Microscopic structure of the low-lying negative-parity states in the proton-neutron symplectic model

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Abstract. The proton-neutron symplectic shell-model approach is applied to the description of the microscopic structure of the low-lying negative-parity states of the $K^\pi = 0^-$ and $K^\pi = 1^-$ bands in $^{154}$Sm and $^{238}$U without the introduction of additional degrees of freedom that are inherent to other approaches to odd-parity nuclear states. 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 for these two nuclei. Additionally, the low-energy $B(E1)$ transition strengths between the states of the ground band and $K^\pi = 0^-$ band for the two nuclei are calculated in the extended proton-neutron symplectic model and compared with experiment. The results obtained reproduce well the experimental data for the two nuclei under consideration without the use of an effective charge, which could be considered as a significant achievement of the present approach.

1. Introduction

Experimental spectra in heavy nuclei show the emergence of simple collective patterns represented primarily by the nuclear collective rotation. 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 [1, 2]. Usually, within the phenomenological approach to negative-parity states additional degrees of freedoms are introduced, like octupole or/and dipole (cluster) ones. The microscopic shell-model structure of these low-lying negative-parity rotational states, from another side, is still a challenge for the microscopic many-particle nuclear theory. This is particularly so because the model space dimensionalities rule out the use of standard shell-model theory. As a consequence, different algebraic models which capitalize on symmetries, exact or approximate, have been developed to reduce the model space in manageable size.

In the present work, we present the results of the proton-neutron symplectic shell-model approach [3, 4, 5, 6, 7] which has been applied to the description of the microscopic structure of the low-lying negative-parity states in strongly deformed nuclei, in particular for the $K^\pi = 0^-$ and $K^\pi = 1^-$ bands in $^{154}$Sm and $^{238}$U. Since 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, one needs only to consider the odd symplectic irrep(s) in order to involve the negative-parity states. In this way, we are able to treat the low-lying positive- and negative-parity collective bands on equal footing within the framework of the microscopic symplectic-based shell-model scheme simply by
considering the even and odd irreducible representations of Sp(12,R), without the introduction of additional degrees of freedom inherent to other approaches to odd-parity nuclear states.

2. 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 [8]:

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

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

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

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

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 on two type 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 \(ROT_p(3) \otimes ROT_n(3) \supset ROT(3)\) 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.[8].

The shell-model chain of \(Sp(12,R)\) algebra relates the PNSM to the shell-model nuclear theory and thus providing 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

\[
b_{\alpha,s}^\dagger = \sqrt{\frac{m_\alpha \omega}{2\hbar}} \left( x_{is}(\alpha) - \frac{i}{m_\alpha \omega} p_{is}(\alpha) \right), \tag{5}
\]

\[
b_{\alpha,s} = \sqrt{\frac{m_\alpha \omega}{2\hbar}} \left( x_{is}(\alpha) + \frac{i}{m_\alpha \omega} p_{is}(\alpha) \right).
\]

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 [3]:

\[
F_{ij}(\alpha, \beta) = \sum_{s=1}^{m} b_{\alpha,s}^\dagger b_{j\beta,s}^\dagger, \quad G_{ij}(\alpha, \beta) = \sum_{s=1}^{m} b_{\alpha,s} b_{j\beta,s}, \tag{6}
\]

\[
A_{ij}(\alpha, \beta) = \frac{1}{2} \sum_{s=1}^{m} (b_{\alpha,s}^\dagger b_{j\beta,s} + b_{j\beta,s}^\dagger b_{\alpha,s}). \tag{7}
\]
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

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

for the indices $a \equiv i\alpha$ and $b \equiv j\beta$ taking the values $1, \ldots, 6$. If we introduce 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 an $U(6)$ coupling of these tensor products to the lowest-weight $U(6)$ state $|\sigma\rangle$, one constructs the whole basis of states for an $Sp(12, R)$ irrep

\[
|\Psi(\sigma n p \epsilon \eta)\rangle = [P^{(n)}(F) \times |\sigma\rangle^{\rho E}],
\]

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

\[
Sp(12, R) \supset U(6) \supset SU_p(3) \otimes SU_n(3) \supset SU(3) \supset SO(3) \supset SO(2),
\]

which defines a shell-model coupling scheme. Under different subgroups in (10) are given the corresponding quantum numbers that characterize their irreducible representations plus some multiplicity indices. In this way, the symplectic bandhead (0h\omega space) is determined by the $\sigma$ quantum number. The core collective excitations ($np-nh$ shell-model configurations) are determined by the $n$ and $E$ quantum numbers, whereas the proton/neutron and total deformations are determined by $(\lambda, \mu_n)$ ($\alpha = p, n$) and $(\lambda, \mu)$ respectively. Finally, the rotation is given by the standard angular momentum quantum number $L$ and its third projection $M$.

### 3. Application

We apply the theory to two well deformed nuclei, namely $^{154}\text{Sm}$ and $^{238}\text{U}$. Since in heavy mass regions the spin-orbit interaction is strong, we use the pseudo-$SU(3)$ scheme to determine the relevant irreducible representations of $Sp(12, R)$. The low-lying positive-parity states in $^{154}\text{Sm}$ were described in the lowest even $Sp(12, R)$ irreducible representation, which we denote here as $0h\omega$ $0p-0h$ [30]. Then the negative-parity states are ascribed to the irreducible collective space of the PNSM spanned by the lowest odd $Sp(12, R)$ irrep $1h\omega$ $0p-0h$ [31]. These two $Sp(12, R)$ irreps were given in Refs.[4] and [5], respectively. Similarly, the low-lying positive- and negative-parity states in $^{238}\text{U}$ are described in the state space, spanned by the lowest even $0h\omega$ $0p-0h$ [54] and odd $1h\omega$ $0p-0h$ [55] $Sp(12, R)$ irreducible representations, respectively. These collective subspaces are also restricted to the fully symmetric $U(6)$ irreps only.

For the description of the low-lying positive- and negative-parity states in $^{154}\text{Sm}$ we used the following Hamiltonian

\[
H_I = N h\omega - \frac{1}{2} \chi [Q_p \cdot Q_n - (Q_p \cdot Q_n)_{TE}] - (\xi + \xi_{sym}) C_2 [SU(3)] + aL^2 + \epsilon (N_{h.h.} - N_0),
\]

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). The trace-equivalent part $(Q_p \cdot Q_n)_{TE}$ [9] is subtracted from the collective potential in order to preserve the mean-field shell structure [10, 11, 12].
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 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 0hω and 1hω 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 [3]. Without this term, the negative-parity states would appear at energy $\sim 1h\omega$. 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 in $^{154}$Sm, we use the following parametrization for the inertia parameter $a$: $a = a_0/(1 + 0.63(\Delta N_0))$, where $(\Delta N_0)$ is the eigenvalue of the operator $\Delta N_0 = (N_{b.h.} - N_0)$ described above. We also introduce an additional parameter $\xi_{sym}$ which role is to shift the SU(3) irreps with either $\lambda$ or $\mu$ odd relative to those with $\lambda$ and $\mu$ both even [13], for which $\xi_{sym}$ is zero, as the former belongs to different symmetry types ($B_\alpha$, $\alpha = 1, 2, 3$, rather than $A$) of the intrinsic Vierergruppe [14, 15], $D_2$.  

**Figure 1.** Comparison of the excitation spectra in $^{154}$Sm and $^{238}$U with experiment. The values of the model parameters in MeV are $\chi = 0.0032$, $\xi = 0.0053$, $a_0 = 0.013$, $\epsilon = -6.809$, and $\xi_{sym} = 0$ for $^{154}$Sm, and $\chi = 0.0055$, $\xi = 0.0034$, $a = 0.006$, $k = 0.0101$, $\epsilon = -6.272$ and $\xi_{sym} = 0$ for $^{238}$U, respectively.
Since the full major-shell mixing proton-neutron quadrupole-quadrupole interaction in Eq. (11) is not able to provide the required amount of vertical mixing of U(6) and SU(3) irreps, needed to build up the enhanced quadrupole collectivity, present in $^{238}$U, for the description of collective dynamics in this nucleus we used the following slightly modified Hamiltonian

$$H_{II} = N\hbar \omega - \frac{1}{2} \chi \vec{Q}_p \cdot \vec{Q}_n - (\xi + \xi_{sym}) C_2 [SU(3)] + aL^2$$

$$- k \sum_{\alpha \neq \beta} \left( A^2(\alpha, \alpha) \cdot G^2(\beta, \beta) + G^2(\alpha, \alpha) \cdot G^2(\beta, \beta) + h.c. \right) + \epsilon(N_{b,h.} - N_0),$$

which contain a rather general term of vertical mixing, lying in the enveloping algebra of Sp(12,$\mathcal{R}$). As we said, the $Q_p$, $Q_n$ interaction favors the horizontal mixing over the vertical one, thus it can be replaced by its in-shell U(6)-restricted part $\vec{Q}_p', \vec{Q}_n$, in which $\vec{Q}_{\alpha,m} \simeq A^{2m}(\alpha, \alpha)$ are the components of the truncated Elliott SU(3) quadrupole moment for the proton and neutron subsystems, respectively.

For obtaining the microscopic structure of the low-lying positive- and negative-parity states in $^{154}$Sm and $^{238}$U, the model Hamiltonians (11) and (12), respectively, were diagonalized in the irreducible collective spaces of Sp(12,$\mathcal{R}$) which are defined by the corresponding even and odd symplectic representations, including the shell-model harmonic oscillator configurations from 20 major shells. In Fig. 1, we compare the excitation energies of the $K^\pi = 0_1^-$ and $K^\pi = 1_1^-$ bands together with the ground, $\beta$ and $\gamma$ bands in $^{154}$Sm and $^{238}$U with experiment. Further, in Fig. 2 we compare the odd-even staggering between the states of the ground band and $K^\pi = 0_1^-$ band in $^{154}$Sm and $^{238}$U with experiment. From the latter, we see a good reproduction of the observed staggering function. The staggering pattern of almost constant amplitude [16], shown in Fig. 2 (especially for $^{154}$Sm), also indicates the good (quasi-dynamical) SU(3) character of the states of the ground and $0_1^-$ bands. Usually, this staggering function is introduced in the literature as a measure of the octupole correlations.

![Figure 2](image.png)

**Figure 2.** (Color online) Comparison of the theoretical and experimental staggering function $\Delta E_{\gamma,1}(L) = \frac{1}{16} (6\Delta E(L) - 4\Delta E(L-1) - 4\Delta E(L+1) + \Delta E(L+2) + \Delta E(L-2))$ [16] between the states of the ground band and $0_1^-$ band in $^{154}$Sm and $^{238}$U, respectively.

In Figs. 3 and 4, we give the relevant decompositions of the wave functions of the $K^\pi = 0_1^-$ and $K^\pi = 1_1^-$ bands for three different angular momentum values in $^{154}$Sm and $^{238}$U. For $^{154}$Sm, the calculations show that practically there are no admixtures from the higher shells and hence the presence of a very good U(6) dynamical symmetry. For $^{238}$U, the predominant U(6) irrep that contributes to the structure is that of the lowest weight state (i.e. symplectic bandhead), plus small admixtures from the first few higher shells. From the two figures, 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 figures thus indicates a new kind of symmetry, called quasi-dynamical symmetry [17]. This symmetry is associated with the mathematical concept of embedded representations [18]. Thus, the results for the microscopic structure of the states of $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ negative-parity bands in $^{154}$Sm and $^{238}$U reveal, correspondingly, the presence of a good SU(3) and U(6) quasi-dynamical symmetry, respectively.

**Figure 3.** The SU(3) decomposition of the wave functions of the $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ bands in $^{154}$Sm for three different angular momentum values.

**Figure 4.** The U(6) decomposition of the wave functions of the $K^\pi = 0^-_1$ and $K^\pi = 1^-_1$ bands in $^{238}$U for three different angular momentum values.

With the wave functions obtained we calculate [7] the interband $B(E1)$ transition strengths between the states of the ground band and $K^\pi = 0^-_1$ band in the two nuclei $^{154}$Sm and $^{238}$U. The results are shown in Fig. 5. We recall, that the intraband $B(E2)$ transition strengths between the states of the ground band in these two nuclei, given in Refs. [4, 6], were reproduced very well. We point out that in the calculations, for both the $B(E2)$ and $B(E1)$ transition strengths, no effective charge was used, i.e. $e = 1$. In this regard, remember that the E1 transition operator in self-IBM and spdf-IBM contains three adjustable parameters. Thus, the results obtained for the transition probabilities can be considered as a significant achievement of the present approach.

4. Conclusions
In the present work, 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 and $^{238}$U. For obtaining...
Figure 5. Comparison of the calculated $B(E1)$ values in Weisskopf units between the states of the ground band and $K^\pi = 0^-_1$ band in $^{154}$Sm and $^{238}$U with experiment. No effective charge is used.

the microscopic structure of the low-lying states under consideration, 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 relevant lowest odd irreducible representations 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 for these two nuclei. The calculations show 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. In the case of $^{238}$U, the results show small admixtures from the higher major shells and a highly coherent mixing of different $U(6)$ irreps which is manifested by the presence of a good $U(6)$ quasi-dynamical symmetry in the microscopic structure of the collective states. Additionally, the low-energy $B(E1)$ transition strengths between the states of the ground band and $K^\pi = 0^-_1$ band for the two nuclei are calculated in the extended proton-neutron symplectic model and compared with experiment. The results obtained reproduce well the experimental data for the two nuclei under consideration without the use of an effective charge, which could be considered as a significant achievement of the present approach.

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