Band structures and deformations of rare-earth nuclei

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Abstract.

We make a systematic theoretical study of Ba, Ce, Nd, Sm, Gd, Dy, Er, Yb, Hf and neighbouring nuclei covering a range of neutron numbers using deformed Hartree-Fock and angular momentum projection theory and present some results here.

1. Introduction

The rotational motion in nuclei is broadly described by the classic model of Bohr and Mottelson and the Nilsson model [1]. For finer description of the states in deformed nuclei, such as band-crossing, rotation-alignment and signature effects in the spectra and electromagnetic transitions etc., one needs a many-body description of the system using two-body interaction among nucleons. In this work we use the deformed Hartree-Fock and Angular Momentum Projection technique and a simple residual interaction to study the spectra, electromagnetic matrix elements and K-isomers of nuclei in the rare-earth region, particularly, Ba, Ce, Nd, Sm, Gd, Dy, Er and Hf isotopes.

2. Deformed Hartree-Fock (HF)

A deformed single-particle state is a superposition of states of various j. Assuming axial symmetric deformation,

\[ | \alpha m > = \sum_j C_j^{\alpha m} | jm > . \]  

(1)

The mixing amplitudes C are the variational parameters in Hartree-Fock theory leading to energy minimization. In the uncoupled representation, the Hartree-Fock equations are [2-5]

\[ (\epsilon_j - \epsilon_{\alpha m})C_j^{\alpha m} + \sum_{j_1j_2j_3j_4m_2} V(j_1m_2j_2m_2; jm_j_4m_2)\rho_{j_4m_2j_2m_2}C_j^{\alpha m} = 0. \]  

(2)

The density matrix is

\[ \rho_{j_4m_2j_2m_2} = \sum_{\alpha(occupied)} C_{j_2}^{\alpha m_2} C_{j_4}^{\alpha m_2}. \]  

(3)
Equations (2) and (3) are solved by iteration to find a self-consistent solution for a nucleus.

2.1. Angular Momentum Projection:
A deformed intrinsic state is a superposition of states of good angular momentum \[ | \Phi_K > = \sum_{I} C_{IK} | \Psi_{IK} > \].

One needs to project out states of good angular momenta from the intrinsic state \( | \Phi_K > \) with the Angular Momentum Projection operator,
\[
P_K^{IM} = \frac{2I + 1}{8\pi^2} \int d\Omega D^I_{MK}^* (\Omega) R(\Omega).
\]

It is important to restore rotational symmetry by such projection operator. As pointed out by Peierls and Yoccoz in their original paper [6], the wave function obtained by using such projection operator gives the correct number of degrees of freedom of a many particle system, since the extra three Euler angles are integrated out to give a state of good angular momentum. The Hamiltonian and multipole matrix elements are given as follows:

\[
\langle \Psi_{K2}^I | H | \Psi_{K1}^I \rangle = \frac{2I + 1}{2} \frac{1}{(N_{K1K2}^I N_{K2K2}^I)^{1/2}} \int d\theta \sin \theta d\theta d_{K2K1}^I K \{ \langle \phi_K^I | H e^{-i\theta J} | \phi_K^I \rangle \}
\]

\[
\langle \Psi_{K1}^I || T^\lambda || \Psi_{K2}^I \rangle =
\]

\[
\frac{(2I_2 + 1)(2I_1 + 1)}{2(N_{K1K1}^I N_{K2K2}^I)^{1/2}} \times \sum_\nu C_{K_1 \nu K_1}^{I_1 \lambda I_1} \int_0^\pi d\theta sin \theta d_{K_2 \nu K_2}^{I_2} (\theta) \times \langle \Phi_K^I | T^\lambda_\nu e^{-i\theta J} | \Phi_K^I \rangle,
\]

where the \( N_{KK'}^I \) stands for wave function overlap (for details refer to [2-5,7-9]).

2.2. Band mixing:
In general two states \( | \Psi_{K1}^I > \) and \( | \Psi_{K2}^I > \) projected from two intrinsic configurations are not orthogonal to each other even if \( | \Phi_{K1} > \) and \( | \Phi_{K2} > \) are orthogonal. Thus, whenever necessary, we do band-mixing using the following equation:

\[
\sum_{K'} (H_{KK'}^I - E_J N_{KK'}^I) C_{K'}^I = 0.
\]

3. Results

We present here deformation parameter \( \beta \), energy spectra, \( B(E2; 0^+ \rightarrow 2^+) \) values and results for \( K^- \) isomers for some deformed nuclei of the rare-earth region [3,5]. In a short space we are able to give a few representative results only. Many more results, including \( B(E2) \) values for higher \( J \) states and magnetic moments, are available with us (also see some of the references given in this paper). It is significant that for the lighter mass nuclei (such as sd shell nuclei), deformed Hartree-Fock and Angular Momentum Projection method gives an adequate description of nuclear spectra [10]. In fact it has been shown that this method gives equivalent result as shell model diagonalization [11]. Here, we have used the above deformed Hartree-Fock and Angular momentum Projection formalism to calculate the deformations, band structures (energies and
B(E2) values of rotational bands) and bands built on various intrinsic states for a number of isotopes in the rare-earth region. In this work and many of our previous works, we use model space consisting of $s_{1/2}, d_{3/2}, d_{5/2}, g_{7/2}, h_{9/2}, i_{13/2}$ orbits for protons and $p_{1/2}, p_{3/2}, f_{5/2}, f_{7/2}, h_{9/2}, i_{13/2}$ orbits for neutrons (Z=50, N=82 core). A surface delta residual interaction is used in the studies. We present here Table and Figures containing results of our calculation and some comparison with available experimental data. Some more results can be seen in some of the references cited.

In Figure 1 we have plotted the quadrupole deformation parameters obtained by deformed Hartree-Fock calculation for Gd, Dy, Er and Yb nuclei. These are prolate deformed nuclei and the main features of the deformation parameters appears satisfactory. The quadrupole deformation peaks around N=100 for these nuclei.

In Figures 2 and 3, we have shown the spectra of $^{168}$Er and $^{164}$Hf (E versus J plot) respectively. For $^{168}$Er the lowest few rotational states known experimentally are quite well reproduced in the present theory. $^{164}$Hf is a very neutron-deficient nucleus away from the stability valley. We have plotted the $K = 0^+$ ground band for this nucleus as well as the $K = 1^+$ rotation-aligned (RAL) band (involving $i_{13/2}$ neutrons in low Ω orbits). The $K = 1^+$ RAL band shows pronounced signature effect [4,5,7-9]. It crosses the ground band around $J = 14\hbar$. Although experimental data for $^{164}$Hf are so far scarce, this nucleus should be amenable to study by (HI,xn) reactions with gamma-ray arrays.

**Figure 1.** Quadrupole deformation parameter for Gd, Dy, Er and Yb isotopes.

**Figure 2.** Excitation energy of $^{168}$Er with angular momentum. The experimental values are also shown for comparison, wherever available.

**Figure 3.** The $K = 0^+$ and RAL band energy with various angular momentum $J$ is shown for $^{164}$Hf.
In Figure 4 and 5, we have plotted the B(E2; 0+ → 2+) values for Gadolinium and Dysprosium nuclei. Some of the experimentally known B(E2; 0+ → 2+) values are also given in these figures. Since we are using a small model space (only one major shell for each of protons and neutrons) one needs effective charges for evaluating the electromagnetic matrix elements. Effective charges 1.8e and 0.8e are used for protons and neutrons respectively.

In Figure 6, we have plotted the energy spectra of the K = 0+ ground band and the K = 6+ and K = 8− K-isomeric bands of 172Hf and compare with the available experimental data. The quality of agreement appears good.

In Figures 7 and 8, we show the Hartree-Fock orbits and the spectra of the low energy bands of 169Re [5]. The lowest energy intrinsic states have K = 9/2− and K = 1/2−. The angular momentum projected spectra of these two bands are shown in Figure 4 and compared with available experimental data. The K = 9/2− band is crossed by a K = 11/2− band with neutron excitation to 13/2 orbits across the neutron Fermi surface around Jπ = 29/2−, leading to an anomalous spacing of energy levels around this J. This agrees fairly with the compression of energy levels seen in the experimental spectrum (see comparison in Figure 8).

The K = 1/2− band of 169Re is based on the mπ = 1/2− state which is mainly of h9/2 proton origin, with a very small h11/2 admixture. It leads to two branches on angular momentum
projection. The favored branch has $J^\pi = 1/2^-, 5/2^-, 9/2^-, 11/2^-$, ...... with $J = 5/2^-$ the lowest in energy. Except for the anomalously low $J = 3/2^-$ of experiment, all other aspects of the favored branch are well reproduced in the calculation. The unfavored branch has not been seen experimentally so far and is predicted in the calculation.

Table 1. Bandhead Energy, Quadrupole moment and Magnetic moment of some Isomeric configurations.

| Isotope | $K^\pi$ | BHE | $Q_S\ [eb]$ | $\mu\ [\mu_N]$ |
|---------|---------|-----|-------------|----------------|
|         | Th.     | Expt. | Th. | Expt. | Th. | Expt. |
| $^{172}$Hf | $6^+$ | 1.210 | 1.685 | 3.29 | 5.4726 | 5.59 ± 0.61 |
| $^{173}$Hf | $8^-$ | 1.311 | 2.006 | 3.55 | 7.63 | 7.955 ± 0.65 |
| $^{178}$Hf | $23^-$ | 0.494 | 1.982 | 4.17 | 7.0858 | 6.63 ± 0.23 |
| $^{178}$Hf | $8^-$ | 1.097 | 1.479 | 4.651 | 7.542 |
| $^{177}$Lu | $23^-$ | 0.707 | 0.970 | 5.315 | 5.71 | 2.590 | 2.93 ± 0.17 |
| $^{179}$W | $33^-$ | 1.741 | 3.535 | 5.394 | 4.73 | 6.076 | 8.31 |

We have studied the K-isomers of some of the nuclei in this region of deformed nuclei and present a few such results in Table 1 for Hafnium and $^{177}$Lu and $^{179}$W nuclei (where the proton and neutron Fermi surfaces are near orbits with relatively high $\Omega$). The band-head energies, spectroscopic quadrupole moments and the magnetic moments of the band-head states are presented and are compared with experimental data. There is a fair degree of agreement between our calculation and the experimental data.
In [12, 13] the experimental results of bands in deformed nuclei have been reasonably well interpreted in the framework of the HF and J projection model. We have many such results for nuclei in this region [5,12, 13 and refs. there in]. On the whole deformed Hartree-Fock and Angular Momentum Projection theory, with band mixing, is able to describe well the essential aspects of the spectra of the deformed nuclei in the rare-earth region [9]. It is good to see that the deformed HF and Angular Momentum Projection method, so successful for the lighter sd shell nuclei, gives quantitative results for the spectra of deformed nuclei in the rare-earth region. In some earlier works the Deformed Hartree-Fock and Angular Momentum Projection theory gave quite sensible results for the shapes and spectra of mercury nuclei [7,14]. Thus the model is an accurate representation of the shell model dynamics for deformed nuclei [11] and is able to explain the various features of rotational bands in a theoretically satisfactory way. It is a number-conserving theory and gives states of good angular momenta.

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