 $e^2$ fm$^4$, while they underestimate the experiment for larger oscillator strengths where highly deformed configurations are energetically less favorable. In addition, if only the leading most deformed ($0^4$) Sp($3, R$) irrep is considered, that is without the mixing due to both ($12$) $S_\sigma = 1$ irreps, the $B(E2 : 2^+_1 \rightarrow 0^+_g)$ values increase only by 5–12%. In this regard, note that in addition to its large projection onto the realistic eigenstates, the leading ($04$)Sp($3, R$) irrep is sufficient for a good reproduction of the NCSM B(E2) estimate.

8.2. Ground state in $^{16}$O nucleus

A closed-shell nucleus has only one possible 0p-0h Sp($3, R$) irrep with a symplectic bandhead coinciding with the single closed-shell Slater determinant. In the case of $^{16}$O the single Sp($3, R$) irrep has the following quantum labels: $N_{\sigma} = 34.5$, $(\lambda_{\sigma} \mu_{\sigma}) = (00)$ and $S_{\sigma} = 0$. As in the $^{12}$C case, we generated translationally invariant basis states for this irrep according to formula (92) up to $6\hbar \Omega$ subspace.
Figure 10. Probability distribution for the (a) $0^+_g$, (b) $2^+_1$ and (c) $4^+_1$ states in $^{12}\text{C}$ and (d) $0^+_g$ in $^{16}\text{O}$ over $0\hbar/\Omega$ (blue, lowest) to $6\hbar/\Omega$ (green, highest) subspaces for the most dominant 0p-0h \( \text{Sp}(3, \mathbb{R}) \) irreps case (left) and NCSM (right) together with the \((04)\) irrep contribution (black diamonds) in $^{12}\text{C}$ as a function of the $\hbar/\Omega$ oscillator strength in MeV for $N_{\text{max}}=6$.

Table 6. Probability distribution of the NCSM ground state in $^{16}\text{O}$ obtained with (a) $\hbar/\Omega = 12$ MeV and (b) $\hbar/\Omega = 15$ MeV across the 0p-0h \( \text{Sp}(3, \mathbb{R}) \) irrep.

<table>
<thead>
<tr>
<th>$\hbar/\Omega$</th>
<th>0\hbar/\Omega</th>
<th>2\hbar/\Omega</th>
<th>4\hbar/\Omega</th>
<th>6\hbar/\Omega</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Sp}(3, \mathbb{R}) ) \ $(00)S_\sigma = 0$</td>
<td>38.73</td>
<td>23.92</td>
<td>11.89</td>
<td>5.28</td>
<td>79.82</td>
</tr>
<tr>
<td>NCSM</td>
<td>38.73</td>
<td>28.78</td>
<td>18.80</td>
<td>12.66</td>
<td>98.97</td>
</tr>
<tr>
<td>$\hbar/\Omega = 15$ MeV</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \text{Sp}(3, \mathbb{R}) ) \ $(00)S_\sigma = 0$</td>
<td>50.53</td>
<td>15.87</td>
<td>6.32</td>
<td>2.30</td>
<td>75.02</td>
</tr>
<tr>
<td>NCSM</td>
<td>50.53</td>
<td>22.58</td>
<td>14.91</td>
<td>10.81</td>
<td>98.83</td>
</tr>
</tbody>
</table>

Consistent with the outcome for $^{12}\text{C}$, the projection of the ground state onto the symplectic basis reveals a large \( \text{Sp}(3, \mathbb{R}) \)-symmetric content in the ground-state wavefunction (table 6). Here, we again retained only the largest amplitudes of the NCSM states, those sufficient to account for at least 98% of the norm. The results show that 75–80% of the NCSM ground state fall within a subspace spanned by the leading 0p-0h \( \text{Sp}(3, \mathbb{R}) \) irrep \( (00)S_\sigma = 0 \) and this overlap is increasing with decreasing value of $\hbar/\Omega$.

8.3. Relevance of Elliott SU(3) model

The results can also be interpreted as a further strong confirmation of the Elliott SU(3) model since the projection of the NCSM states onto the $0\hbar/\Omega$ space (figure 10, blue (right) bars) is a
projection of the NCSM results onto the wavefunctions of the SU(3) model. For example, for $^{12}$C the $0h\Omega$ SU(3) symmetry ranges from just over 40% of the NCSM $0^+_\text{gs}$ for $h\Omega = 11$ MeV to nearly 65% for $h\Omega = 18$ MeV (figure 10, blue (left) bars) with 80–90% of this symmetry governed by the leading $0^4$ irrep. These numbers are consistent with what has been shown to be a dominance of the leading SU(3) symmetry for SU(3)-based shell-model studies with realistic interactions in $0h\Omega$ model spaces. It seems the simplest of the Elliott collective states can be regarded as a good first-order approximation in the presence of realistic interactions, whether the latter is restricted to a $0h\Omega$ model space or the richer multi-$h\Omega$ NCSM model spaces.

9. Multiple-particle–multiple-hole symplectic irreps

Comparison of Sp$(3, \mathbb{R})$ symmetry-adapted and $\alpha$-cluster wavefunctions indicates that the restriction of the symplectic model subspace to the dominant $0p-0h$ irreps is not sufficient to describe highly deformed states with a pronounced $\alpha$-cluster structure [84, 85, 121, 126]. We therefore augmented the symplectic model space with symplectic irreps built over all $2h\Omega 2p-2h$ and the most deformed $4h\Omega 4p-4h$ Sp$(3, \mathbb{R})$ bandheads and analyzed their role for description of the given realistic NCSM eigenstates [88].

The total number of the $2h\Omega 2p-2h$ symplectic bandheads is around $10^3$ in the case of $^{12}$C, and approximately half of this amount for $^{16}$O. However, similar to the case of 0p-0h symplectic bandheads, only a relatively small fraction of the $2h\Omega 2p-2h$ symplectic bandheads project at the non-negligible level onto the low-lying NCSM wavefunctions. Specifically, the projection yields 20 most dominant $2h\Omega 2p-2h$ symplectic bandheads. These bandheads are then utilized to generate the corresponding Sp$(3, \mathbb{R})$ translationally invariant irreps up to $N_{\text{max}} = 6$ ($6h\Omega$ model space).

9.1. Ground-state rotational band in $^{12}$C nucleus

In the case of $^{12}$C, the expansion of the 0p-0h symplectic model subspace to include the most important $2h\Omega 2p-2h$ Sp$(3, \mathbb{R})$ irreps improves the overlaps between the NCSM eigenstates for the $J = 0, 2$ and 4 states in the ground-state rotational band and the Sp$(3, \mathbb{R})$-symmetric basis by about 5% (figure 11). (Note that for these states the $4h\Omega 4p-4h$ symplectic irreps are found to be negligible.) Overall, approximately 85% of the NCSM eigenstates fall within a subspace spanned by the most-significant 3 0p-0h and 20 2h\Omega 2p-2h Sp$(3, \mathbb{R})$ irreps. As one varies the $h\Omega$ oscillator strength, the projection changes slightly reaching close to 90% for $h\Omega = 11$ MeV (figures 11 and 12).

Among the $2h\Omega 2p-2h$ symplectic irreps, those with bandheads specified by the $(\lambda, \mu)$ quantum numbers (24) and (13) play the most important role, followed by the (62) irrep. The significance of the first two $(\lambda, \mu)$ sets, in addition to the 0p-0h Sp$(3, \mathbb{R})$ irrep contribution, indicate a propensity of the $2h\Omega$ components in the NCSM ground-state band toward oblate deformed shapes. However, the most prolate deformed configuration is also embraced as suggested by projection onto the (62) class of the symplectic bandheads. The symplectic excitations above the relevant Sp$(3, \mathbb{R})$ bandheads point to the development of a more complex shape structure as seen, for example, in figure 13 for the $^{12}$C ground state. Among these, the stretched symplectic states appear to be of a special interest as they usually possess larger overlaps with the realistic states under consideration as compared to the other symplectic excitations. The stretched states are those with $\mu = \mu_{\alpha}$ and maximum value of $\lambda$, namely $\lambda_{\alpha} + N_{\alpha}$ for $N_{\alpha} h\Omega$ excitations above the symplectic bandhead. These correspond to horizontal (same $\mu$) increments of two $\lambda$ units in the plane of figure 13 starting from the bandhead.
configuration. The dominance of the highly deformed symplectic states within the most important $2\hbar\Omega 2p-2h$ $Sp(3, \mathbb{R})$ irreps also enhances the corresponding $B(E2 : 2^+_1 \rightarrow 0^+_0)$ values.

9.2. Ground state in $^{16}$O nucleus

A much more interesting scenario is observed for the low-lying $0^+$ states in $^{16}$O. Here, the projection of the NCSM eigenstates onto the symplectic model subspace can also yield insight into the $\alpha$-cluster structure of the realistic states based on the $\alpha+^{12}$C cluster model [84, 85, 121, 126].

As compared to the outcome of the $0p-0h$ analysis, the inclusion of the $2\hbar\Omega 2p-2h$ $Sp(3, \mathbb{R})$ irreps constructed over the most significant symplectic bandheads improves the overlaps of the selected symplectic basis with the NCSM eigenstate for the $^{16}$O ground state by about 10%. As a result, the ground state in $^{16}$O as calculated by NCSM projects at the 85–90% level onto the $J = 0$ symplectic symmetry-adapted basis (figures 14 and 16(a)) with a total dimensionality of only $\approx 0.001\%$ of the NCSM space.

The $0p-0h$ symplectic model subspace analysis for the $^{16}$O ground state reveals the dominance of the $(00)S_0 = 0$ symplectic irrep, which varies from 80% down to 75% of the NCSM realistic wavefunction for values of the oscillator strength $\hbar\Omega = 12–16$ MeV, respectively. The $0\hbar\Omega$ projection of the $(00)S_0 = 0Sp(3, \mathbb{R})$ irrep reflects the spherical shape preponderance in the ground state of $^{16}$O (figure 15(a)), specifically around 40–55% for the
same $\hbar\Omega$ range. In addition, a relatively significant mixture of slightly prolate deformed shapes are observed and they are predominantly associated with stretched symplectic excitation states (along the horizontal $\lambda\omega$ axis in figure 15(a)). Among them, the most significant mode with a projection onto the NCSM state of $\sim13\%$ (for $\hbar\Omega = 16$ MeV) up to $\sim25\%$ (for $\hbar\Omega = 12$ MeV) is described by the $2\hbar\Omega$ (20) $1p−1h$ and weaker $2p−2h$ $Sp(3,\mathbb{R})$-symmetric excitations built over the $(00)S_{sr} = 0$ symplectic bandhead. This $2\hbar\Omega$ (20) symplectic configuration projects at the 65% level [84] on the corresponding $\alpha+^{12}\text{C}$ cluster model wavefunction. Orthogonal to these excitations, the $(20)S_{sr} = 0$ $2p−2h$ symplectic bandhead constructed at the $2\hbar\Omega$ level are found to be the most dominant among the $2\hbar\Omega$ $2p−2h$ $Sp(3,\mathbb{R})$ bandheads when compared to the NCSM eigenstates (table 7 and figure 15(a)). This means that the appearance of the $2\hbar\Omega$ $2p−2h$ $Sp(3,\mathbb{R})$ bandheads in the ground state of $^{16}\text{O}$ is governed in such a way to preserve the shape coherence of all the significant $2\hbar\Omega$ configurations.

### 9.3. First excited $0^+$ state in $^{16}\text{O}$ nucleus

We also analyzed the symplectic structure of the $0^+_2$ NCSM eigenstate in $^{16}\text{O}$, which likewise was calculated using the JISP16 interaction in a $N_{\text{max}} = 6$ space. This state is of a special interest because its microscopic description requires one to take into account highly deformed spatial multiple-particle–multiple-hole configurations. We therefore focused our investigation.
on determining whether such highly deformed multiple-particle–multiple-hole symplectic irreps are realized within the NCSM eigenstate. It is important to note that this state is not fully converged and the 6ℏΩ model space is quite restrictive for the development of strong 4p−4h correlations. This is because a very limited range of shells is accessed in the 4p−4h excitations, specifically, the sd and the pf shells for \( N_{\text{max}} = 6 \) 4p−4h configurations. Note that only two particles can reach the pf shell under the \( N_{\text{max}} = 6 \) constraint.

The results indicate that the 0\( ^+_1 \) NCSM eigenstate is dominated by the 2ℏΩ configurations composing 45−55% of the wavefunction. This is different from what we have observed in the \( ^{12}\text{C} \) ground-state rotational band and the \( ^{16}\text{O} \) ground state that are mostly governed by \( 0\hbar\Omega \)
configurations with a clear dominance of the 0p-0h Sp(3, R) irreps. The projection of this NSCM wavefunction onto the symplectic basis reveals, for the first time, a large contribution of the 2Ω 2p−2h Sp(3, R) irreps (see table 7 and figure 16(b)). This contribution tends to decrease with increasing hΩ oscillator strength. It reaches 47% for hΩ = 12 MeV and declines down to 33% for hΩ = 16 MeV, with a clear dominance of the leading, (42), 2Ω 2p−2h irrep (figure 15(b)). It is important to note that the bandhead of this leading irrep projects at the 100% level onto the α+12C cluster model wavefunction possessing the same, (42), SU(3) character [84]. The role of the 0p-0h Sp(3, R) irrep within the NCSM eigenstate is also important, increasing from 29% (for hΩ = 12 MeV) up to 45% (for hΩ = 16 MeV). The main contribution to this percentage comes from the (20) configuration, which has significant overlaps with the corresponding α+12C cluster model wavefunction [84]. This suggests that the cluster structure of the 0^+_2 NCSM eigenstate has already started to emerge in the 6hΩ
model space. Overall, the symplectic basis projects at the 80% level onto the first excited $0^+_2$ state, which turns to be a superposition of the $0p-0h$ and $2\hbar/Omega_1 2p-2h$ symplectic irreps.

In addition to the above, the outcome suggests that the leading most deformed $4\hbar/Omega_1 4p-4h$ symplectic irrep, $(\lambda_{\sigma} \mu_{\sigma}) = (84 \alpha)$, which is identical to the most deformed $\alpha+^{12}\text{C}$ cluster model wavefunction with the relative motion of the clusters carrying eight oscillator quanta [84], contribute rather insignificantly (0.31–0.16%) to the $6\hbar/Omega_1$-NCSM first excited $0^+_2$ state. Nevertheless, this (84) contribution is several orders of magnitude higher than the (84) contribution to the ground state, which was found to be $\approx 10^{-4}\%$. The results suggest the need for exploring the $\text{Sp-NCSM}$ scheme with model spaces beyond $N_{\text{max}} = 6$ to achieve convergence of such higher-lying collective modes.

10. Symplectic invariance within the spin parts of realistic eigenstates

As one varies the oscillator strength $\hbar/Omega_1$, the overall overlaps slightly increase toward smaller harmonic oscillator frequencies (see e.g. figures 12 and 14). In order to explain this behavior, we examined the spin components of the converged NCSM eigenstates with respect to the same spin carrying $\text{Sp}(3, \mathbb{R})$ irreps.

The NCSM eigenstates are superpositions of different spin components, and hence can be schematically written as

$$|\text{NCSM}; J M_J\rangle = \sum_{s=0}^{S_{\text{max}}} \alpha_s |S = s; J M_J\rangle.$$  \hspace{1cm} (95)

Here, $S_{\text{max}}$ signifies the maximum allowed spin for the given nucleus, e.g. $S_{\text{max}} = 6$ and 8 for $^{12}\text{C}$ and $^{16}\text{O}$ nuclei, respectively, $|S = s; J M_J\rangle$ denotes spin $S = s$ component of the NCSM eigenstate and $\alpha_s$ is the probability amplitude. We can carry out a spin decomposition of the NCSM eigenstates by making use of operator $\hat{P}(S_{\text{min}})$ defined as

$$\hat{P}(S_{\text{min}}) = \prod_{s=S_{\text{min}}}^{S_{\text{max}}} \left(1 - \frac{\hat{S}^2}{s(s+1)}\right).$$  \hspace{1cm} (96)

We performed the spin decomposition for the well-converged NCSM eigenstates, that is, the ground-state band of $^{12}\text{C}$ and the ground state of $^{16}\text{O}$. The probability amplitudes of
the spin components reveal that the renormalization of the bare interaction through the Lee–Suzuki similarity transformation for different values of $\hbar/\Omega_1$ influences the spin mixing within the NCSM eigenstates (see figure 17). The $S = 0$ part ($S = 1$ and $S = 2$ parts) of all NCSM eigenstates investigated decreases (increases) toward higher $\hbar/\Omega_1$ frequencies (figure 17). As the spin $S = 2$ components gain importance, the total projection of the NCSM eigenstates onto the symplectic space declines slightly, as there is no dominant symplectic symmetry structure within the $S = 2$ components of the investigated NCSM wavefunctions.

Another striking property is revealed when the spin projections of the converged NCSM eigenstates are examined. Specifically, the spin-zero part of all three NCSM eigenstates for $^{12}\text{C}$ is almost entirely projected (95%) onto only six $S_\sigma = 0$ symplectic irreps, with as much as 90% of the spin-zero components of the NCSM eigenstates accounted for solely by the leading $(04)$ irrep. As for the $S = 1$ part, the overlap with the two $S_\sigma = 1$ $(12)$ symplectic irreps is around 80% for the $0^+_1$ and $2^+_1$ and around 70% for $4^+_1$. Clearly, the $S = 1$ part is remarkably well described by merely two $\text{Sp}(3, \mathbb{R})$ irreps. In summary, the $S = 0$ and $S = 1$ parts of the NCSM wavefunctions are very well explained by only three $0p-0h \text{Sp}(3, \mathbb{R})$ irreps. Similar results are obtained for the ground state of $^{16}\text{O}$. The leading $S_\sigma = 0$ symplectic irrep, $(00)$, projects at the 90% level onto the $S = 0$ component of the $0^+_{gs}$ eigenstate, and the inclusion of the few most significant $2p-2h \text{Sp}(3, \mathbb{R})$ irreps increases this projection up to 95% (see figure 18).

Furthermore, as shown in figure 18, the $\text{Sp}(3, \mathbb{R})$ symmetry and hence the geometry of the nucleon system being described is nearly independent of the $\hbar/\Omega$ oscillator strength.
The symplectic symmetry is present with equal strength in the spin parts of the NCSM wavefunctions for $^{12}$C as well as $^{16}$O regardless of whether the bare or the effective interactions are used. This suggests that the Lee–Suzuki transformation, which effectively compensates for the finite space truncation by renormalization of the bare interaction, does not affect the Sp(3, $R$) symmetry structure of the spatial wavefunctions [9]. Further, these results suggest that the symplectic structure detected in the present analysis for 6$\hbar$Ω model space is what would emerge in NSCM evaluations with a sufficiently large model space to justify the use of the bare interaction.

11. Dimension of symplectic model space

The typical dimension of a symplectic irrep basis in the $N_{\text{max}} = 6$ model space is in the order of $10^2$ as compared to $10^7$ for the full NCSM m-scheme basis space. Note that if one were to include all possible Sp(3, $R$) irreps with $N\hbar\Omega - n\hbar$ bandheads ($N \leq N_{\text{max}}$), and their basis states up to $N_{\text{max}}\hbar\Omega$ subspace, one would span the entire $N_{\text{max}}\hbar\Omega$ model space. Moreover, the space spanned by a given symplectic irrep, $N_{\sigma}(J_{\sigma}, \mu_{\sigma})$, can be decomposed to subspaces of a definite total angular momentum $J$ (see equation (92)) and can be further reduced to only the subspaces specified by the $J$ values under consideration. In the case of the ground-state band
Table 8. Model spaces dimension for different maximum allowed $\hbar\Omega$ excitations, $N_{\text{max}}$, for the NCSM and the three most significant $0p-0h$ $\text{Sp}(3, \mathbb{R})$ irreps limited to $J = 0$, 2 and 4 states in $^{12}\text{C}$. For comparison, the size of the full space of the three $0p-0h$ $\text{Sp}(3, \mathbb{R})$ irreps (all $J$ values) is shown together with the $J = 0$, 2 and 4 model space dimension of all the 13 $0p-0h$ $\text{Sp}(3, \mathbb{R})$ irreps for $^{12}\text{C}$.

<table>
<thead>
<tr>
<th>$N_{\text{max}}$</th>
<th>NCSM</th>
<th>3 $\text{Sp}(3, \mathbb{R})$ irreps</th>
<th>3 $\text{Sp}(3, \mathbb{R})$ irreps</th>
<th>13 $\text{Sp}(3, \mathbb{R})$ irreps</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$J = 0, 2, 4$</td>
<td>all $J$</td>
<td>$J = 0, 2, 4$</td>
</tr>
<tr>
<td>0</td>
<td>51</td>
<td>13</td>
<td>21</td>
<td>30</td>
</tr>
<tr>
<td>2</td>
<td>$1.77 \times 10^4$</td>
<td>68</td>
<td>127</td>
<td>157</td>
</tr>
<tr>
<td>4</td>
<td>$1.12 \times 10^6$</td>
<td>216</td>
<td>444</td>
<td>495</td>
</tr>
<tr>
<td>6</td>
<td>$3.26 \times 10^7$</td>
<td>514</td>
<td>1098</td>
<td>1169</td>
</tr>
<tr>
<td>8</td>
<td>$5.94 \times 10^8$</td>
<td>1030</td>
<td>2414</td>
<td>2326</td>
</tr>
<tr>
<td>10</td>
<td>$7.83 \times 10^9$</td>
<td>1828</td>
<td>4674</td>
<td>4103</td>
</tr>
<tr>
<td>12</td>
<td>$8.08 \times 10^{10}$</td>
<td>2979</td>
<td>8388</td>
<td>6651</td>
</tr>
</tbody>
</table>

Table 9. Model spaces dimension for different maximum allowed $\hbar\Omega$ excitations, $N_{\text{max}}$, for the NCSM and the single $0p-0h$ $\text{Sp}(3, \mathbb{R})$ irrep limited to $J = 0$ states in $^{16}\text{O}$.

<table>
<thead>
<tr>
<th>$N_{\text{max}}$</th>
<th>NCSM</th>
<th>(00) $\text{Sp}(3, \mathbb{R})$ irrep</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$J = 0$</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>$1.24 \times 10^3$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>$3.44 \times 10^3$</td>
<td>4</td>
</tr>
<tr>
<td>6</td>
<td>$2.61 \times 10^7$</td>
<td>7</td>
</tr>
<tr>
<td>8</td>
<td>$9.70 \times 10^8$</td>
<td>11</td>
</tr>
<tr>
<td>10</td>
<td>$2.27 \times 10^{10}$</td>
<td>16</td>
</tr>
<tr>
<td>12</td>
<td>$3.83 \times 10^{11}$</td>
<td>23</td>
</tr>
</tbody>
</table>

of $^{12}\text{C}$, these are $J = 0$, 2 and 4, and for the ground state of $^{16}\text{O}$ it is $J = 0$. As the model space, $N_{\text{max}}$, is increased the dimension of the $J = 0$, 2 and 4 symplectic space built on the 13 $0p-0h$ $\text{Sp}(3, \mathbb{R})$ irreps grows very slowly compared to the NCSM space dimension (table 8 and figure 19(a)). The dominance of only three irreps additionally reduces the dimensionality of the symplectic model space (table 8), which in the $12\hbar\Omega$ model space constitutes only $3.7 \times 10^{-6}\%$ of the NCSM space size. The space reduction is even more dramatic in the case of $^{16}\text{O}$ (table 9 and figure 19(b)).

Further reduction in the symplectic model space size can be achieved by considering $\text{Sp}(3, \mathbb{R})$ irreps carrying a total spin $S \leq 2$. This reduction is based on the fact that the low-lying states in light nuclei do not favor high-spin components as they are shifted upward in energy by the spin–orbit part of the internucleon interaction [127].

The symplectic model subspace remains a very small fraction of the NCSM basis space, even when the most dominant $2\hbar\Omega$ $2p-2h$ $\text{Sp}(3, \mathbb{R})$ irreps are included. The reduction is even more dramatic in the case of $^{16}\text{O}$, where only the $J = 0$ subspace can be taken into account for the $0^+$ states under consideration (figure 19(b)). This means that the space spanned by the set of relevant symplectic basis states is computationally manageable even when high-$\hbar\Omega$ configurations are included [9].

12. Summary

In this review, we presented underlying principles of the Sp-NCSM approach and described the construction of translationally invariant basis states of a general symplectic $\text{Sp}(3, \mathbb{R})$ irrep
Figure 19. NCSM space dimension as a function of the maximum $\hbar\Omega$ excitations, $N_{\text{max}}$, compared to that of the $\text{Sp}(3, \mathbb{R})$ subspace: (a) $J = 0, 2$ and 4 for $^{12}\text{C}$ and (b) $J = 0$ for $^{16}\text{O}$.

and the expansion of the latter in the $m$-scheme basis, the same basis currently used within the NCSM framework. We have shown that \textit{ab initio} NCSM calculations with the JISP16 nucleon–nucleon interaction display a very clear symplectic structure, which is unaltered whether bare or effective interactions for various harmonic oscillator strengths are used. This demonstrates the importance of the $\text{Sp}(3, \mathbb{R})$ symmetry in light nuclei while reaffirming the value of the simpler SU(3) model upon which it is based. The results further suggest that a Sp-NCSM extension of the NCSM may be a practical scheme for achieving convergence to measured B(E2) values without the need for introducing an effective charge as well as for modeling cluster-like phenomena by extending the NCSM model space only along the relevant symplectic states leading to a dramatically smaller dimensionality as compared to a full model space.

Acknowledgments

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Appendix A. Matrix elements of the symplectic generators

Matrix elements of the one-body part of the $A_{LM}^{(20)}$ symplectic generator in the spherical harmonic oscillator basis are given as

$$
\langle n_l f | j f m_j | n_l i | j i m_i \rangle A_{LM}^{(20)} (n_l i | j i m_i, n_l f | j f m_j, \{ l_l l_f \}) = \frac{A - 1}{\sqrt{2A}} \delta_{n_j n_i + 2} (-1)^\phi \sqrt{2L + 1} \sqrt{2j_i + 1} C_{j, m_j, L, M, m_f, m_i}^{j, m_j, l_l, l_f} \sum_{n_l i} \left( \begin{array}{ccc} l_i & 1 & l_f \\ j_f & l_f & j_i \end{array} \right) \langle n_l f | b | n_l i \rangle \langle n_l j | b | n_l j \rangle
$$

where $\phi = \frac{1}{2} + \frac{j_i}{L} + j_f + l_i$ and $A$ denotes the total number of nucleons.
An additional two-body term must be subtracted from the symplectic raising generator (72) to remove the spurious center-of-mass motion. The two-body matrix elements of the \( A_{\text{EM}}^{(20)} \) symplectic generator can be written as

\[
\langle n_1^{I_1} j_1^{m_1}; n_2^{I_2} j_2^{m_2}; A_{\text{EM}}^{(20)} | n_1^{I_1} j_1^{m_1}; n_2^{I_2} j_2^{m_2} \rangle = \delta_{\eta l_1+1} \delta_{\eta l_2+1} \sqrt{\frac{\eta}{A}} (-1)^{I_2} \sqrt{(2j_1 + 1) (2j_2 + 1)} \langle n_1^{I_1} j_1^{m_1} | b\rangle \langle n_1^{I_1} j_1^{m_1} | n_2^{I_2} j_2^{m_2} \rangle \times \left\{ \begin{array}{c} l_1 \frac{1}{2} \frac{1}{2} \frac{1}{2} l_1' j_1' j_1' \\ j_1' 1 1 \end{array} \right\} \left\{ \begin{array}{c} l_2 \frac{1}{2} \frac{1}{2} \frac{1}{2} l_2' j_2' j_2' \\ j_2' 1 1 \end{array} \right\} \sum_{\alpha, \beta = 0, 1} C_{j_1 m_1 j_2}^{\alpha \beta} C_{j_2 m_2 j_1}^{\alpha \beta} C_{j_1 m_1 j_2}^{\beta \alpha} C_{j_2 m_2 j_1}^{\beta \alpha} (A_2)
\]

with \( \chi = j_1 + l_1 - j_2 - l_2 + L/2 \).

The matrix elements of the symplectic lowering operators \( B_{\text{EM}}^{(02)} \) are readily obtained from relations (A.1) and (A.2) upon replacing \( b \) with \( b^\dagger \) and \( b^\dagger \) with \( b \). Note that both phase factors \( \phi \) and \( \chi \) remain unaltered.

Matrix elements of the one-body part of the \( C_{\text{EM}}^{(11)} \) symplectic generators are given by

\[
\langle n_1^{I_1} j_1^{m_1}; C_{\text{EM}}^{(11)} | n_1^{I_1} j_1^{m_1} \rangle = \sqrt{\delta_{\eta l_1}} \frac{\sqrt{3} A - 1}{A} (-1)^{\phi} \sqrt{2I + 2} \sqrt{2j_1 + 1} e^{j_1 m_1} \times \left\{ \begin{array}{c} l_1 \frac{1}{2} \frac{1}{2} \frac{1}{2} l_1' j_1' j_1' \\ j_1' 1 1 \end{array} \right\} \langle n_1^{I_1} j_1^{m_1} | b\rangle \langle n_1^{I_1} j_1^{m_1} | n_1^{I_1} j_1^{m_1} \rangle, (A.3)
\]

with \( \phi = \frac{1}{2} + j_1 + l_1 + L \).

The two-body matrix elements the \( C_{\text{EM}}^{(11)} \) can be written as

\[
\langle n_1^{I_1} j_1^{m_1}; n_2^{I_2} j_2^{m_2}; C_{\text{EM}}^{(11)} | n_1^{I_1} j_1^{m_1}; n_2^{I_2} j_2^{m_2} \rangle = \delta_{\eta l_1+1} \delta_{\eta l_2+1} \left\{ \begin{array}{c} l_1 \frac{1}{2} \frac{1}{2} \frac{1}{2} l_1' j_1' j_1' \\ j_1' 1 1 \end{array} \right\} \left\{ \begin{array}{c} l_2 \frac{1}{2} \frac{1}{2} \frac{1}{2} l_2' j_2' j_2' \\ j_2' 1 1 \end{array} \right\} \sum_{\alpha, \beta = 0, 1} C_{j_1 m_1 j_2}^{\alpha \beta} C_{j_2 m_2 j_1}^{\alpha \beta} C_{j_1 m_1 j_2}^{\beta \alpha} C_{j_2 m_2 j_1}^{\beta \alpha} (A.4)
\]

with \( \chi = j_1 + l_1 + j_2 + l_2 + L \).

The reduced matrix elements of the harmonic oscillator ladder operators, \( b^\dagger \) and \( b \), given in a phase convention with the radial part of the harmonic oscillator wavefunctions positive at infinity have the form,

\[
\langle n_1^{I_1} j_1^{m_1} | b^\dagger \rangle \langle n_1^{I_1} j_1^{m_1} \rangle = \left(-\sqrt{l_1} \sqrt{n_1 + 1} + 2 \delta_{l_1, l_1 - 1} + \sqrt{l_1} + \sqrt{n_1 + 1} + 3 \delta_{l_1, l_1 + 1}\right) \delta_{n_1, n_1}, \quad (A.5)
\]

\[
\langle n_1^{I_1} j_1^{m_1} | b \rangle \langle n_1^{I_1} j_1^{m_1} \rangle = \left(-\sqrt{l_1} \sqrt{n_1 + 1} \sqrt{n_1 + 1} + 2 \delta_{l_1, l_1 - 1} + \sqrt{l_1} + \sqrt{n_1 + 1} + 3 \delta_{l_1, l_1 + 1}\right) \delta_{n_1, n_1}. \quad (A.6)
\]

References