Algebraic benchmark for prolate-oblate coexistence in nuclei
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We present a symmetry-based approach for prolate-oblate and spherical-prolate-oblate shape coexistence, in
the framework of the interacting boson model of nuclei. The proposed Hamiltonian conserves the SU(3) and
SU(3) symmetry for the prolate and oblate ground bands and the U(5) symmetry for selected spherical states.
Analytic expressions for quadrupole moments and E2 rates involving these states are derived and isomeric states
are identified by means of selection rules.

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A prominent feature in atomic nuclei, exemplifying a quantal mesoscopic system, is their ability to accommodate
distinct shapes in their low-lying spectrum. Such shape coexistence in the same nucleus is known to occur widely
across the nuclear chart [1,2]. The increased availability of rare isotope beams and advancement in high-resolution spec-
troscopy open new capabilities to investigate such phenomena in nuclei far from stability [3]. Notable empirical examples
include the coexistence of prolate and oblate shapes in the neutron-deficient Kr [4], Se [5], and Hg [6] isotopes and the
triple coexistence of spherical, prolate, and oblate shapes in $^{246}$Pb [7]. A detailed microscopic interpretation of nuclear
shape coexistence is a formidable task. In a shell model description of nuclei near shell closure, it is attributed to the
occurrence of multiparticle-multihole intruder excitations. For medium-heavy nuclei, this necessitates drastic truncations of
large model spaces, e.g., by Monte Carlo sampling [8,9] or by a bosonic approximation of nucleon pairs [10–16]. In a
mean-field approach, based on energy density functionals, the critical point where the corresponding multiple minima are
near degenerate.

The indicated basis states are specified by quantum numbers which are the labels of irreducible representations
of the $\hat{SU}(3)$ algebras in each chain. For a given $\lambda, \mu$, we associate with chains of nested subalgebras. These solvable limits admit
analytic solutions, with closed expressions for observables, quantum numbers, and definite selection rules. The DS chains
with leading subalgebras U(5), SU(3), $\overline{SU}(3)$, and SO(6) correspond to known paradigms of nuclear collective structure:
spherical vibrator and prolate-, oblate-, and $\gamma$-soft deformed rotors, respectively. This identification is consistent with the
geometric visualization of the model, obtained by an energy surface, $E_N(\beta, \gamma)$, defined by the expectation value of the
Hamiltonian in the coherent (intrinsic) state [23,24],

$$
|\beta, \gamma; N\rangle = (N!)^{-1/2}(b^\dagger)^N|0\rangle,
$$

where $b^\dagger = \beta \cos \gamma d^\dagger_1 + \beta \sin \gamma (d^\dagger_{-1} + d^\dagger_{-2})/\sqrt{2} + s^\dagger$. Here
($\beta, \gamma$) are quadrupole shape parameters whose values at the global minimum of $E_N(\beta, \gamma)$ define the equilibrium shape
for a given Hamiltonian. The shape can be spherical ($\beta = 0$) or deformed ($\beta > 0$) with $\gamma = 0$ (prolate), $\gamma = \pi/3$ (oblate),
$0 < \gamma < \pi/3$ (triaxial), or $\gamma$ independent. The standard DS Hamiltonians support a single minimum in their energy surface
and hence serve as benchmarks for the dynamics of a single quadrupole shape. In the present Rapid Communication, we
propose a novel algebraic benchmark for describing the coexistence of prolate-oblate (P-O) shapes with equal $\beta$

deformations and triple coexistence of spherical-prolate-oblate (S-P-O) shapes. We focus on the dynamics in the vicinity of the
critical point where the corresponding multiple minima are near degenerate.

The DS limits appropriate to prolate and oblate shapes correspond, respectively, to the chains [22]

$$
U(6) \supset SU(3) \supset SO(3) \quad |N, (\lambda, \mu), K, L\rangle, \quad (2a)
$$

$$
U(6) \supset \overline{SU}(3) \supset SO(3) \quad |N, (\bar{\lambda}, \bar{\mu}), \bar{K}, L\rangle, \quad (2b)
$$

The indicated basis states are specified by quantum numbers which are the labels of irreducible representations
(irreps) of the algebras in each chain. For a given $N$, the allowed $SU(3)$ [$\overline{SU}(3)$] irreps are $\lambda, \mu = (2N - 4k - 6m, 2k)
[(\bar{\lambda}, \bar{\mu}) = (2k, 2N - 4k - 6m)]$ with $k, m$ non-negative integers. The multiplicity label $K$ ($\bar{K}$) corresponds geometrically to
the projection of the angular momentum ($L$) on the symmetry axis. The basis states are eigenstates of the Casimir operator
$C_2 = [SU(3)]_1$ or $\bar{C}_2 = [\overline{SU}(3)]_1$, where $C_2 = [SU(3)]_1 = 2Q^{(2)} + \frac{1}{2} L^{(1)}, L^{(1)}, Q^{(2)} = d^\dagger s + s^\dagger d^\dagger - \frac{1}{2} \sqrt{\beta} (d^\dagger d^\dagger)^{2}, L^{(1)} = \sqrt{10}(d^\dagger d^\dagger)^{1/2}$.
$\hat{d}_\mu = (-1)^\mu d_{-\mu}$, and $\hat{C}_2[\text{SU}(3)]$ is obtained by replacing $Q^{(2)}_2$ by $\tilde{Q}^{(2)}_2 = d^2 s + s' d + \frac{1}{\sqrt{7}}(d'\tilde{d})^{(2)}$. The generators of SU(3) and $\tilde{\text{SU}}(3)$, $Q^{(2)}_2$ and $\tilde{Q}^{(2)}_2$, and corresponding basis states, are related by a change of phase $(s',s) \rightarrow (s',-s)$, induced by the operator $R_\eta = \exp(i\pi/2\eta)$, with $\eta = s'$. The DS Hamiltonian involves a linear combination of the Casimir operators in a given chain. The spectrum resembles that of an axially deformed rotovibrator composed of SU(3) or SU(3) multiplets forming rotational bands, with $L(L+1)$ splitting generated by $\hat{C}_2[\text{SO}(3)] = L^{(1)}, L^{(1)}$. In the SU(3) or SU(3) DS limit, the lowest irrep $(2N,0)$ or $(0,0N)$ contains the ground band $g(K=0)$ or $g(\bar{K}=0)$ of the oblate (oblate) deformed nucleus. The first excited irrep $(2N-4,2)$ or $(2,2N-4)$ includes both the $\beta(K=0)$ and $\gamma(\bar{K}=2)$ or $\beta(\bar{K}=0)$ and $\gamma(\bar{K}=2)$ bands. Hence, we denote such oblate and oblate bands by $(g_1,\beta,1)$ and $(g_2,\beta,2)$, respectively. Since $R_\eta Q^{(2)}_2 R_\eta^{-1} = -Q^{(2)}_2$, the SU(3) and SU(3) DS spectra are identical and the quadrupole moments of corresponding states differ in sign.

The phase transition between prolate and oblate shapes has been previously studied by varying a control parameter in the IBM Hamiltonian. However, this section mainly discusses the case of spherical-deformed DS for selected spherical states. The construction is based on SU(3) DSs for the prolate and oblate ground bands and the U(5) DS for selected spherical states. The construction is based on an intrinsic-collective pictures of the Hamiltonian, with higher-order SU(3)-invariant IBM interactions. P-O coexistence was considered within the IBM with configuration mixing, using different Hamiltonians for the normal and intruder configurations and a number-conserving mixing term [9–12]. In the present work, we adapt a different strategy. We construct a single number-conserving Hamiltonian which retains the virtues of SU(3) and SU(3) DSs for the prolate and oblate ground bands and the U(5) DS for selected spherical states. The construction is based on an intrinsic-collective resolution of the Hamiltonian, with a procedure used formerly in the study of spherical-deformed shapes.

The intrinsic part of the critical-point Hamiltonian is required to satisfy

\[
\hat{H}|N, (\lambda,\mu) = (2N,0), K = 0, L = 0, (3a) \\
\hat{H}|N, (\bar{\lambda},\bar{\mu}) = (0,2N), \bar{K} = 0, L = 0, (3b)
\]

Equivalently, $\hat{H}$ annihilates the intrinsic states of Eq. (1), with $\beta = \sqrt{2}, \gamma = 0$ and $\beta = -\sqrt{2}, \gamma = 0$, which are the lowest- and highest-weight vectors in the irreps $(2N,0)$ and $(0,2N)$ of SU(3) and SU(3), respectively. The resulting Hamiltonian is found to be

\[
\hat{H} = h_0 P_0^1 \hat{h}_0 P_0 + h_2 P_0^1 \hat{h}_2 P_2 + \eta_3 G_3^1 \cdot \hat{G}_3, (4)
\]

where $P_0^1 = d^1 d^1 + 2 s^2 s^2, G_3^1 = \sqrt{7}(d^1 d^1 + d^1 d^1)$, $G_{3,\mu} = (-1)^{\mu} G_{3,-\mu}$, $\hat{d}_\mu = \sum_\mu d_\mu^\dagger d_\mu$ and the centered dot denotes a scalar product. The corresponding energy surface, $E(N, (\beta,\gamma)) = N(N-1)(N-2)\tilde{E}(\beta,\gamma)$, is given by

\[
\tilde{E}(\beta,\gamma) = ((\beta^2 - 2)(h_0 + h_2 \beta^2) + \eta_3 \beta^6 \sin^2(3 \gamma)) \\
\times (1 + \beta^2)^{-3}. (5)
\]

The surface is even for $\beta$ and $\Gamma = \cos 3 \gamma$, and can be transcribed as $\bar{E}(\beta,\gamma) = z_0 + (1 + \beta^2)^{-3}[A\beta^6 + B\beta^6 \Gamma^2 + D\beta^4 + F\beta^2]$, with $A = -4h_0 + 2h_2 + \eta_3$, $B = -\eta_3$, $D = (11h_0 + 4h_2)$, $F = 4(h_2 - 4h_0)$, $z_0 = 4h_0$. It is the most general form of a surface accommodating degenerate prolate and oblate extrema with equal $\beta$ deformations, for a Hamiltonian with cubic terms $[34,35]$. For $h_0, h_2, \eta_3 > 0$, $\bar{H}$ is positive definite and $\bar{E}(\beta,\gamma)$ has two degenerate global minima, $\beta = \sqrt{2}, \gamma = 0$ and $\beta = -\sqrt{2}, \gamma = \pi/3$ [or equivalently $\beta = \sqrt{2}, \gamma = 0$], at $\bar{E} = 0$, $\beta = 0$ is always an extremum, which is a local minimum (maximum) for $F > 0$ $(F < 0)$, at $\bar{E} = 4h_0$. Additional extremal points include (x) a saddle point: $[\beta_*^2 = 2(4h_0 - h_2)/h_0 - h_2, \gamma = 0, \pi/3]$, at $\bar{E} = 4(h_0 + 2h_2)\eta_3$, and (y) a local maximum and a saddle point: $[\beta_*^2, \gamma = \pi/6]$, at $\bar{E} = 1(1 + \beta_*^2\gamma^2 - 2\beta_*^4) + 2F] + z_0$, where $\beta_*^2$ is a solution of $(D - 3A)\beta_*^4 + 2(F - D)\beta_*^2 = F = 0$. The saddle points, when they exist, support a barrier separating the various minima, as seen in Fig. 1.

The members of the prolate and oblate ground bands, Eq. (3), are zero-energy eigenstates of $\bar{H}(4)$, with good SU(3) and SU(3) symmetry, respectively. For large $N$, the spectrum is harmonic, involving $\beta$ and $\gamma$ vibrations about the respective deformed minima, with frequencies

\[
\epsilon_{\beta_1} = \epsilon_{\beta_2} = \frac{8}{9}(h_0 + 2h_2)N^2, (6a) \\
\epsilon_{\gamma_1} = \epsilon_{\gamma_2} = 4\eta_3 N^2. (6b)
\]

For $h_0 = 0$, also $\beta = 0$ becomes a global minimum at $\bar{E} = 0$, resulting in three degenerate minima, corresponding to triple coexistence of prolate, oblate, and spherical shapes. $\hat{H}(h_0 = 0)$
has the following U(5) basis state:
\[
\hat{H}(h_0 = 0|N,n_d = \tau = L = 0) = 0,
\]
as an eigenstate. Equivalently, it annihilates the intrinsic state of Eq. (1), with \(\beta = 0\). The additional normal modes involve quadrupole vibrations about the spherical minimum, with frequency
\[
\epsilon = 4\hbar^2 N^2.
\]
When \(\beta = 0\) is only a local minimum, the \((n_d = L = 0)\) state experiences a shift of order \(4\hbar^2 N^3\).

The Hamiltonian of Eq. (4) is invariant under a change of sign of the \(s\) bosons and hence commutes with the \(\mathcal{R}_s\) operator mentioned above. Consequently, all nondenerate eigenstates of \(\hat{H}\) have well-defined \(s\) parity. This implies vanishing quadrupole moments for an \(E2\) operator, which is odd under such sign change. To overcome this difficulty, we introduce a small \(s\)-parity-breaking term, \(a\beta_2 = a[-\bar{C}_2[\text{SU}(3)] + 2\bar{N}(2\bar{N} + 3)]\), which contributes to \(E(\beta, \gamma), \bar{a}(1 + \beta^2)^{-\frac{1}{2}}(\beta^2-2) + 2\bar{\beta}^2(2 - 2\bar{\beta}^2\beta^2\gamma^2),\) with \(\bar{a} = a/(N - 2)\). The linear \(\Gamma\) dependence distinguishes the two deformed minima and slightly lifts their degeneracy, as well as that of the normal modes (6). Replacing \(\beta_2\) by \(\tilde{\beta}_2\), associated with \(\bar{C}_2[\text{SU}(3)]\), leads to similar effects but interchanges the role of prolate and oblate bands. Identifying the collective part with \(\bar{C}_2[\text{SO}(3)]\), we arrive at the following complete Hamiltonian:
\[
\hat{H}' = \hat{H}(h_0, h_2, \eta_3) + \alpha \tilde{\beta}_2 + \rho \bar{C}_2[\text{SO}(3)],
\]
where \(\hat{H}(h_0, h_2, \eta_3)\) is the Hamiltonian of Eq. (4).

Figures 1(a)-(1-b)-(1-c) [1(d)-(1-e)-(1-f)] show \(\bar{E}(\beta, \gamma)\), \(\bar{E}(\beta, \gamma = 0)\) and the bandhead spectrum of \(\hat{H}'\) (9), with parameters ensuring P-O [S-P-O] minima. The prolate \(g_1\) band remains solvable with energy \(E_{g1}(L) = \rho L(L + 1)\). The oblate \(g_2\) band experiences a slight shift of order \(\frac{\alpha}{2} N^2\) and displays a rigid-rotor-like spectrum. In the case of P-O coexistence, the SU(3) and SU(3) decomposition in Fig. 2 demonstrates that these bands are pure DS basis states, with \((2N, 0)\) and \((0, 2N)\) characters, respectively, while excited \(\beta\) and \(\gamma\) bands exhibit considerable mixing. In the case of triple S-P-O coexistence, the prolate and oblate bands show similar behavior. A new aspect is the simultaneous occurrence in the spectrum [Fig. 1(f)] of spherical type of states, whose wave functions are dominated by a single \(n_d\) component. As shown in Fig. 3, the lowest spherical states have quantum numbers \((n_d = L = 0)\) and \((n_d = 1, L = 2)\), and hence coincide with pure U(5) basis states, while higher spherical states have a pronounced (\(~70\%) \(n_d = 2\) component. This structure should be contrasted with the U(5) decomposition of deformed states (belonging to the \(g_1\) and \(g_2\) bands) which, as shown in Fig. 3, have a broad \(n_d\) distribution. The purity of selected sets of states with respect to SU(3), SU(3), and U(5), in the presence of other mixed states, are the hallmarks of a partial dynamical symmetry [36,37]. It is remarkable that a simple Hamiltonian, as in Eq. (9), can accommodate simultaneously several incompatible symmetries in a segment of the spectrum.

Since the wave functions for the members of the \(g_1\) and \(g_2\) bands are known, one can derive analytic expressions for their quadrupole moments and \(E2\) transition rates. Considering the \(E2\) operator
\[
T(E2) = e_B d^1 d s + s^1 d,
\]
with an effective charge \(e_B\), the quadrupole moments are found to have equal magnitudes and opposite signs,
\[
Q_L = \mp e_B \sqrt{\frac{16\pi}{40} \frac{L}{2L + 3} \frac{4(2N - L)(2N + L + 1)}{3(2N - 1)}},
\]
where the minus (plus) sign corresponds to the prolate-\(g_1\) (oblate-\(g_2\)) band. The \(B(E2)\) values for intraband \((g_1 \rightarrow g_1, g_2 \rightarrow g_2)\) transitions,
\[
B(E2; g_1, L + 2 \rightarrow g_1, L) = e_B^2 \frac{3(L + 1)(L + 2)(4N - 1)^2(2N - L)(2N + L + 1)}{18(2N - 1)^2},
\]
are the same. These properties are ensured by the fact that \(\mathcal{R}'T(E2)\mathcal{R}^{-1} = \mp T(E2)\). Interband \((g_2 \rightarrow g_1) E2\) transitions, are extremely weak. This follows from the fact that the \(L\) states of the \(g_1\) and \(g_2\) bands vanish, respectively, the \((2N, 0)\) and \((0, 2N)\) irrep of SU(3) and SU(3), \(T(E2)\) as a \((2,2)\) tensor under both algebras can thus connect the \((2N, 0)\) irrep of
g1 only with the (2N − 4, 2) component in g2, which, however, is vanishingly small. The selection rule \( g_1 \leftrightarrow g_2 \) is valid also for a more general \( E2 \) operator, obtained by adding \( Q^{(2)} \) or \( \tilde{Q}^{(2)} \) to the operator of Eq. (10) since the latter, as generators, cannot mix different irreps of SU(3) or \( \text{SU}(3) \). By similar arguments, \( E0 \) transitions in between the \( g_1 \) and \( g_2 \) bands are extremely weak, since the relevant operator, \( T(E0) \propto \hat{n}_d \), is a combination of \( (0, 0) \) and \( (2, 2) \) tensors under both algebras. Accordingly, the \( L = 0 \) bandhead state of the higher \( (g_2) \) band cannot decay to the lower \( g_1 \) band and hence displays characteristic features of an isomeric state. In contrast to \( g_1 \) and \( g_2 \), excited \( \beta \) and \( \gamma \) bands are mixed and hence are connected by \( E2 \) transitions to these ground bands. Their quadrupole moments are found numerically to resemble, for large \( N \), the collective model expression \( Q(K, L) = \frac{3K^2 - (L + 1)(L + 2)}{(L + 1)(2L + 3)} q_K \), with \( q_K > 0 \) \((q_K < 0)\) for prolate (oblate) bands.

In the case of triple \((S-P-O)\) coexistence, since \( T(E2) \) obeys the selection rule \( \Delta n_d = \pm 1 \), the spherical states, \((n_d = L = 0) \) and \((n_d = 1, L = 2)\), have no quadrupole moment and the \( B(E2) \) value for their connecting transition, obeys the \( U(5) \)-DS expression \([22]\)

\[
B(E2; n_d = 1, L = 2 \rightarrow n_d = 0, L = 0) = \varepsilon_0^2 N. \tag{13}
\]

These spherical states have very weak \( E2 \) transitions to the deformed ground bands, because they exhaust the \( (n_d = 0, 1) \) irreps of \( U(5) \), and the \( n_d = 2 \) component in \( (L = 0, 2, 4) \) states of the \( g_1 \) and \( g_2 \) bands is extremely small, of order \( N^{-3/2} \). There are also no \( E0 \) transitions involving these spherical states, since \( T(E0) \) is diagonal in \( n_d \). The lowest \( (n_d = L = 0) \) state has, therefore, the attributes of a spherical isomer state. The analytic expressions of Eqs. (11)–(13) are parameter-free predictions, except for a scale, and can be used to compare with measured values of these observables and to test the underlying SU(3), \( \text{SU}(3) \), and \( U(5) \) partial symmetries.

The proposed Hamiltonian \((9)\) involves three-body interactions. Similar cubic terms were encountered in previous studies within the IBM, in conjunction with triaxiality \([38,39]\), band anharmonicity \([40,41]\), and signature splitting \([42,43]\) in deformed nuclei. Higher-order terms show up naturally in microscopic-inspired IBM Hamiltonians derived by a mapping from self-consistent mean-field calculations \([15,44]\). Near shell closure \( H' \) \((9)\) can be regarded as an effective number-conserving Hamiltonian, which simulates the excluded intruder configurations by means of higher-order terms. Indeed, the energy surfaces of the IBM with configuration mixing \([11,12,45]\) contain higher powers of \( \beta^2 \) and \( \beta^3 \cos 3y \), as in Eq. (5). Recalling the microscopic interpretation of the IBM bosons as images of identical valence-nucleon pairs, the results of the present study suggest that for nuclei far from shell closure, shape coexistence can occur within the same valence space.

As discussed, the coexisting prolate and oblate ground bands of \( H' \) \((9)\) are unmixed and retain their individual SU(3) and \( \text{SU}(3) \) characters. This situation is different from that encountered in the neutron-deficient Kr \([4]\) and Hg \([6]\) isotopes, where the observed structures are strongly mixed. It is in line with the recent evidence for shape coexistence in neutron-rich Sr isotopes, where spherical and prolate-deformed configurations exhibit very weak mixing \([46]\). Band mixing can be incorporated in the present formalism by adding kinetic rotational terms which do not affect the shape of the energy surface \([28–30,35]\) but may destroy the partial symmetry property of the states. The evolution of structure away from the critical point can be studied by varying the coupling constant \( \alpha \) in Eq. (9). Larger values of \( \alpha \) will shift the energy of the nonyrast ground band (the oblate \( g_2 \) band in the example considered). In the case of a triple \( S-P-O \) coexistence, adding an \( n_d \) term to \( H'(n_\beta = 0) \) will leave the \( n_d = 0 \) spherical ground state unchanged but will shift the prolate and oblate bands to higher energy. The same method of intrinsic-collective resolution can be used to identify appropriate Hamiltonians for an asymmetric prolate-oblate coexistence with different \( \beta \) deformations. Details of such extensions and refinements will be reported elsewhere.

In summary, we have presented a number-conserving rotational-invariant Hamiltonian which captures essential features of P-O and S-P-O coexistence in nuclei. It preserves particular symmetries for certain prolate and oblate bands and spherical states, with closed expressions for \( E2 \) moments and transition rates, which are the observables most closely related to the nuclear shape. These attributes turn the proposed framework into a suitable algebraic benchmark for the study of shape coexistence in nuclei, providing a convenient starting point, guidance, and test ground for more detailed treatments of this intriguing phenomena.

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