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Nuclear Shape Phase Transition in Er-Yb-Hf Isotopes Using the Interacting Boson Model

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In terms of the standard interacting boson model (sd-IBM)with one and two body interactions , the nuclear shape phase transition from spherical vibrator U(S) to axially deformed rotator SU(3) is studied in intrinsic coherent state . The results are applied to the even even Er-Yb-Hf Isotopic chain. A fitting procedure is performed to get the parameters of the model for each nucleus of the isotopic chain in order to obtain a minimum root mean square (rms) deviation between the calculated and the experimental selected energy levels, E2 transition rates and two- neutron separation energies. The potential energy surfaces (PES 'S) and the critical points are analyzed in a search for shape phase transitions . The behavior of energy and B(E2) ratios in the ground state band are examined.

Keywords: *Nuclear shape phase transition, IBM, PES,s , energy and B(E2) ratios*

1. INTRODUCTION

The original version of interacting boson model (sd- IBM-1) provides an elegant and powerful tool for description of collective nuclei [1].In this model , collective excitations in even- even nuclei are described in terms of a system of fixed number N of bosons of two types : monopole (s) and quadrupole (d) bosons with angular momenta $L^{\pi} = 0^{+}$ and 2^{+} respectively. The six boson creation operators [$s^{\dagger}$, $d_{\mu}^{\dagger}$ ($\mu = 0, \pm 1, \pm 2$)] and six boson annihilation operators [s, $\tilde{d}_{\mu}$ ($\mu = 0, \pm 1, \pm 2$)] , satisfy standard boson commutator relations. The structure of the model is determined by the U (6) group algebra generated by 36 bilinear - combinations of these boson operators. The IBM Hamiltonian can be expressed as a superposition's of the first and second order Casimir operators of the groups entering the reduction chains of the U (6) group. The group structure leads to only three limiting dynamical symmetries U (5), SU (3) and O (6), which correspond to the three limiting cases, vibrational, rotational and γ - unstable nuclei respectively.

Recently the study of shape phase transitions is one of the most exciting topics nuclear structure .The interacting boson model (IBM) [1] and the geometric collective model (GCM) [2-4] represent two major models that successfully describe nuclear shape transitions [5-12].Shape phase transitions from one nuclear shape to another were first discussed [13] applying catastrophe theory [14] obtained in the classical limits of the IBM. A first order phase transition has been found in the transition U(5)- SU(3) , while a second order phase transition in U(5)-O(6). In particular the critical symmetry E(5) [15] has been suggested to describe critical points in the phase transition from spherical U(5) to γ – unstable O(6) shapes, while X(5) [16] is designed to describe critical points in the phase transition from spherical U(5) to axially deformed SU(3) shapes. In addition, the Y(5) symmetry [17] has suggested the importance of considering phase transition from axially deformed to triaxial nuclei . Since the IBM was formulated from the beginning in terms of creation and annihilation boson operators, its geometric interpretation in terms of the shape variable is usually done by introducing the intrinsic coherent state [18, 19] with two shape deformation parameters β and γ.

The purpose of this paper is to investigate shape phase transitions within the IBM-1 using intrinsic coherent state for Er-Yb-Hf isotopic chains , in which the occurrence of shape transitions from U(5) to SU(3) has been predicted, and show the dependence of the potential energy surfaces PES 's on the total number of bosons. The paper is organized as follows. In section 2, we constructed the IBM Hamiltonian in terms of multipole operators and using the intrinsic coherent state. In section 3 we generated the PES 's. The location of the critical points in the shape transition is identified in section 4. In section 5, a systematic study of Er-Yb-Hf isotropic chains related to the U(5)- SU(3) shape transition is given .The main conclusion arising from the present results are discussed in section 6.

2. THEORETICAL PROCEDURE

The Hamiltonian adopted in the following includes a vibrational term and rotational term include quadrupole quadrupole interaction i.e breaking the SU(3) Hamiltonian by inclusion of the vibrational term which characterize the U(5) dynamical symmetry

$$H = \varepsilon\, \hat{n}_d + a_1 \hat{L}\,.\,\hat{L} + a_2\, Q^x.\, Q^x \tag{1}$$

Where (dot) denotes scalar product, $\hat{n}_d$ is the boson number operator, $\hat{L}$ is the angular momentum operator and Q^x is the boson quadrupole operator defined as:

$$\hat{n}_d = \left(\mathrm{d}^{\dagger}\ \mathrm{x}\ \tilde{\mathrm{d}}\right)^{(0)} \tag{2}$$

$$\hat{L} = \sqrt{10}\ \left(\mathrm{d}^{\dagger}\ \mathrm{x}\ \tilde{\mathrm{d}}\right)^{(1)} \tag{3}$$

$$\hat{Q}^x = \left(\mathrm{s}^{\dagger}\ \mathrm{x}\ \tilde{\mathrm{d}} + \mathrm{d}^{\dagger}\ \mathrm{x}\ \tilde{\mathrm{s}}\right)^{(2)} + x\,(\mathrm{d}^{\dagger}\ \mathrm{x}\ \tilde{\mathrm{d}})^{(2)} \tag{4}$$

Here $\tilde{\mathrm{s}} = \mathrm{s}$, $\tilde{\mathrm{d}}_m = (-1)^m\, \mathrm{d}_{-m}$ and χ is a structure parameter.

Equation (1) defines an IBM-1 Hamiltonian in terms of four model parameters ε, a_1 , a_2 and χ . The connection between the IBM, PES's, geometric shapes and shape phase transitions can be investigated by introducing the intrinsic coherent state defined by [20]

$$|N\beta\gamma\rangle = \frac{1}{\sqrt{N!}}\,(b_c^{\dagger})^N\,|0\rangle \tag{5}$$

based on the boson creation operator of the form

$$b_c^{\dagger} = \frac{1}{\sqrt{1+\beta^2}}\left[\mathrm{s}^{\dagger} + \beta\,\cos\, d_0^{\dagger} + \frac{1}{\sqrt{2}}\beta\,\sin\gamma\left(d_2^{\dagger} + d_{-2}^{\dagger}\right)\right] \tag{6}$$

N is the total number of bosons which is equal to the number of nucleon pairs in the valence space, (β, γ) are the basic deformation parameters which determine the geometry of the nuclear surface. Spherical shapes are characterized by β = 0 and deformed ones by β ≠ 0. The angle γ allows one to distinguish between axially symmetric deformed nuclei, $\gamma = 0^0$ for prolate and $\gamma = 60^0$ for oblate deformation and $0^0 < \gamma < 60^0$ for triaxial nuclei.

3. THE POTENTIAL ENERGY SURFACES (PES,S)

The PES's are determined by calculating the expectation value of the Hamiltonian

$$E(N,\beta,\gamma,x) = \frac{\langle N\ \beta\ \gamma|H|N\ \beta\ \gamma\rangle}{\langle N\ \beta\ \gamma|N\ \beta\ \gamma\rangle} \tag{7}$$

The intrinsic coherent state $|N\beta\gamma\rangle$ is normalized.

For distinct values of (β,γ) , we have the overlap

$$\langle N\,\hat{\beta}\,\hat{\gamma}|H|N\,\beta\,\gamma\rangle = \frac{\left[1+\beta\hat{\beta}\cos(\gamma-\hat{\gamma})\right]^N}{(1+\beta^2)^{\frac{N}{2}}\left(1+\hat{\beta}^2\right)^{\frac{N}{2}}}$$

$$N \to \infty$$

$$\to exp.\left[N\beta\hat{\beta}\cos(\gamma-\hat{\gamma}) - \frac{1}{2}N\left(\beta^2+\hat{\beta}^2\right)\right] \quad (8)$$

The matrix elements of each operators in the Hamiltonian are calculated using the concept of Ginocchio and Kirson [21].

The expectation value E (N, β, γ , χ)in the ground state can be written in the form

$$E(N,\beta,\gamma,x) = \sum_{k,l}\frac{a_{kl}\,\beta^{2k+3l}cos^l 3\gamma}{(1+\beta^2)^2} + a_0 \quad (9)$$

Hamiltonian parameters ε, a_1,a_2 in equation (1), and are given by :

$$a_{10} = [\varepsilon + 6a_1 + (x^2 - 8 + 4N)a_2]N \quad (10)$$

$$a_{01} = -4\sqrt{\frac{2}{7}}\; x\, a_2(N-1)N \quad (11)$$

$$a_{20} = \left[\varepsilon + 6a_1 + (\frac{2N+5}{7}x^2 - 4)a_2\right]N \quad (12)$$

$$a_0 = 5a_2N \quad (13)$$

4. CRITICALITY CONDITIONS

To examine the PES's , a phase transitions might occur when the order parameters a_{kl} varied and pass through a critical points. Since the parameter a_{01} controls the steepness of the potential, therefore, the dynamical fluctuations is strongly affects the energies of excited intrinsic states. The parameter a_{01} = 0 gives a γ - flat potential and a decrease of a_{01} introduces a γ - dependence, the potential with a minimum at γ =0. Changing a_{01} will indeed induce a γ - unstable to symmetric rotor transition. It best to simultaneously vary a_{10} and a_{20} as well.

One needs to determine the locus of points for which the first derivative of equation (9) must be zero and the second derivative must be positive, this gives for γ =0, the following

$$\beta[2a_{10} + 3a_{01}\beta + (4a_{20} - 2a_{10})\beta^2 - a_{01}\beta^3] = 0 \quad (14)$$

And

$$a_{10} + 3a_{01}\beta + (6a_{20} - 8a_{10})\beta^2 - 8a_{01}\beta^3 - (6a_{20} - 3a_{10})\beta^4 + a_{01}\beta^5 \; > 0 \quad (15)$$

One minimum occurs at β=0, this corresponding to the spherical phase

($a_{10} > a^2_{01}$ / 4 | a_{20} |) and a deformed phase β>0 appears for a_{01} < 0 and ($a_{10} < a^2_{01}$ / 4 | a_{20} |).

For $x = -\sqrt{7}/2$, γ > 0 and a_1= 3 a_2 / 8 and eliminating the contribution of the one body terms of the quadrupole - quadrupole interaction , the PES / Nε take the form

$$\frac{E(\beta)}{N\varepsilon} = \frac{(1-4\lambda)\beta^2 + 2\sqrt{2}\,\lambda\,\beta^3 + (1-\frac{1}{2}\lambda)\beta^4}{(1+\beta^2)^2} + \frac{5}{\varepsilon}a_2 \quad (16)$$

With $\lambda = -a_2(N-1)/\varepsilon$

If $(2\sqrt{2}\,\lambda)^2 = 4(1-4\lambda)(1-\frac{1}{2}\lambda)$, the critical point is at λ_c = 2/9 or $\varepsilon = -(9/2)(N-1)\,a_2$ and the equilibrium value of the deformation parameter at λ_c is $\beta_c = (2\sqrt{2}\,\lambda)/2(1-1/2\,\lambda) = 1/2\sqrt{2}$

For the vibrational limit U (5), the corresponding critical point is at β=0, while for the rotational limit SU(3) with $x = -\sqrt{7}/2$, ε = 0 and a_1 = 0 and eliminating the contribution of the one body terms of the quadrupole - quadrupole interaction , yield

$$a_{10} = 4a_2(N-1)N \tag{17}$$

$$a_{01} = 2\sqrt{2}a_2(N-1)N \tag{18}$$

$$a_{20} = \frac{1}{2}a_2(N-1)N \tag{19}$$

and the PES take the form

$$E(\beta) = \frac{1}{2}a_2N(N-1)\frac{8\beta^2 + 4\sqrt{2}\,\beta^3 + \beta^4}{(1+\beta^2)^2} \tag{20}$$

and the equilibrium value is obtained by solving the equation

$$4 + 3\sqrt{2}\beta - 3\beta^2 - \sqrt{2}\beta^3 = 0 \tag{21}$$

which yield $\beta = \sqrt{2}$ (for prolate γ =0)

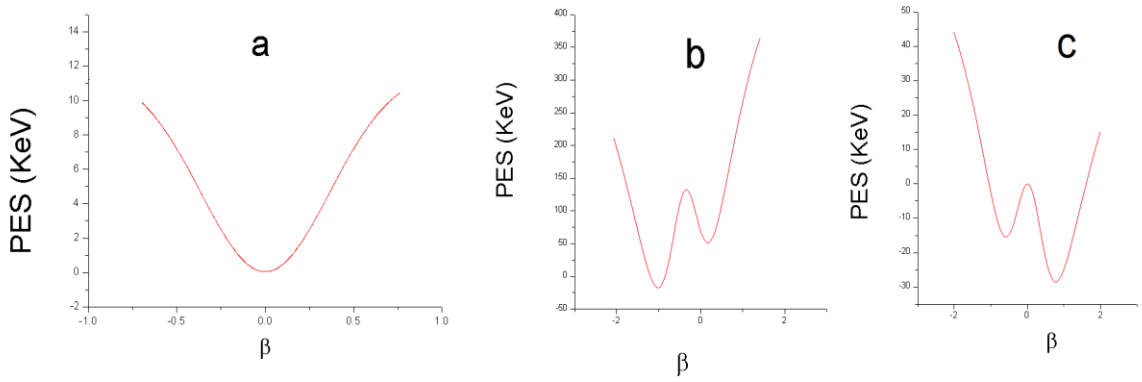

Fig1. *Illustrate the PES,s for the pure harmonic oscillator and the axial symmetric rotator.*

Figure (1). The PES's as a function of the deformation parameter β(a)for vibrator(a_{10} =4 5,a_{01} = a_{20} =0) and(b),(c) for symmetric rotator(a_{10} =-110,a_{01} = -40 , a_{20} =580),(a_{10} =-135,a_{01} = -45, a_{20} =80).

To investigate the U(5)- SU(3), we show in Figure(2) , the PES's for N=10 and $x = -\sqrt{7}/2$ for a set of significant values of the model parameters listed in Table(1) .

Table1. *The set of IBM parameters to describe shape - phase transition from vibrator (q) to rotator (f), the critical point is at (c). The boson number N=10 and structure parameter χ is fixed at* $-\sqrt{7}/2$

Curve	a_0	a_{10}	a_{01}	a_{20}
A	0	10	0	10
B	-0.6337	0.6521	-3.2265	4.6448
C	-0.6400	0.5600	-3.2583	4.5920
D	-0.6775	0.0068	-3.4492	4.2751
F	-1.2500	-8.4375	-6.3639	-0.5625

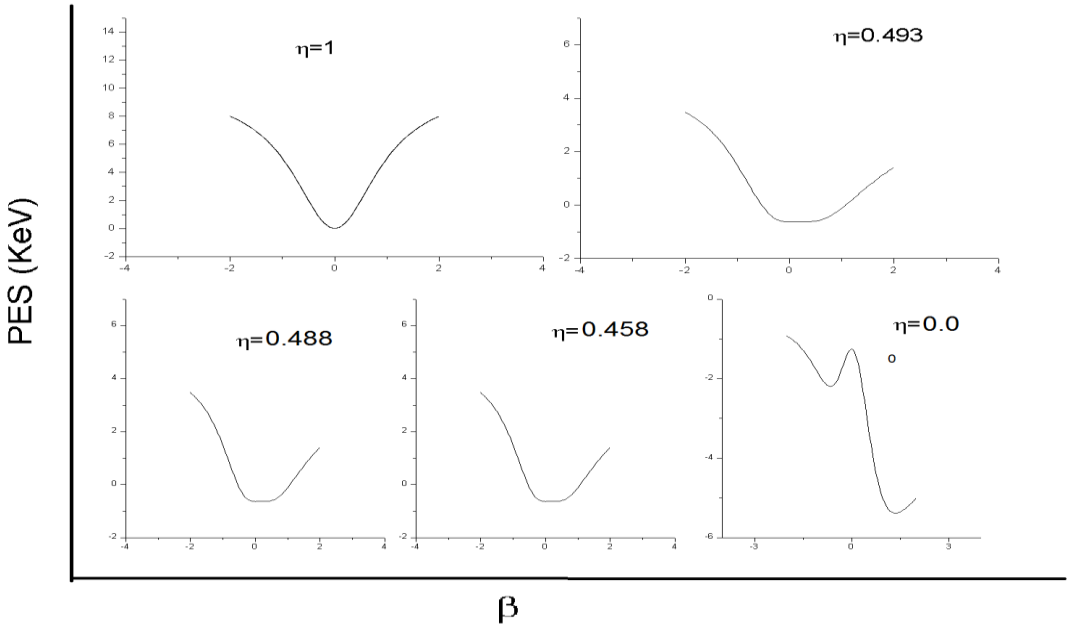

Fig2. *The PES's as a function of the deformation parameter βfor shape phase transition from vibrator(panel a) to rotator (panel f) , the critical point is at(panel c).The boson number is N=10 and the structure parameter χ is fixed at $-\sqrt{7}/2$.*

We observe the evoluation from a spherical potential (a) whose minimum is found at β=0, to potential with well deformed (f) . In particular (c), the spherical and the prolate deformed minima are degenerate and this condition defines the critical point of the first order phase transition.

5. ENERGY RATIOS AND ELECTRIC QUADRUPOLE TRANSITION PROBABILITIES.

To get the characteristics of the evoluation of the collectivity in even- even nuclei, the behavior of the energy ratios $R_{I/2}$ = E (I)/ E (2) will be studied

$$R_{1/2} = \begin{cases} \frac{I}{2} & for \;\; U(5) \\ I(I+1) & for \;\; U(3) \end{cases} \tag{22}$$

While energy levels give important clues as to the existence of symmetries, better inferences are gained by a study of electric quadrupole transition between states. The E2 transitions provide more stringent test of the model. In the IBM, the most general E2 transition operator is written as [22]

$$T(E2) = \alpha_2 \left(s^{\dagger} \times \tilde{d} + d^{\dagger} \times \tilde{s} \right)^{(2)} + \beta_2 \, (d^{\dagger} \times \tilde{d})^{(2)} \tag{23}$$

where α_2 is the boson effective charge determined from the fit to the B(E2,$2_1^+ \rightarrow 0_1^+$) and β_2 may be determined from the quadrupole moment Q(2_1^+). The ratio $\beta_2 / \alpha_2 = x = -\sqrt{7}/2$ in the SU (3) limit.

It is commonly assumed that the ratios of the B (E2) reduced transition probabilities between levels of the ground state band takes the values between vibrational and rotational limits. The B(E2) ratios for the dynamical symmetry limits U(5) and SU(3) of the IBM are :

$$B_{I+2/2} = \frac{B(E2, I+2 \rightarrow I)}{B(E2, 2_1^+ \rightarrow 0_1^+)} = \begin{cases} \frac{1}{2}(I+2)(1-\frac{I}{2N}) & for \;\; U(5) \\ \frac{15}{2}\frac{(I+2)(I+1)}{(2I+3)(2I+5)}\left(1-\frac{I}{2N}\right)(1+\frac{I}{2N+3}) & for \;\; U(3) \end{cases} \tag{24}$$

i.e $B_{4/2} \rightarrow 2$ for U(5) and $B_{4/2} \rightarrow 10/7$ for SU(3)

6. APPLICATION TO EVEN- EVEN ER-YB- HF ISOTOPES

Nuclei in rare – earth elements are well known examples of the U(5) – SU(3) transitions which exhibit a transition of nuclear shape from spherical to deformed form. In our calculations we will apply the formalism outlined in the previous sections to the rare earth $^{154\text{-}168}$ Er, $^{156\text{-}172}$ Yb and $^{160\text{-}175}$ Hf isotopes with total number of bosons from 8 to 16.

First , energy levels $E(I_i)$, E2 transition rates B(E2) and two neutron separation energies $S_2n(I)$ are selected and fitted with our IBM -1 Hamiltonian equation (1).

A computer simulated search program has been used to get a minimum root – mean- square (rms) deviations between the experimental data and the calculated ones derived from our present four parameters model. The quality of the fitting is indicated by the common definition of the chi:

$$x\left(E(I)\right) = \sqrt{\frac{1}{N_E}\sum_i (E^{exp}(I_i) - E^{cal}(I_i))^2}$$

$$x\left(B(E2)\right) = \sqrt{\frac{1}{N_{B(E2)}}\sum_i (B(E2)_i^{exp} - B(E2)_i^{cal})^2}$$

$$x\left(S_n\right) = \sqrt{\frac{1}{N_{S_n}}\sum_i ({S_n}^{exp}(i) - {S_n}^{cal}(i))^2}$$

Where the sums are over the available data points N_E, $N_{B\,(E2)}$ and N_{Sn} in number respectively. The experimental data are taken from the National Nuclear Data Center (NNDC) and (ENSDF) [23]. The best adopted model parameters a_0,a_{10},a_{01} and a_{20} for each nucleus are listed in Table (2).

Table2. *The model parameters a_0,a_{10},a_{01},a_{20} (all in KeV) as derived in fitting procedure used in the calculation for Er-Yb -Hf isotopic chains*

Nuclei	A	N_B	a_0	a_{10}	a_{01}	a_{20}
	154	9	-0.3750	4.1458	1.0904	6.4219
	156	10	-0.6875	0.0471	-1.6404	4.8612
	158	11	-0.7875	-1.6586	-2.0541	4.4739
$_{68}$Er	160	12	-0.865	-3.0403	-2.3636	4.1401
	162	13	-0.9375	-5.0526	-2.5496	3.7667
	164	14	-1.0500	-7.8687	-2.1596	2.9444
	166	15	-1.1375	-10.5018	-2.1110	2.1506
	168	16	-1.0250	-8.7062	-2.3668	3.5595
	156	8	-0.5125	2.2587	-0.16687	5.1262
	158	9	-0.7250	-0.2876	-0.5704	4.3347
	160	10	-0.8625	-2.4411	-1.1617	3.7145
$_{70}$Yb	162	11	-0.9000	-4.8400	-1.6163	3.6775
	164	12	-0.9125	-4.1093	-2.2319	3.7655
	166	13	-0.9125	-4.5813	-2.7158	3.9681
	168	14	-0.9250	-5.3088	-3.1366	4.0554
	170	15	-0.8750	-4.6984	-3.9287	4.7078
	172	16	-0.7750	-2.8232	-5.9652	5.5202
	160	8	-0.7000	0.1474	-0.6285	4.0422
	162	9	-0.8125	-1.4686	-1.0284	3.7269
	164	10	-0.8750	-2.6354	-1.5153	3.5734
	166	11	-0.8625	-2.8484	-1.9547	3.9131
$_{72}$Hf	168	12	-0.8750	-3.4630	-2.4694	4.0390
	170	13	-0.8375	-3.1845	-3.3950	4.4970
	172	14	-0.8250	-3.2764	-3.8524	4.8711
	174	15	-0.7625	-2.2645	-5.0213	5.5373
	176	16	-0.5625	-3.6497	-5.0031	5.4584

The structure parameters χ was fixed at $-\sqrt{7}/2$. For all nuclei in the isotopic chains investigated here, the geometric character can be declared by plotting the PES's obtained from the IBM-1 Hamiltonian versus the deformation parameters β .This is illustrated in Figures (3-5).

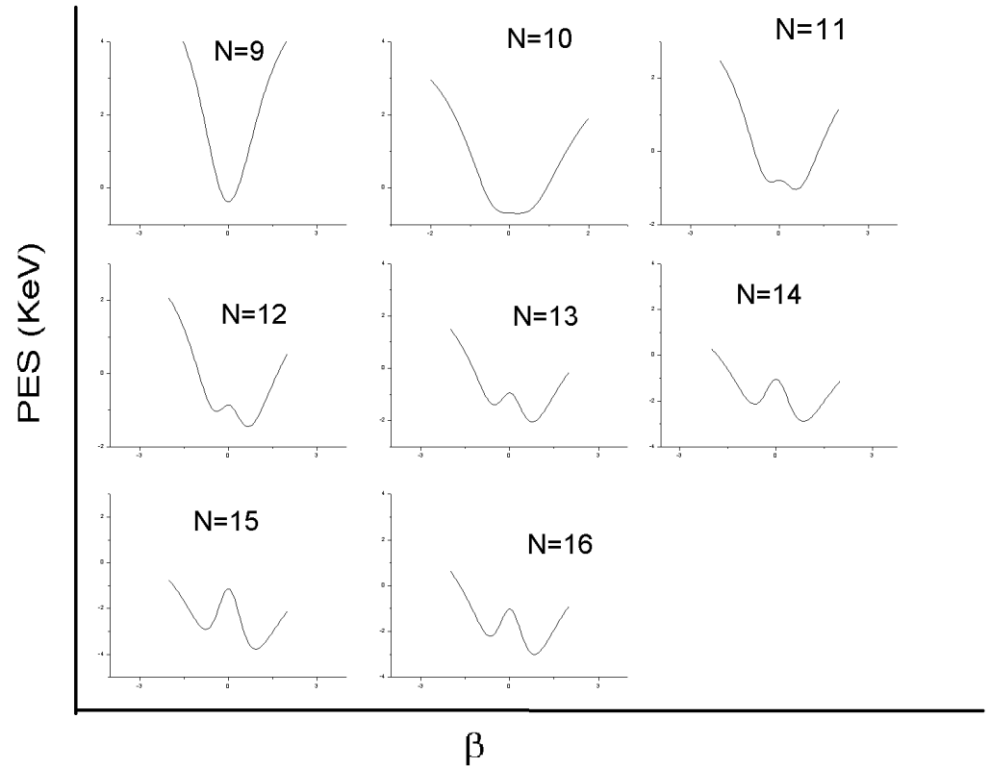

Fig3. *Er*

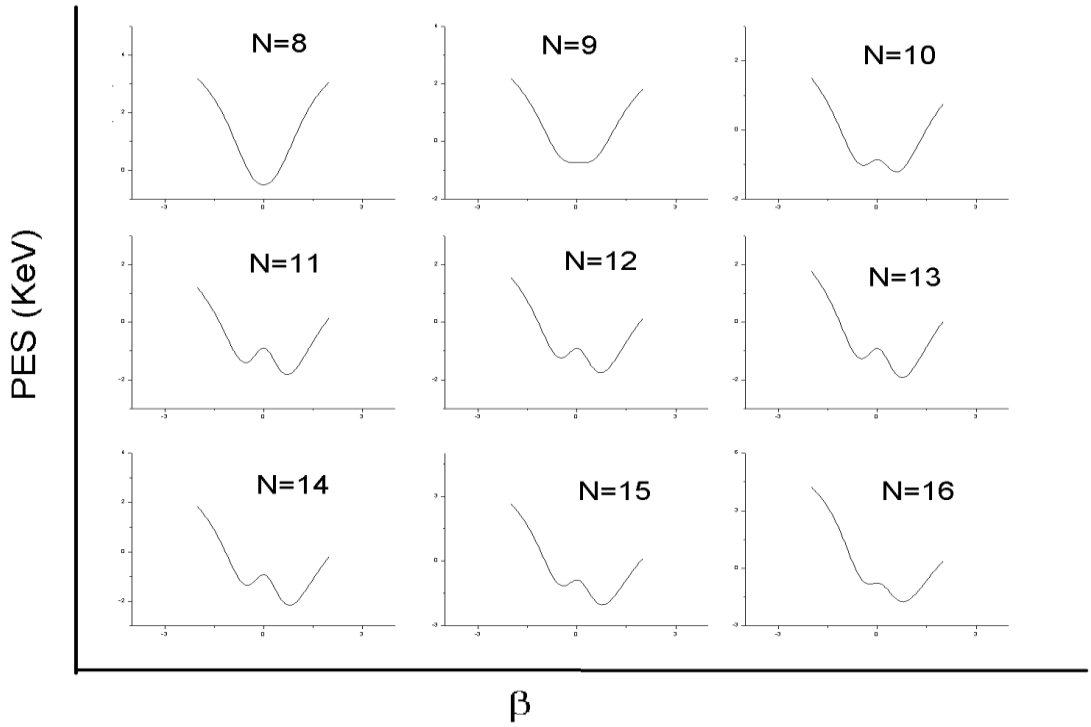

Fig4. *Yb*

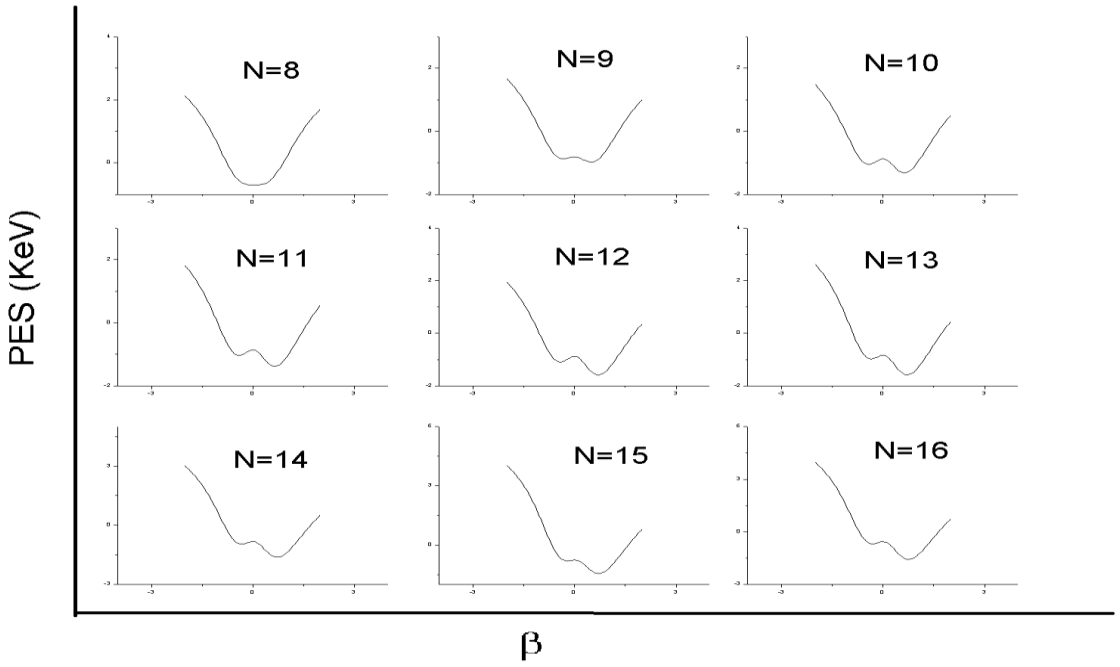

Fig5. *Hf*

We observe that the nuclei in each isotopic chain evolve from spherical to axially symmetric well deformed when moving from the lighter to heavier isotopes, i.e U(5)-SU(3) first order shape phase transition.

In Figure (6) we give the energy ratios $R_{I/2} = E(I) / E(2)$ for the $I^{\pi} = 4^{+},6^{+},8^{+}$ and 10^{+} levels of the critical nuclei $^{156\text{-}160}$Er , $^{158\text{-}162}$Yb and $^{160\text{-}164}$Hf compared with those of the dynamical symmetry limits U(5) and SU(3).

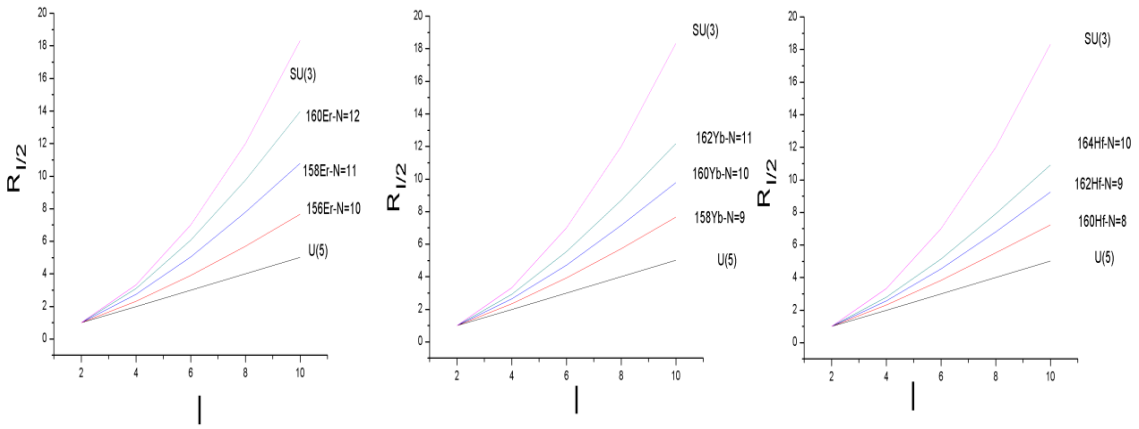

Fig6. *Normalized excitation energies $R_{I/2} = E(I_1^{+}) / E(2_1^{+})$ for $^{156,\ 158,160}$Er (N=10,11,12) , ^{158,160,162}Yb (N=9,10,11) and ^{160,162,164}Hf (N=8,9,10) nuclei and comparison to U(5) and SU(3) predictions.*

We can see that the IBM data lie between the two limits. In Figure (7), we give the calculated ratios $B_{I+2\ /\ 2} = B(E2, I+2 \rightarrow I) / B(E2, 2_1^{+} \rightarrow 0_1^{+})$ in the ground state band for the boson number N=11 which is a measure of nuclear collectivity. A comparison in made with dynamical symmetries U(5) and SU(3) predictions.

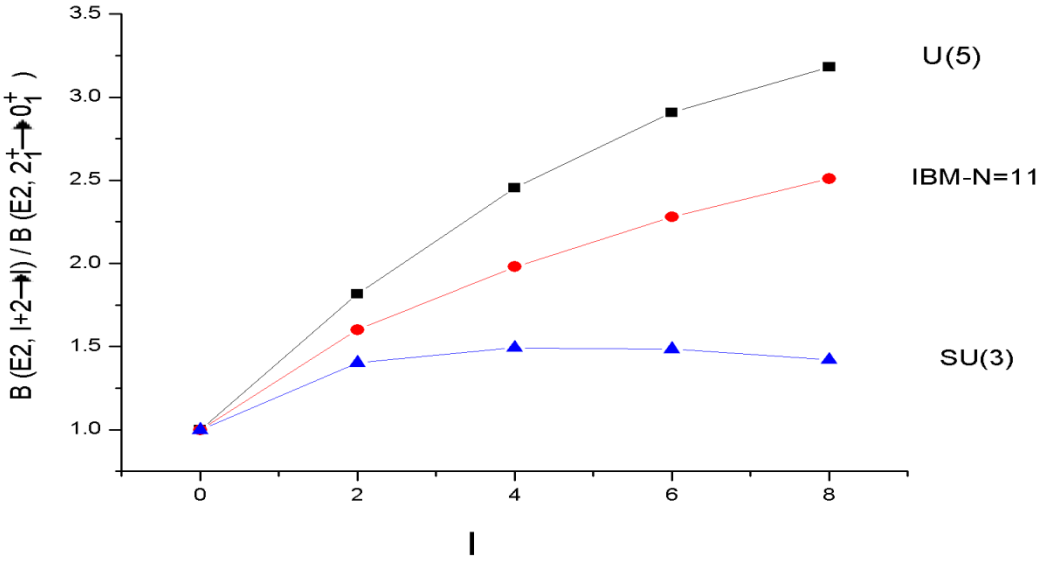

Fig7. *The calculated ratios B (E2, I+2→I) / B (E2, $2_1^+ \rightarrow 0_1^+$) for the yrast band at the critical boson number N=11 compared to the dynamical symmetries U(5) and SU(3) predictions.*

7. CONCLUSION

We have analyzed the PES'S and the critical points of the U(5) - SU(3) nuclear shape phase transition obtained from the sd- IBM and in the boson intrinsic coherent state framework . The validity of the model is examined for the rare- earth chains Er-Yb-Hf with neutron number from 86 to 104.

The parameters of the model were obtained by performing a computer simulated search program in order to obtain a minimum root mean square (rms) derivation between the calculated and the experimental selected excitation energies, B(E2) values and two neutron separation energies.

Our analysis revealed a shape transition from spherical vibrator to axially deformed rotor when moving from the lighter to heavier isotopes.

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