Microscopic structure of the low-lying negative-parity states in ^{154}Sm

H. G. Ganev

Joint Institute for Nuclear Research, Dubna, Russia
and Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria

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The proton-neutron symplectic model with Sp(12,R) dynamical algebra is applied to the description of the microscopic structure of the low-lying negative-parity states of the $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ bands in ^{154}Sm without the introduction of additional degrees of freedom that are inherent to other approaches to odd-parity nuclear states. For this purpose, the model Hamiltonian is diagonalized in a U(6)-coupled basis, restricted to state space spanned by the fully symmetric U(6) irreps of the lowest odd irreducible representation of Sp(12,R). In this way, the positive- and negative-parity collective bands are treated on equal footing within the framework of the microscopic symplectic-based shell-model scheme. A good description of the energy levels of the two bands under consideration, as well as the reproduction of some energy splitting quantities which are usually introduced in the literature as a measure of the octupole correlations, is obtained. The microscopic structure of low-lying collective states with negative-parity in ^{154}Sm shows that practically there are no admixtures from the higher shells and hence the presence of a very good U(6) dynamical symmetry. Additionally, the structure of the collective states under consideration shows also the presence of a good SU(3) quasidynamical symmetry.

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I. INTRODUCTION

Experimental spectra in heavy nuclei show the emergence of simple collective patterns represented primarily by the nuclear collective rotation. In this way, the low-lying spectra of well deformed even-even nuclei consist of different rotational bands—ground state, β, γ, etc.—of positive parity, whose properties are described very successfully within the macroscopic nuclear structure physics theories, like the Bohr-Mottelson (BM) [1] and the interacting boson model (IBM) [2] ones.

In some mass regions several bands of negative parity are also observed in the low-lying nuclear spectra in even-even nuclei, like $K^\pi = 0^-$, 1^-, and 2^- bands [3,4]. The most well studied of them is the $K^\pi = 0^-$ band, usually interpreted as an octupole vibrational band, connected to the ground state band by enhanced $E1$ transitions. Sometimes, as suggested to be the case of static octupole deformation [4], the ground state and $K^\pi = 0^-$ bands intertwine into a single alternating parity band.

Negative parity states have been described within different approaches mainly by inclusion of additional octupole and/or dipole (cluster) degrees of freedom. The bands of negative-parity states are often associated with the reflection asymmetry in the intrinsic frame of reference. In the geometrical approach this is achieved by including of the $\alpha_{30} \equiv \beta_3$ deformation [5]. In the IBM [2] the description of negative-parity states requires the introduction of f and/or p bosons with negative parity in addition to the standard s and d bosons ($spdf$-IBM) [6,7]. An alternative interpretation of the low-lying negative-parity states has been provided in different cluster models [8,9] in which the dipole degrees of freedom are related to the relative motion of the clusters. Based on the Bohr Hamiltonian, different critical point symmetries including axial quadrupole and octupole deformations have been proposed [10–13], extending the concept of critical point symmetries introduced for the description of positive-parity states.

From another perspective, the standard shell model allows the microscopic description of both the positive- and negative-parity states by considering the single-particle excitations to the higher major oscillator shells which differ, respectively, with even and odd number with respect to the valence shell. For instance, the negative-parity states of the even-even sd nuclei have been considered to arise from either exciting a p particle to the ds shell or exciting a ds particle to the fp shell [14]. It is well known, however, that with the increase of the number of valence particles and/or the single-particle states available, the model space dimensionalities grow rapidly and rule out the use of standard shell-model theory. As a consequence, different approaches have been proposed to truncate the many-particle configuration space. Among them, the algebraic models based on the symmetries, exact or approximate, provide elegant and very efficient methods for reducing the model space in manageable size. In addition, different truncation schemes have been used to reorganize the available shell-model spaces in such a way that their symmetry-adapted bases already capture the essential features of the observed nuclear properties.

The first microscopic, algebraic model of nuclear rotations is the SU(3) model of Elliott [15], which exploits the U(3) $\supset$ SU(3) $\supset$ SO(3) group-subgroup chain to classify the many-particle states and to construct the effective nucleon-nucleon interaction. The group U(3) is the symmetry group of the three-dimensional harmonic oscillator, which is chosen to approximate the nuclear mean filed. This model of nuclear structure was successfully applied to the light deformed *p*- and *sd*-shell nuclei and showed how states with rotational properties could emerge within the framework of the nuclear shell model. The nucleons within the fully occupied shells are treated as inactive, constituting an inert core, and the nuclear rotational states are described in terms of valence shell $0\hbar\omega$ configurations. The latter suggests that the negative-parity states within the framework of the SU(3) model can also be described by considering the available configurations of the adjacent major shell, constituting the $1\hbar\omega$ harmonic oscillator subspace. For example, while the leading SU(3) irreducible representation (8,0) of the $0\hbar\omega$ subspace provides a basis of states for the ground band in ^{20}Ne in the Elliott model, the SU(3) irreducible representation (9,0) of the $1\hbar\omega$ subspace, given in Ref. [14], turns out to be appropriate for the description of the 0^-_1 band observed experimentally in the spectrum [3].

From another side, it was shown that the dynamical group of the harmonic oscillator Hamiltonian is the noncompact symplectic group $\mathrm{Sp}(6,R)$[1] [16], which contains the Elliott SU(3) as a subgroup. Along this line, a natural multi-major shell extension of the Elliott SU(3) model, which includes core collective excitations, related to the giant resonances, was proposed and is presented by the one-component $\mathrm{Sp}(6,R)$ symplectic model [17,18]. Thus, in this regard, both the SU(3) and $\mathrm{Sp}(6,R)$ models define a relevant coupling scheme for identifying the collective dynamics and performing large shell-model mixed representation calculations.

The early applications of the $\mathrm{Sp}(6,R)$ model and its submodels—reviewed in Ref. [19]—were with algebraic or schematic interactions, and, with a few exceptions, have been performed within a single symplectic irrep and all done for the positive-parity states only. More recent applications of the $\mathrm{Sp}(6,R)$ model, with algebraic and schematic interactions, include [20–22] for light and intermediate-mass nuclei, and [23] for the low-lying rotational states of the ground band in ^{166}Er. Recently, *ab initio* large-scale no-core shell model calculations with realistic interactions, inspired from QCD, have also been done in large multishell spaces in a $\mathrm{U}(3)\times\mathrm{SU}(2)_{S_p}\times\mathrm{SU}(2)_{S_n}$ symmetry-adapted basis for light to intermediate-mass nuclei [24–26], which revealed the symplectic $\mathrm{Sp}(6,R)$ symmetry which was not assumed *a priori*. However, already for very light nuclei, such calculations assuming all possible single-particle excitations across the major shells (i.e., considering all particles as active: the no-core shell model) require the use of supercomputers, and it is inconceivable that corresponding calculations could be carried out in the near future for heavy nuclei. Additionally, the most important point revealed by the calculations within the framework of the one-component $\mathrm{Sp}(6,R)$ symplectic model [17,18] is that the standard spherical shell model is not appropriate for the description of the rotational states of strongly deformed heavy nuclei [23,27]. This is so, in particular, because the conventional shell-model configurations available are not enough deformed to describe observed quadrupole collectivity. As a result, the observed low-lying rotational states of strongly deformed heavy nuclei have a negligible overlap with the available standard shell-model states [23,27]. In this case the relevant Hilbert spaces for heavy mass nuclei become even much larger than the conventional shell model dictates and add further computational complexity.

An alternative, symmetry-based, microscopic shell-model approach to the structure of strongly deformed heavy nuclei is provided by the pseudo-SU(3) scheme [28–30], based on the observation that, because of the spin-orbit interaction, the single-particle energy levels of the shell model regroup into pseudo-oscillator shells. As a result, another good SU(3) symmetry appears, called pseudo-SU(3) symmetry. Based on this symmetry, the $\mathrm{Sp}(6,R)$ pseudosymplectic model and its contracted version for heavy nuclei have been developed [31] and applied to the description of the microscopic structure of the low-lying rotational states of the ground or ground and γ bands for some heavy well-deformed even-even nuclei from the rare earth and actinide regions [31,32].

In the shell model the many-particle Hilbert space of the nucleus is separated into energy-ordered subspaces. The subset of nucleons then is supposed to occupy the single-particle states of a closed-shell core, whereas the remaining nucleons are restricted to a finite-dimensional valence space. Shell-model calculations in such subspaces have been successful in describing subsets of nuclear properties in light nuclei and, to some extent, in heavier singly-closed-shell nuclei and in nuclei close to doubly-closed shells. In contrast to the conventional shell model which divides the many-body Hilbert space of nuclear systems into different shells (i.e., horizontally), the one-component symplectic $\mathrm{Sp}(6,R)$ model organizes the many-particle configuration space vertically, dividing the full Hilbert space into a direct sum of different symplectic slices or vertical cones. Each symplectic slice represents an irreducible collective space for the microscopic collective model and is a small fraction of the full nuclear state space. Each subspace of the $\mathrm{Sp}(6,R)$ model contains a set of collective rotational and high-energy vibrational states of a nucleus, the latter related to the giant resonance degrees of freedom.

Symplectic states in the one-component symplectic model, adapted to the $\mathrm{Sp}(6,R)\supset\mathrm{U}(3)\supset\mathrm{SU}(3)\supset\mathrm{SO}(3)$ chain, are the shell model configurations that are eigenstates of the harmonic oscillator Hamiltonian with energy $(E_0+2n)\hbar\omega$ carrying good SU(3) symmetry. From the shell-model perspective, therefore, the $\mathrm{Sp}(6,R)$ symplectic model is an extension of the conventional oscillator shell model that goes beyond the single valence major shell and includes, in addition, the *n*p-*n*h coherent admixtures, required to build up the enhanced quadrupole collectivity without the use of effective charges. Symplectic raising operators change the number of harmonic oscillator quanta by two units and hence preserve the parity of the states within the considered symplectic irrep.

Symplectic groups, however, admit two types of irreducible representations: even and odd ones which contain all the harmonic oscillator shell-model states with even and odd number of excitation quanta, respectively. This allows one to

[1]The notation $\mathrm{Sp}(2n,R)$ is used for the group of linear canonical transformations in $2n$-dimensional phase space. Some authors denote the $\mathrm{Sp}(2n,R)$ group by $\mathrm{Sp}(n,R)$.

account for both the positive- and negative-parity states. In this way all the many-particle states of the harmonic oscillator Hamiltonian fall into two types of irreducible representations of the symplectic group. Thus, in order the negative-parity states to be involved in the symplectic-based shell-model theory, one needs simply to consider the odd symplectic irrep(s).

Recently, the fully microscopic proton-neutron symplectic model (PNSM) of nuclear collective motion with Sp(12,R) dynamical algebra was introduced by considering the symplectic geometry and possible collective flows in the two-component many-particle nuclear system [33]. From a hydrodynamic perspective, the PNSM appears as a two-fluid irrotational-flow collective model of Bohr-Mottelson type, coupled to the intrinsic U(6) vortex degrees of freedom which are related to the valence shell protons and neutrons. The need to consider of intrinsic degrees of freedom and their coupling to the irrotational-flow collective dynamics was realized a long time ago (cf. Ref. [19] and references therein). The U(6) intrinsic degrees of freedom play an important role in the construction of the microscopic wave functions because they allow one to ensure the full antisymmetry of the total wave function and are responsible for the appearance of the low-lying collective states. In this way the extra degrees of freedom contained in this larger U(6) algebraic structure therefore embrace the basic SU(3) rotor as well as the low-lying vibrational degrees of freedom.

From the shell-model perspective, the PNSM appears [34] as a natural multi-major-shell extension of the generalized proton-neutron SU(3) scheme, which takes into account the core collective excitations associated with the giant resonance vibrational degrees of freedom. The microscopic U(6) structure, related to the valence proton and neutron degrees of freedom, also contains many SU(3) irreps appropriate for the description of different excited bands. In this way, both the vertical and horizontal mixings of different SU(3) irreducible representations are naturally contained in the PNSM, thus providing a relevant shell-model coupling scheme for shell-model based calculations and a single microscopic framework for the simultaneous description of the low-lying bands of collective states in strongly deformed nuclei, which exhibit a simple rotational patterns and both the high-lying (giant resonance) and [in contrast to the Sp(6,R) case] low-lying shape vibrational excitations. The latter were shown to correspond to the relative angular excitation of the proton subsystem with respect to the neutron one [35]. In other words, the low-lying states in the PNSM could thus be described by a microscopically based U(6) structure along the lines of the popular IBM [2], albeit, in contrast to the latter, renormalized by their coupling to the giant resonance vibrations.

The PNSM has been applied for the simultaneous description of the microscopic structure of the ground, γ, and β bands in ^{166}Er [36], using the $SU_p(3) \otimes SU_n(3)$ symmetry-adapted basis, which is appropriate for the case of generic nonfully symmetric irreducible representations of Sp(12,R). The PNSM was further used to study the microscopic structure of the low-lying collective states of the ground, β, and γ bands in ^{154}Sm [35] and ^{238}U [37], using the more general U(6)-coupled basis, restricted to the symplectic state space spanned by the fully symmetric U(6) vectors. The calculations showed that when the collective quadrupole dynamics is covered already by the symplectic bandhead structure, as in the case of ^{154}Sm, the results show the presence of a very good U(6) dynamical symmetry [35]. In the case of ^{238}U, when there is an observed enhancement of the intraband $B(E2)$ transition strengths, then the results show small admixtures from the higher major shells and a highly coherent mixing of different irreps which is manifested by the presence of a good U(6) quasidynamical symmetry in the microscopic structure of the collective states under consideration [37].

In the present paper, the proton-neutron symplectic model with Sp(12,R) dynamical algebra, which naturally involves vertical as well as horizontal mixing of different SU(3) irreducible representations, is further applied to the description of the microscopic structure of low-lying negative-parity states of the $K^\pi = 0_1^-$ and $K^\pi = 1_1^-$ bands in ^{154}Sm without the introduction of additional degrees of freedom that are inherent to other approaches to odd-parity nuclear states. For this purpose, the model Hamiltonian is diagonalized in a U(6)-coupled basis, restricted to state space spanned by the fully symmetric U(6) irreps of the lowest odd irreducible representation of Sp(12,R). In this way, the positive- and negative-parity collective bands are treated on equal footing within the framework of the microscopic symplectic-based shell-model scheme simply by considering the lowest even and odd Sp(12,R) irreducible representations, respectively. The results obtained in this work extend the previously obtained ones in the framework of the PNSM for the lowest three collective bands of positive parity in ^{154}Sm [35]. In this regard, the present paper represents a further step towards the more comprehensive treatment of collective motion in this nucleus within the microscopic symplectic-based framework. Moreover, to my knowledge, these are the first symplectic-based shell-model calculations which have been performed for the description of negative-parity states in atomic nuclei.

II. THE PROTON-NEUTRON SYMPLECTIC MODEL

Collective observables of the proton-neutron symplectic model, which span the Sp(12,R) algebra, are given by the following one-body operators [33]:

$$Q_{ij}(\alpha,\beta) = \sum_{s=1}^{m} x_{is}(\alpha)x_{js}(\beta), \tag{1}$$

$$S_{ij}(\alpha,\beta) = \sum_{s=1}^{m} (x_{is}(\alpha)p_{js}(\beta) + p_{is}(\alpha)x_{js}(\beta)), \tag{2}$$

$$L_{ij}(\alpha,\beta) = \sum_{s=1}^{m} (x_{is}(\alpha)p_{js}(\beta) - x_{js}(\beta)p_{is}(\alpha)), \tag{3}$$

$$T_{ij}(\alpha,\beta) = \sum_{s=1}^{m} p_{is}(\alpha)p_{js}(\beta), \tag{4}$$

where $i, j = 1, 2, 3$; $\alpha, \beta = p, n$ and $s = 1, \ldots, m = A - 1$. In Eqs. (1)–(4), $x_{is}(\alpha)$ and $p_{is}(\alpha)$ denote the coordinates and corresponding momenta of the translationally invariant Jacobi vectors of the m-quasiparticle two-component nuclear system, and A is the number of protons and neutrons.

The PNSM dynamical algebra Sp(12,R) has many subalgebra chains, which roughly can be divided into two types of chains: the collective model and the shell model chains. The form (1)–(4) of the symplectic algebra Sp(12,R) is naturally adapted to the collective model chain, which reveals the dynamical content of symplectic symmetry. Among the subalgebras of this chain are, for example, the general collective motion in six dimensions GCM(6) and the coupled two-rigid rotor model $\mathrm{ROT}_p(3) \otimes \mathrm{ROT}_n(3) \supset \mathrm{ROT}(3)$ Lie algebras. The GCM(6) algebra introduces the SO(6) intrinsic vortex degrees of freedom, which coupled to the giant resonances allows for the continuous range of rotational dynamics from rigid to irrotational flow. For more details about the dynamical content of the PNSM, we refer the reader to Ref. [33].

The shell-model chain of Sp(12,R) algebra relates the PNSM to the shell-model nuclear theory and thus provides a connection to the microscopic fermion physics. It provides a shell-model coupling scheme and a basis for detailed microscopic shell-model calculations. The shell-model chain is naturally expressed in terms of the harmonic oscillator creation and annihilation operators

$$b^{\dagger}_{i\alpha,s} = \sqrt{\frac{m_\alpha \omega}{2\hbar}}\left(x_{is}(\alpha) - \frac{i}{m_\alpha \omega} p_{is}(\alpha)\right),$$
$$b_{i\alpha,s} = \sqrt{\frac{m_\alpha \omega}{2\hbar}}\left(x_{is}(\alpha) + \frac{i}{m_\alpha \omega} p_{is}(\alpha)\right). \tag{5}$$

Then the symplectic generators take an alternative form as all bilinear combinations of the harmonic oscillator raising and lowering operators that are $O(m)$ invariant [34]:

$$F_{ij}(\alpha,\beta) = \sum_{s=1}^{m} b^{\dagger}_{i\alpha,s} b^{\dagger}_{j\beta,s}, \tag{6}$$

$$G_{ij}(\alpha,\beta) = \sum_{s=1}^{m} b_{i\alpha,s} b_{j\beta,s}, \tag{7}$$

$$A_{ij}(\alpha,\beta) = \frac{1}{2}\sum_{s=1}^{m} (b^{\dagger}_{i\alpha,s} b_{j\beta,s} + b_{j\beta,s} b^{\dagger}_{i\alpha,s}). \tag{8}$$

An Sp(12,R) unitary irreducible representation is characterized by the U(6) quantum numbers $\sigma = [\sigma_1, \ldots, \sigma_6]$ of its lowest-weight state $|\sigma\rangle$, i.e., $|\sigma\rangle$ satisfies

$$G_{ab}|\sigma\rangle = 0;$$
$$A_{ab}|\sigma\rangle = 0, \quad a < b;$$
$$A_{aa}|\sigma\rangle = \left(\sigma_a + \frac{m}{2}\right)|\sigma\rangle \tag{9}$$

for the indices $a \equiv i\alpha$ and $b \equiv j\beta$ taking the values $1, \ldots, 6$. If one introduces the U(6) tensor product operators $P^{(n)}(F) = [F \times \ldots \times F]^{(n)}$, where $n = [n_1, \ldots, n_6]$ is a partition with even integer parts, then by a U(6) coupling of these tensor products to the lowest-weight state $|\sigma\rangle$, one constructs the whole basis of states for an Sp(12,R) irrep

$$|\Psi(\sigma n \rho E \eta)\rangle = [P^{(n)}(F) \times |\sigma\rangle]^{\rho E}_{\eta}, \tag{10}$$

where $E = [E_1, \ldots, E_6]$ indicates the U(6) quantum numbers of the coupled state, η labels a basis of states for the coupled U(6) irrep E, and ρ is a multiplicity index. In this way one obtains a basis of Sp(12,R) states that reduces the subgroup chain $\mathrm{Sp}(12,R) \supset \mathrm{U}(6)$. To fix the basis η one has to consider further the reduction of the U(6) to the three-dimensional rotational group SO(3). Thus, in order to completely classify the basis states, I use the following reduction chain [34,35]:

$$\begin{array}{ccccccc} \mathrm{Sp}(12,R) & \supset & & & & & \\ \sigma & n\rho & & & & & \\ & \supset \mathrm{U}(6) & \supset & \mathrm{SU}_p(3) \otimes \mathrm{SU}_n(3) & & & \\ & E & \gamma & (\lambda_p,\mu_p)\ (\lambda_n,\mu_n) & & & \\ & \supset \mathrm{SU}(3) & \supset & \mathrm{SO}(3) & \supset & \mathrm{SO}(2), & \\ & \varrho\ (\lambda,\mu) & \kappa & L & & M & \end{array} \tag{11}$$

which defines a shell-model coupling scheme. Under different subgroups in Eq. (11) are given the corresponding quantum numbers that characterize their irreducible representations plus some multiplicity indices. For more details concerning the shell-model classification of the collective states in ^{154}Sm, see Ref. [35]. Thus, each Sp(12,R) irreducible representation, denoted as $\langle\sigma\rangle = \langle\sigma_1 + \frac{m}{2}, \ldots, \sigma_6 + \frac{m}{2}\rangle$, is determined by the symplectic bandhead $\sigma = [\sigma_1, \ldots, \sigma_6]$ that is fixed by the underlying proton-neutron shell-model structure. So, the theory becomes completely compatible with the Pauli principle.

TABLE I. The U(6) irreps contained in the odd Sp(12,R) irreducible representation $\langle\sigma\rangle = \langle 73 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}\rangle$, appropriate for description of the negative-parity states in ^{154}Sm.

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[35], [34, 1], 2[33, 2], [32, 3],
[32, 2, 1], [31, 4], [31, 2, 2]
[33], [32, 1], [31, 2]
[31]

III. APPLICATION

The shell-model considerations based on the pseudo-SU(3) scheme [28–30] give for the positive-parity states in ^{154}Sm the following symplectic irrep: $\langle\sigma\rangle = \langle 72 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}\rangle$ [35], which is determined by the intrinsic U(6) structure of the corresponding lowest-weight state $\sigma = [72, 42, 42, 42, 42, 42]_6 \equiv [30]_6$. Then the odd irrep $\langle\sigma\rangle = \langle 73 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}, 42 + \frac{153}{2}\rangle$ of Sp(12,R), shown in Table I and determined by the symplectic bandhead $\sigma = [73, 42, 42, 42, 42, 42]_6 \equiv [31]_6$ of the $1\hbar\omega$ space, will be of relevance for the description of the negative-parity states in ^{154}Sm. More details about the construction and structure of the shell-model representations of the PNSM can be found in Ref. [34].

In the present application, I consider only the many-particle Hilbert space spanned by the fully symmetric U(6) vectors only, which are expected to dominate the low-lying

TABLE II. Symplectic classification of the SU(3) basis states, associated with the negative-parity states in ^{154}Sm.

$2n$	$[E_1,\ldots,E_6]$	(λ_p,μ_p)	(λ_n,μ_n)	(λ,μ)
0	[31]	⋯ (13,0) ⋯	⋯ (18,0) ⋯	(31, 0), (29, 1), (27, 2), ..., (11,10),(9,11),(7,12)
2	[33]	⋯ (15,0) ⋯	⋯ (18,0) ⋯	(33, 0), (31, 1), (29, 2), ..., (9,12),(7,13),(5,14)
4	[35]	⋯ (17,0) ⋯	⋯ (18,0) ⋯	(35, 0), (33, 1), (31, 2), ..., (7,14),(5,15),(3,16)
⋮	⋮	⋮	⋮	⋮

energy spectrum. The symplectic classification of the SU(3) basis states for the negative-parity states in ^{154}Sm according to the decompositions given by Eq. (11) for the Sp(12,R) irrep $\langle\sigma\rangle = \langle 73+\frac{153}{2}, 42+\frac{153}{2}, 42+\frac{153}{2}, 42+\frac{153}{2}, 42+\frac{153}{2}, 42+\frac{153}{2}\rangle$, restricted to the space of fully symmetric U(6) partitions, is given in Table II.

A. The model Hamiltonian

In present application, for the negative-parity states, the following model Hamiltonian is used:

$$H = N\hbar\omega - \tfrac{1}{2}\chi[Q_p\cdot Q_n - (Q_p\cdot Q_n)_{TE}] - \xi C_2[\mathrm{SU(3)}] + aL^2 + \epsilon(N_{b.h.} - N_0). \tag{12}$$

where $N = N_p + N_n$ and $Q_\alpha \equiv Q(\alpha,\alpha)$ with $\alpha = p, n$ are the full major-shell mixing quadrupole tensor operators and are given by Eq. (1). A similar Hamiltonian has been used in the pseudo-SU(3) scheme calculations within the framework of the contracted symplectic model [31,32]. The trace-equivalent part $(Q_p\cdot Q_n)_{TE}$ [38] is subtracted from the collective potential in order to preserve the mean-field shell structure [31,32,39] under the action of the proton-neutron quadrupole-quadrupole interaction. The SU(3) second-order Casimir operator C_2[SU(3)] splits energetically different SU(3) multiplets and in this way determines the bandhead energies of excited bands with respect to the ground state band. The term $\epsilon(N_{b.h.} - N_0)$ is introduced in the model to take into account the energy difference between the even and odd symplectic bandheads. $N_{b.h.}$ is the number operator of the symplectic bandhead which eigenvalues for the $0\hbar\omega$ and $1\hbar\omega$ shell-model subspaces are given by N_0 and $N_0' = N_0 + 1$, respectively. N_0 denotes the minimum number of oscillator quanta allowed by the Pauli principle [34]. Without this term, the negative-parity states would appear at energy $\sim 1\hbar\omega$. Indeed, setting $\epsilon = 0$, one obtains for the energy of the first excited negative-parity state 1^- of $K^\pi = 0^-_1$ band $E_{1^-} = 8.16$ MeV, which is comparable with the intershell distance $1\hbar\omega = 7.649$ MeV for ^{154}Sm that comes from different symplectic bandheads (determined by the minimum Pauli allowed number of quanta N_0 and $N_0 + 1$, respectively). The major shell separation energy $\hbar\omega$ is determined by the standard formula $41A^{-1/3}$ MeV. The term aL^2, which represents a residual rotor part, allows the experimentally observed moment of inertia to be reproduced without altering the wave functions. In order to account for experimentally observed different moments of inertia of the negative-parity bands with respect to the positive-parity ones, I use additionally the following parametrization for the inertia parameter a : $a = a_0/(1+\frac{1}{3}\langle\Delta N_0\rangle)$, where $\langle\Delta N_0\rangle$ is the eigenvalue of the operator $\Delta N_0 = (N_{b.h.} - N_0)$ described above. The form $a_0/(1+\frac{1}{3}\langle\Delta N_0\rangle)$ is chosen in a way that it is valid for both the positive- (for which $\langle\Delta N_0\rangle = 0$ and its reduces to the inertia parameter $a = a_0$ used in Ref. [35]) and negative-parity states. Such kind of parametrizations which introduce a deformation dependence of the moment of inertia are used in the literature, e.g. Refs. [40,41], to account for different moments of inertia for different bands. The inertia parameter does not affect the wave function, its role is just to fine tune the observed moment of inertia. In this regard, the parameter a_0 could be used instead of $a_0/(1+\frac{1}{3}\langle\Delta N_0\rangle)$ at the price of slightly worst energy agreement. (The parameter $a_0/(1+\frac{1}{3}\langle\Delta N_0\rangle)$ is 75% of a_0.)

The Hamiltonian (12) preserves the symplectic symmetry, thus having Sp(12,R) as its dynamical algebra in the sense that the physical operators are obtained in terms of its generators, and the whole negative-parity spectrum is provided by a single irreducible representation of it.

B. The energy spectra

The model Hamiltonian (12) is diagonalized in the irreducible collective space of Sp(12,R), spanned by the fully symmetric U(6) vectors only, considering the particle-hole collective excitations up to energy $41\hbar\omega$. The results for the low-lying energy levels of the $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ bands together with the ground, β, and γ bands are compared with experiment [3] in Fig. 1. The theoretical energies of the three lowest positive-parity bands in ^{154}Sm are taken from Ref. [35]. The model parameters χ, ξ, a are determined by fitting to the low-lying positive-parity states of the ground, β, and γ bands. Their values in MeV, respectively, are [35] $\chi = 0.0032$, $\xi = 0.0053$, and $a_0 = 0.013$. The adopted value of the last Hamiltonian parameter, related to the negative parity bands, is $\epsilon = -6.809$.

In Fig. 2, the SU(3) decomposition of the wave functions (probability distribution) of 1^- states of the $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ bands in ^{154}Sm is shown. From the latter one sees that the SU(3) dynamical symmetry is broken due to the mixing of different irreps. From another side, almost all SU(3) irreducible representations, contributing to the structure, belong to a single U(6) irreducible representation, namely that of the symplectic bandhead. More precisely, the U(6) irrep of the lowest-weight state exhausts up to 98.569% and 98.573% of the structure of the 1^- state of the $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ bands, respectively. This indicates that the states under consideration possess a good U(6) dynamical symmetry. The same picture is obtained for the other collective states. Compared to the SU(3) decomposition of the positive-parity states in ^{154}Sm (cf. Fig. 7 of Ref. [35]), in the present case one sees a wider distribution over different SU(3) irreps, which is due to the extra energy coming from the difference $|1\hbar\omega - \epsilon| \approx 0.84$

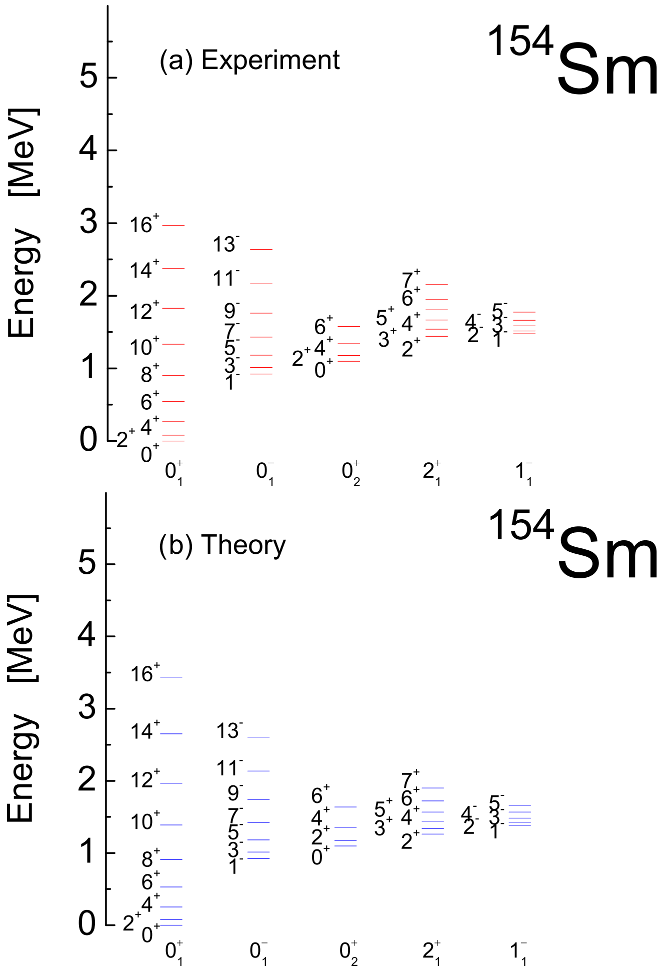

FIG. 1. Comparison of experimental energy levels (a) with the theory (b) for the low-lying positive-parity ground, β, and γ bands (data are from Ref. [35]) and negative-parity $K^{\pi} = 0_1^-$ and $K^{\pi} = 1_1^-$ bands in ^{154}Sm.

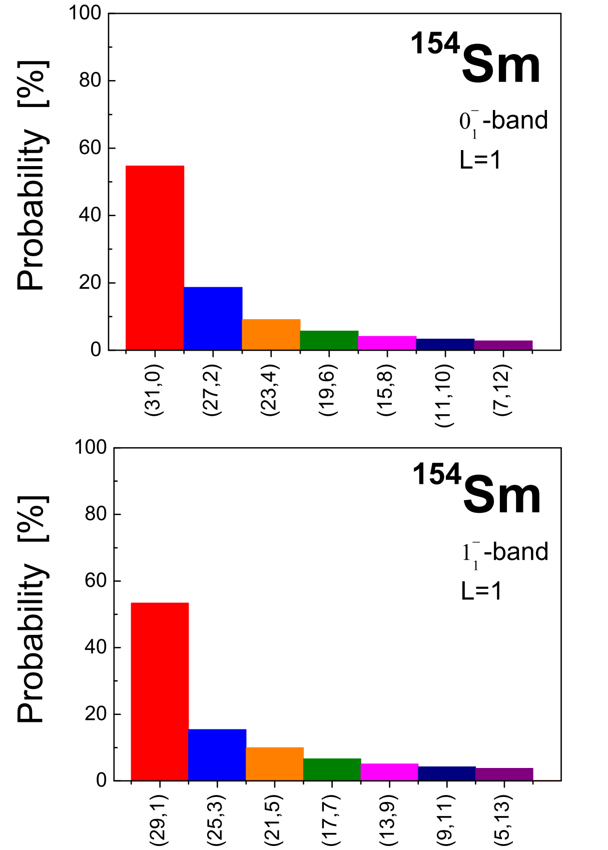

FIG. 2. Calculated SU(3) probability distributions for the wave functions for the 1^- states of the $K^{\pi} = 0_1^-$ and $K^{\pi} = 1_1^-$ bands.

MeV. But nevertheless, the microscopic structure of the 1^- collective states of the two bands under consideration retain the simple picture in which only a few SU(3) irreps dominate the structure.

Additionally, in Fig. 3, I show the SU(3) decomposition of the wave functions of $K^{\pi} = 0_1^-$ and $K^{\pi} = 1_1^-$ bands, respectively, for three different values of the angular momentum in each band. From the figure, one sees a highly coherent mixing in which the squared amplitudes are practically L independent, at least for low angular momenta for which the Coriolis and centrifugal forces are not so strong. The figure thus indicates a new kind of symmetry, called quasidynamical symmetry [42]. This symmetry is associated with the mathematical concept of embedded representations [43]. Thus, the results for the microscopic structure of the states of the two negative-parity bands under consideration in ^{154}Sm reveal, in addition to the good U(6) symmetry, the presence also of a good SU(3) quasidynamical symmetry, in the sense given in Refs. [23,42].

C. The energy staggering

Different energy spin-dependent quantities have been introduced [44–46] as a measure of octupole correlations. For example, the signature-splitting index $S(L)$ [45], which is also a convenient measure for deviation from the pure rotational behavior, is defined as

$$S(L) = \frac{[E_{L+1} - E_L] - [E_L - E_{L-1}]}{E_{2_1^+}}, \tag{13}$$

which describes the normalized position of a negative-parity level L^- relative to the positive-parity one with spin and parity $(L \pm 1)^+$. Large nonzero values of this quantity are usually associated with the soft octupole vibrations built on the ground state in well quadrupole-deformed nuclei, in which the negative-parity states are well separated from the positive-parity ones. An alternating parity band, formed by merging of the opposite parity sequences of states, is respectively represented by approximately zero values of $S(L)$ pointing out the equal spacing of the levels constituting the band.

I compare the calculated values of $S(L)$ for ^{154}Sm with experiment in Fig. 4. Here, one sees that the decreasing experimental signature splitting with increasing angular momentum is reproduced by the theory. The signature splitting index for ^{154}Sm gives no hint of strong octupole correlations, as $S(L)$ does not approach 0 (no alternating parity band)

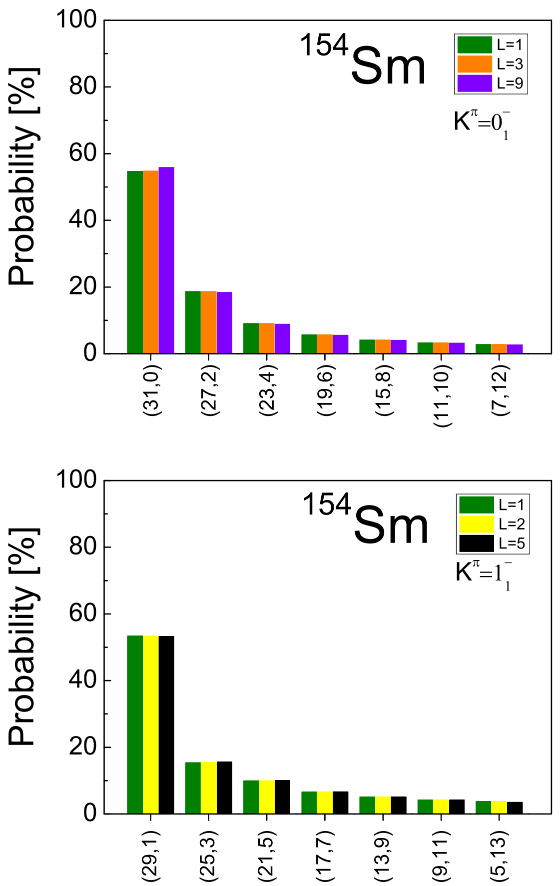

FIG. 3. Calculated SU(3) probability distributions for the wave functions of the $K^{\pi} = 0_1^-$ and $K^{\pi} = 1_1^-$ bands for three different angular momentum values.

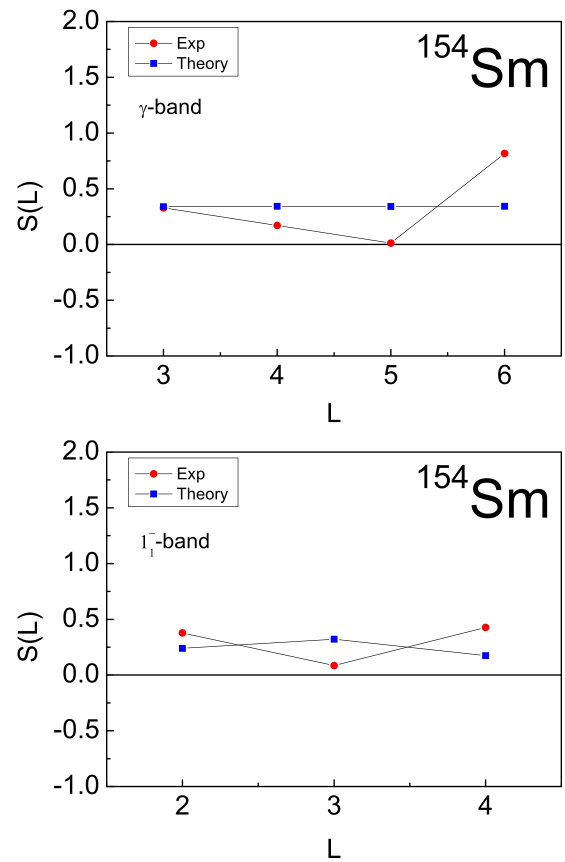

FIG. 5. Theoretical and experimental signature-splitting index $S(L)$ (13) between the states of the γ and $K^{\pi} = 1_1^-$ bands in ^{154}Sm.

in the available data. Additionally, in Fig. 5 I compare the calculated values for the signature-splitting index $S(L)$ with experiment for the γ and $K^{\pi} = 1_1^-$ bands. For the γ band one obtains a small, positive, and constant value of 0.34 that is a characteristic feature of $S(L)$ for the axially symmetric rotor (with value +0.33) [47]. For the $K^{\pi} = 1_1^-$ band, the same constant behavior of small positive value is also more or less observed. Note also the different scales in Figs. 4 and 5.

The function $S(L)$ (13) vanishes for

$$E(L) = E_0 + AL(L+1), \tag{14}$$

but not for

$$E(L) = E_0 + AL(L+1) + B[L(L+1)]^2. \tag{15}$$

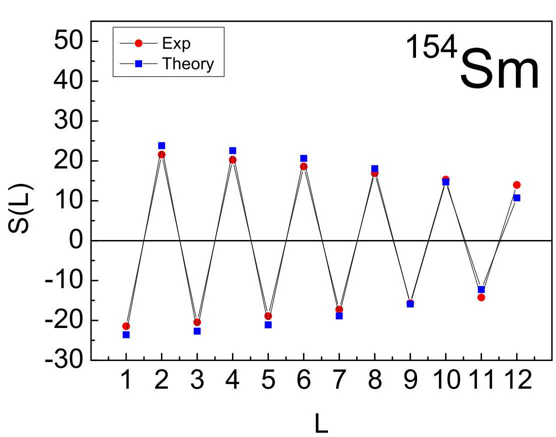

FIG. 4. Theoretical and experimental signature-splitting index $S(L)$ (13) between the states of the ground band and 0_1^- band in ^{154}Sm.

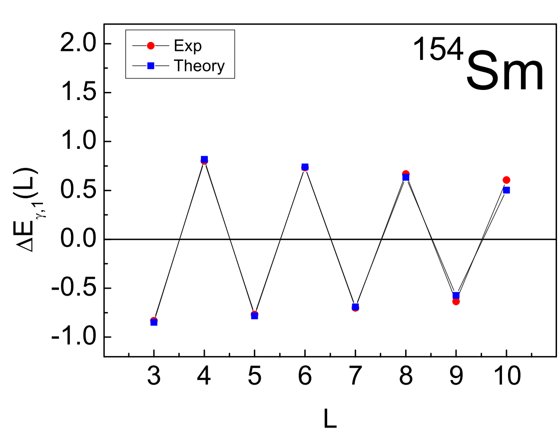

FIG. 6. Theoretical and experimental staggering function $\Delta E_{\gamma,1}(L)$ (16) between the states of the ground band and 0_1^- band in ^{154}Sm.

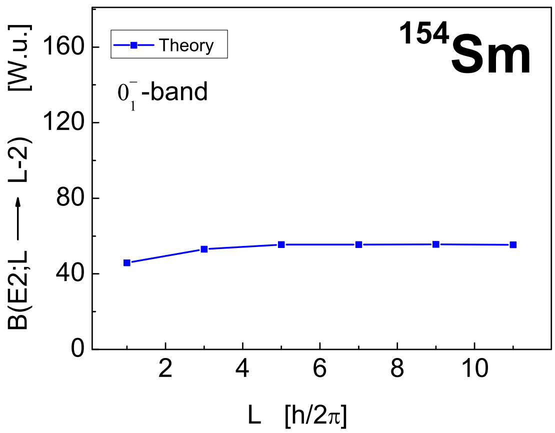

FIG. 7. Calculated intraband $B(E2)$ values in Weisskopf units between the states of the $K^\pi = 0_1^-$ band in ^{154}Sm. No effective charge is used.

Another quantity is also used in practice [46]

$$\Delta E_{\gamma,1}(L) = \frac{1}{16}[6\Delta E(L) - 4\Delta E(L-1) - 4\Delta E(L+1) + \Delta E(L+2) + \Delta E(L-2)], \quad (16)$$

where $\Delta E(L) = E(L+1) - E(L)$. The staggering function (16), in contrast to (13), vanishes for (15) and hence it represents a more sensitive measure for the deviations of the nuclear dynamics from that of pure rotational collective motion. Recall that the pure SU(3) limit of the *spdf*-IBM (and other algebraic models) predicts a staggering of constant amplitude [46].

I consider the odd-even staggering between the states of the ground band and $K^\pi = 0_1^-$ band in ^{154}Sm, which is compared with the experimental pattern in Fig. 6. From the latter, we see a good reproduction of the observed staggering function. The staggering pattern of almost constant amplitude, shown in Fig. 6, also indicates the good (quasidynamical) SU(3) character of the states of the ground and 0_1^- bands.

D. Transition probabilities

It is known that the transition probabilities are more sensitive tests for each model. The $B(E1)$ transitions, connecting the alternating-parity sequences, require some new mathematical efforts and will be considered elsewhere. Here, I restrict myself only to the intraband $B(E2)$ transition strengths in the lowest $K^\pi = 0_1^-$ band, which are a measure of the quadrupole collectivity in the negative-parity states.

In Fig. 7 I show the calculated intraband $B(E2)$ transition strengths between the states of the $K^\pi = 0_1^-$ band, obtained by Eq. (17) of Ref. [35] without the use of an effective charge. Recall, that the intraband $B(E2)$ transition strengths between the states of the ground band, given in Ref. [35], reproduce very well the experimental data with no effective charge. Compared to the ground band, the $B(E2)$ intraband transitions in the $K^\pi = 0_1^-$ band, with the wave functions obtained in the present work, show a reduced quadrupole collectivity. Unfortunately, there are no experimental data available for these $B(E2)$ transition strengths that would allow one to establish the extent to which the quadrupole collectivity in the negative-parity states is captured by the used model Hamiltonian, and possibly the lack of other important correlations in the structure of the wave functions.

IV. CONCLUSIONS

Symplectic symmetries organize the many-particle configuration space vertically, dividing the full Hilbert space into a direct sum of different symplectic slices or vertical cones. Each symplectic slice, preserving the parity and permutational symmetry, represents an irreducible collective space for the microscopic collective model and is a small fraction of the full nuclear state space.

Further, it is well known that the symplectic groups admit two types of irreducible representations: even and odd ones which contain all the harmonic oscillator shell-model states with even and odd number of excitation quanta, respectively. This allows one to account for both the positive- and negative-parity states. In this way all the many-particle states of the harmonic oscillator Hamiltonian fall into the two types of irreducible representations of the symplectic group. Thus, in order for the negative-parity states to be involved in the symplectic-based shell-model theory, one needs simply to consider the odd symplectic irrep(s). The positive- and negative-parity collective bands are then treated on equal footing within the framework of the microscopic symplectic-based shell-model scheme simply by considering the two types of symplectic irreps without the introduction of additional degrees of freedom that are inherent to other approaches to odd-parity nuclear states.

In the present paper, the proton-neutron symplectic model with Sp(12,*R*) dynamical algebra, which naturally involves vertical as well as horizontal mixing of different SU(3) irreducible representations, is applied to the description of the microscopic structure of the low-lying negative-parity states of the $K^\pi = 0_1^-$ and $K^\pi = 1_1^-$ bands in ^{154}Sm. For this purpose, the model Hamiltonian is diagonalized in a U(6)-coupled basis, restricted to state space spanned by the fully symmetric U(6) irreps of the lowest odd irreducible representation of Sp(12,*R*). A good description of the energy levels of the two bands under consideration, as well as the reproduction of some energy splitting quantities which are usually introduced in the literature as a measure of the octupole correlations, is obtained. The microscopic structure of low-lying collective states with negative-parity in ^{154}Sm shows that practically there are no admixtures from the higher shells and hence the presence of a very good U(6) dynamical symmetry. Additionally, the structure of the collective states under consideration shows also the presence of a good SU(3) quasidynamical symmetry.

To my knowledge, these are the first symplectic-based shell model calculations performed for the description of negative-parity states in atomic nuclei.

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