Shell model description of normal parity bands in odd-mass heavy deformed nuclei

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The low-energy spectra and $B(E2)$ electromagnetic transition strengths of ^{159}Eu, ^{159}Tb, and ^{159}Dy are described using the pseudo SU(3) model. Normal parity bands are built as linear combinations of SU(3) states, which are the direct product of SU(3) proton and neutron states with pseudospin zero (for even number of nucleons) and pseudospin 1/2 (for odd number of nucleons). Each of the many-particle states has a well-defined particle number and total angular momentum. The Hamiltonian includes spherical Nilsson single-particle energies, the quadrupole-quadrupole and pairing interactions, as well as three rotor terms which are diagonal in the SU(3) basis. The pseudo SU(3) model is shown to be a powerful tool to describe odd-mass heavy deformed nuclei.

The shell model is a fundamental theory that is applicable in nuclear, atomic, and nonrelativistic quark physics [1]. In its simplest formulation it provides a natural explanation of magic numbers as shell closures and the energy spectra of closed shell ± 1 odd-mass nuclei [2,3]. Powerful computers and special algorithms for diagonalizing large matrices have allowed systematic studies of nuclei of the sd shell [4] and pf shell up to $A = 56$ [5]. New methods for solving large scale shell-model problems in medium mass nuclei have also been developed [6]. A shell-model description of heavy nuclei requires further assumptions that include a systematic and proper truncation of the model space [1].

In light deformed nuclei the dominance of the quadrupole-quadrupole interaction led to the introduction of the SU(3) shell model [7], and with it a very natural means to truncate large model spaces. Although realistic interactions mix different irreducible representations (irreps), the ground state wave function of well-deformed light nuclei normally consists of only a few SU(3) irreps [8–11]. The strong spin-orbit interaction renders the usual SU(3) scheme useless in heavy nuclei, but at the same time pseudospin emerges as a good symmetry [12–14].

Pseudospin symmetry refers to the experimental fact that single-particle orbitals with $j = l - 1/2$ and $j = (l - 2) + 1/2$ in the shell η lie very close in energy and can therefore be labeled as pseudospin doublets with quantum numbers $\tilde{j} = j$, $\tilde{\eta} = \eta - 1$, and $\tilde{l} = l - 1$. The origin of this symmetry has been traced back to the relativistic Dirac equation [15–17]. The pseudo SU(3) model capitalizes on the existence of pseudospin symmetry.

In the simplest version of the pseudo SU(3) model, the intruder level with opposite parity in each major shell is removed from active consideration and pseudo-orbital and pseudospin angular momentum are assigned to the remaining single-particle states. The coupling of a deformed rigid-rotor core with one extra particle in a pseudo SU(3) orbital has been used to describe rotational bands and electromagnetic properties of heavy odd-mass nuclei [18] and identical normal and superdeformed bands [19].

A fully microscopic description of low-energy bands in even-even nuclei has been developed using the pseudo SU(3) model. The first applications used the pseudo SU(3) as a dynamical symmetry, with a single SU(3) irrep describing the whole yrast band up to backbending [20]. A comparison of quantum rotor and microscopic SU(3) states [21] provided a classification of the SU(3) irreps in terms of their transformation properties under π rotations in the intrinsic frame [22] and led to the construction of a K^2 operator which plays a crucial role in the description of the gamma band [23].

On the computational side, the development of a computer code to calculate reduced matrix elements of physical operators between different SU(3) irreps [24] represented a breakthrough in the development of the pseudo SU(3) model. For example, with this code it is possible to include pairing, which is an SU(3) symmetry breaking interaction, in the Hamiltonian and exhibit its close relationship with triaxiality [25,26]. Full-space calculations in the pf shell [27] in an SU(3) basis [11] show that for a description of the low-energy spectra of deformed nuclei the Hilbert space can be truncated to leading irreps of the quadrupole-quadrupole and spin-orbit (or pseudospin-orbit) interactions. However, the inclusion of a pairing-type interaction is essential for a correct description of moments of inertia in such a truncated space.

Once a basic understanding of this overall structure was achieved, a powerful shell-model theory for a description of normal parity states in heavy deformed nuclei emerged. For example, the low-energy spectra of many Gd and Dy isotopes, their $B(E2)$ and $B(M1)$ transition strengths for both their scissors and twist modes [28] and their fragmentation were successfully described with a realistic Hamiltonian [29].

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TABLE I. The 15 pseudo SU(3) irreps used in the description of ^{159}Tb bands.

(λ_π,μ_π)	(λ_ν,μ_ν)	Total (λ,μ)					
(10,4)	(18,4)	(28,8)	(29,6)	(30,4)	(31,2)	(32,0)	(26,9)
(11,2)	(18,4)	(29,6)	(30,4)	(31,2)			
(10,4)	(20,0)	(30,4)					
(11,2)	(20,0)	(31,2)					
(7,7)	(18,4)	(25,11)	(26,9)				
(10,4)	(16,5)	(26,9)					
(8,5)	(18,4)	(26,9)					

TABLE II. Parameters used in Hamiltonian (3).

	χ	G_π	G_ν	a	b	A_{asym}
^{159}Eu	0.00753	0.132	0.106	-0.0508	0.0009	0.0008
^{159}Tb	0.00753	0.132	0.106	0.0198	-0.0031	0.0008
^{159}Dy	0.00753	0.132	0.106	0.0048	0.0006	0.0008

In the present Rapid Communication we introduce a refined version of the pseudo SU(3) formalism which uses a realistic Hamiltonian with single-particle energies plus quadrupole-quadrupole and monopole pairing interactions with strengths taken from known systematics. The model is applied to three odd-mass rare earth nuclei: ^{159}Eu, ^{159}Tb, and ^{159}Dy. The results represent a full implementation of the very ambitious program implied in first applications of the pseudo SU(3) model to odd-mass nuclei performed nearly 30 years ago [14].

Many-particle states of n_α active nucleons in a given normal parity shell η_α, $\alpha=\nu$, or π, can be classified by the following chains of groups:

$$\{1^{n_\alpha^N}\} \quad \{\tilde{f}_\alpha\} \quad \{f_\alpha\}\gamma_\alpha(\lambda_\alpha,\mu_\alpha) \quad \tilde{S}_\alpha K_\alpha$$

$$U(\Omega_\alpha^N)\supset U(\Omega_\alpha^N/2)\times U(2)\supset SU(3)\times SU(2)\supset$$

$$\tilde{L}_\alpha \qquad\qquad J_\alpha^N$$

$$SO(3)\times SU(2)\supset SU_J(2),$$

(1)

where above each group the quantum numbers that characterize its irreps are given and γ_α and K_α are multiplicity labels of the indicated reductions.

The most important configurations are those with highest spatial symmetry [20,11]. This implies that $\tilde{S}_{\pi,\nu}=0$ or 1/2, that is, only configurations with pseudospin zero for even number of nucleons and 1/2 for odd number of nucleons are taken into account.

We will describe ^{159}Tb as a first example. It has 15 protons and 12 neutrons in the 50-82 and 82-126 shells, respectively. The number of nucleons in normal (N) and abnormal (A) parity orbitals is determined by filling the Nilsson levels with a pair of particles for $\beta\sim0.25$ in order of increasing energy. This gives

$$n_\pi^N=9, \quad n_\pi^A=6, \quad n_\nu^N=8, \quad n_\nu^A=4. \quad (2)$$

After decoupling the pseudospin in Eq. (1) we get $\{\tilde{f}_\pi\}=\{2^41\},\{\tilde{f}_\nu\}=\{2^4\}$ with $\tilde{S}_\pi=1/2$ and $\tilde{S}_\nu=0$. Table I lists the 15 pseudo SU(3) irreps, with the largest value of the Casimir operator C_2, which were used in this calculation.

The Hamiltonian contains spherical Nilsson single-particle terms for protons and neutrons $(H_{sp,\pi[\nu]})$, the quadrupole-quadrupole $(\tilde{Q}\cdot\tilde{Q})$ and pairing $(H_{pair,\pi[\nu]})$ interactions as well as three ''rotorlike'' terms which are diagonal in the SU(3) basis:

$$H=H_{sp,\pi}+H_{sp,\nu}-\frac{1}{2}\chi\tilde{Q}\cdot\tilde{Q}-G_\pi H_{pair,\pi}-G_\nu H_{pair,\nu}+aK_J^2$$

$$+bJ^2+A_{asym}\tilde{C}_2. \quad (3)$$

The term proportional to K_J^2 breaks the SU(3) degeneracy of the different K bands [23], the J^2 term represents a small correction to fine tune the moment of inertia, and the last $\tilde{C}_2$ term is introduced to distinguish between SU(3) irreps with λ and μ both even from the others with one or both odd [22].

The Nilsson single-particle energies as well as the pairing and quadrupole-quadrupole interaction strengths were taken from systematics [30,31]; only a and b were used for fitting. Parameter values are listed in Table II and are consistent with those used in the description of neighboring even-even nuclei [29].

Figure 1(a) shows the calculated and experimental [32] $K=\frac{3}{2}$, $\frac{5}{2}$, and $\frac{1}{2}$ bands for ^{159}Tb. The agreement between theory and experiment is in general excellent. The model predicts a continuation of the $K=\frac{5}{2}$ band and overemphasizes staggering in the $K=\frac{1}{2}$ band.

The role played by each term in the Hamiltonian will be discussed in detail elsewhere [33]. In this Rapid Communication we wish to emphasize that the pairing interaction is absolutely essential despite the strong truncation of the Hilbert space. To this end we present in Fig. 1(b) the low-energy spectra of ^{159}Tb with the same Hamiltonian *except that the pairing interaction has been turned off*. It clearly exhibits the importance of the pairing interaction in building up the correct moment of inertia: the spectra *without* pairing is strongly compressed. It can also be seen that pairing affects the other energies in a similar way with an overall effect that resembles the introduction of a multiplicative factor in the Hamiltonian. We conclude that the proposed truncation scheme is justified and works as expected.

Theoretical and experimental [32] $B(E2)$ transition strengths between yrast states in ^{159}Tb are shown in Table III. The $E2$ transition operator that was used is given by [20]

$$Q_\mu=e_\pi Q_\pi+e_\nu Q_\nu\approx e_\pi\frac{\eta_\pi+1}{\eta_\pi}\tilde{Q}_\pi+e_\nu\frac{\eta_\nu+1}{\eta_\nu}\tilde{Q}_\nu, \quad (4)$$

with effective charges $e_\pi=2.3$, $e_\nu=1.3$. These values are very similar to those used in the pseudo SU(3) description of

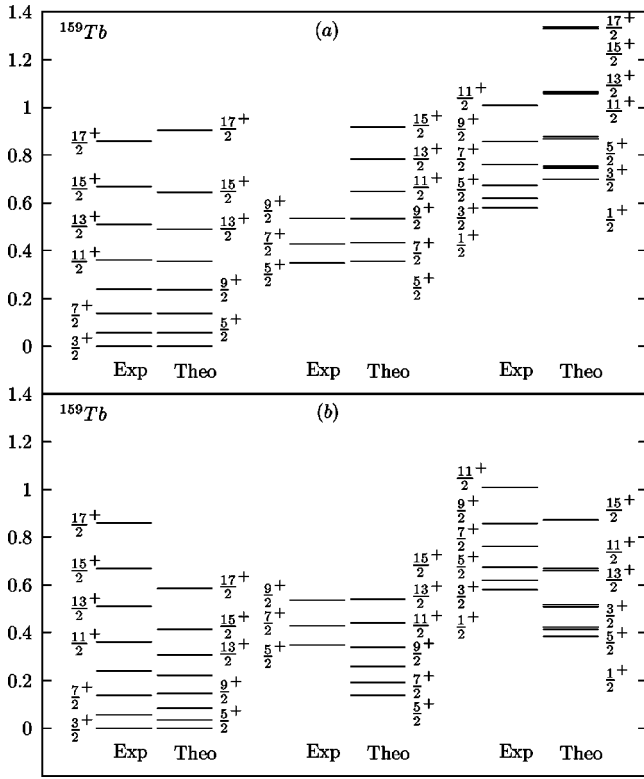FIG. 1. Energy spectra of ^{159}Tb. ''Exp'' represents the experimental results and ''Theo'' the calculated ones. Insert (a) shows the energies obtained with the Hamiltonian parameters listed in Table II, insert (b) shows the energies obtained without pairing.

FIG. 2. (a) Energy spectra of ^{159}Eu and (b) ^{159}Dy, with the same convention of Fig. 1.

even-even nuclei [20,29]. They are larger than those used in standard calculations of $B(E2)$ strengths [30] due to the passive role assigned to nucleons in unique parity orbitals, whose contribution to the quadrupole moments is parametrized in this way.

In Fig. 2(a) we present the low-lying energy spectra of

TABLE III. Theoretical and experimental $B(E2)$ transition strengths for ^{159}Tb.

$J^+ \rightarrow (J+2)^+$	Th. ($e^2\,b^2$)	Expt. ($e^2\,b^2$)
$\frac{3}{2}^+ \rightarrow \frac{7}{2}^+$	1.6503	1.4736 ± 0.2047
$\frac{5}{2}^+ \rightarrow \frac{9}{2}^+$	2.0553	1.8590 ± 0.1023
$\frac{7}{2}^+ \rightarrow \frac{11}{2}^+$	2.1966	2.2180 ± 0.0537
$\frac{9}{2}^+ \rightarrow \frac{13}{2}^+$	2.2464	2.3280 ± 0.0645
$\frac{11}{2}^+ \rightarrow \frac{15}{2}^+$	2.2568	2.1080 ± 0.1433
$\frac{13}{2}^+ \rightarrow \frac{17}{2}^+$	1.4542	1.9867 ± 0.1316

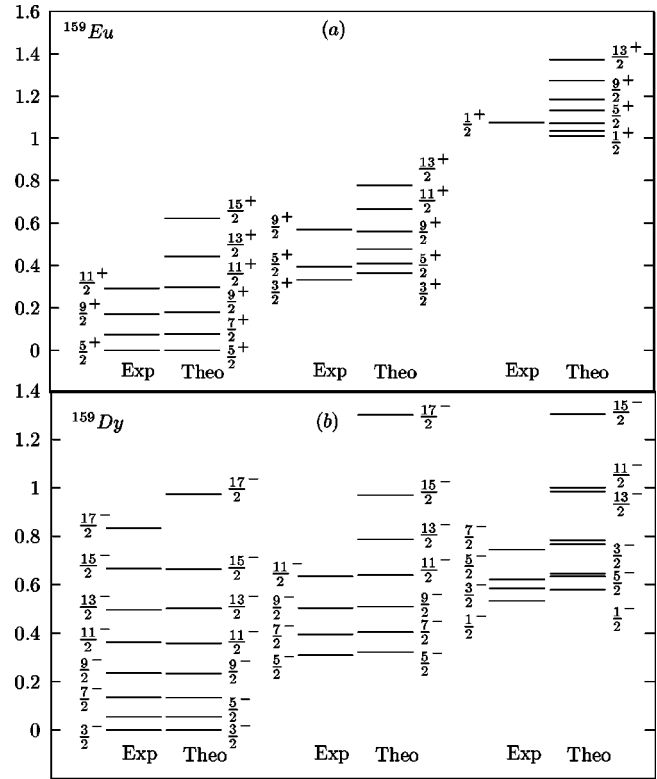| $J^+ \rightarrow (J+1)^+$	Th. ($e^2\,b^2$)	Expt. ($e^2\,b^2$)
$\frac{3}{2}^+ \rightarrow \frac{5}{2}^+$	2.9988	2.8013 ± 0.1458
$\frac{5}{2}^+ \rightarrow \frac{7}{2}^+$	1.6914	1.5691 ± 0.3411
$\frac{7}{2}^+ \rightarrow \frac{9}{2}^+$	1.0471	0.7483 ± 0.0831
$\frac{9}{2}^+ \rightarrow \frac{11}{2}^+$	0.7084	0.6877 ± 0.0675
$\frac{11}{2}^+ \rightarrow \frac{13}{2}^+$	0.5201	0.3761 ± 0.0477
$\frac{13}{2}^+ \rightarrow \frac{15}{2}^+$	0.3726	0.4386 ± 0.0760

^{159}Eu, including the $K=\frac{5}{2},\frac{3}{2}$, and $\frac{1}{2}$ bands built with seven protons in the normal parity subshell $\tilde{\eta}=3$ and 8 neutrons in $\tilde{\eta}=4$. There is a good agreement between the experimental [32] and theoretical results. The model predicts a second $\frac{7}{2}^+$ state in the $K=\frac{3}{2}$ band which is missing in the experimental spectra, as well as several other states in the excited bands.

It is interesting to notice that the ground state in ^{159}Tb is $\frac{3}{2}^+$ while in ^{159}Eu it is $\frac{5}{2}^+$. Reproducing this effect is one of the successes of this theory; realistic single-particle energies are required to get this ordering correct.

The low energy spectra of ^{159}Dy is presented in Fig. 2(b). There are three bands, with $K=\frac{3}{2},\frac{5}{2}$, and $\frac{1}{2}$, respectively. As in the other cases the agreement between theory and experiment is remarkably good. In the $K=\frac{3}{2}$ ground state band the $\frac{17}{2}^-$ state is predicted to have an energy higher than the experimentally observed one. This departure of the experimental ground state band from the rigid rotor behavior may be related with a band crossing. The possibility of describing it by increasing the Hilbert space is under investigation. In the $K=\frac{1}{2}$ band the $\frac{3}{2}^-$ state lies higher than its $\frac{5}{2}^-$ partner which contradicts the experimental results. As in the other cases, the model predicts several excited levels that are as yet undetected.

It has been shown that normal parity bands in odd-mass heavy deformed nuclei can be described quantitatively using the pseudo SU(3) model. Only a few representations with largest C_2 values and pseudo spin 0 or 1/2 are needed. The Hamiltonian uses Nilsson single-particle energies, quadrupole-quadrupole and pairing interactions with

strengths fixed by systematics, and three small rotor terms which with the others yield excellent results for energies and $B(E2)$ values in $A=159$ nuclei.

This work exhibits the usefulness of the pseudo SU(3) model as a shell model, one which can be used to describe deformed rare-earth and actinide isotopes by performing a symmetry dictated truncation of the Hilbert space. It opens up the possibility of a more detailed microscopic description of other properties of heavy deformed nuclei, both with even and odd protons and neutrons numbers, such as g factors, $M1$ transitions, and beta decays.

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