

Variable symmetries in rare earth nuclei and phase transformations.

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Abstract—This paper presents a simple approach using empirical data to determine a first-order phase change in nuclei. The study examines the relationship between χ (a Majorana parameter in Interacting Boson Approximation) and Grodzins systematic ($E_4^+ * B(E2)\uparrow$), which serves as a signature of a quantum phase transformation from prolate to oblate nuclear structure. The observed transition zone at N~90 is explained through shape transformation in a two-level system. The X(5) model is particularly effective in describing rare earth transitional isotopes, with emphasis on Gd-Hf. We are pioneers in conducting this research, and our results substantiate the approach of accuracy of Grodzins systematic in portraying the transitions from spherical U(5) to deformed SU(3) and O(6) patterns within the framework of the Interacting Boson Approximation.

Keywords: Critical point symmetry (CPS), Grodzins systematic $(E_4^+ * B(E2)\uparrow)$, Interacting Boson Approximation (IBA), Phase transition, Quantum phase transition (QPT).

DOI: 10.48047/ecb/2023.12.10.917

I. INTRODUCTION

The field of nuclear physics has greatly benefited, for more than six decades, from the presence of a collection of structural patterns that serve as reference points, illustrating the theoretical limits of structure. These include magic nuclides [1], harmonic oscillators [2], distorted symmetric gyrators [3], and gammaunstable nuclides [4]. Regarding collectivity in nuclei, the symmetries represented by the last three patterns have been formally defined within the framework IBA model [5], specifically under the algebraic structure U(6). This codification ranges from globular U(5) to distorted SU(3), and O(6) boundaries. Such symmetries have a wider application beyond the specific nuclei in which they are observed. They offer straightforward frameworks to describe nuclei with similar structures and act as convenient endpoints [6] for areas of structural transformation within them. Previously researchers first proposed phase transformation utilizing the fundamental state formulation [7-9] of the IBA model [10]. Although the structure depicts the most abrupt shift at the actual point of the phase changeover, there haven't been any analytical explanations for it as of the present. There is currently no description that offers quantum numbers corresponding to particular energy levels or collections of levels, or that specifies the selection procedures that control them, for nuclei at critical points. A manageable and virtually variable-free explanation for the most difficult nuclear systems to examine would be provided by such a description, though it would substantially increase our comprehension of nuclear framework. Unlike the typical thermodynamic phase changeover, QPTs occur at absolute zero temperature, and they arise from variations in a parameter within the Hamiltonian [11, 12].

These changes have garnered significant interest across various physical systems, such as Josephsonjunction arrays and quantum Hall-effect systems [13]. Recently, experimental observations have demonstrated the changeover from Bardeen Cooper-Schrieffer (BCS) coupling exchange [14] to Bose-Einstein condensation (BEC) by growing the potency of the pairing cooperation in ultra cold alkali atoms [15-17]. The changeover from a rigidly-horizontal to a rigidly-bowed configuration has been investigated in non-rigid multi-atomic molecules as well [18]. Recent discussions have focused on geometrical contexts of critical point transitions, specifically employing the Bohr Hamiltonian. Critical point transitions of the unique kinds E(5) [19] and X(5) [20] have been discovered. With modifications in the gamma levels of freedom, these transitions indicate phase shifts of various orders (first and second) between a spinning system and a vibrating system. Analytical solutions in both cases are made possible by the deformation parameter β , which possesses an infinite square well potential. The crucial aspects in the IBA are the specific points within regions of shape transition where different measurements [21], such as $R_{4/2}$ (the ratio of energy between the 4^+ and 2^+ states) or one neutron segregation energies (S_n) experience the highest rate of change. At these points, the first derivatives reach an extreme value, and the second derivatives change direction. The objective of this article is to discover a fresh and straightforward method for measurement in atomic nuclei, which serves as an indicator for QPT in nuclei. This method also enables differentiation among different symmetries and the subsequent changes in phases.

Due to the growing interest in QPT in nuclei, a series of studies have attempted to identify specific signatures or indicators, known as order parameters that can differentiate among1st and 2nd order phase transformations. Iachello and Zamfir [22] conducted a study that highlighted the contrast in the expected dbosons count (n_d) in the initial excited 0^+ level and ground level (v_2) , as well as the isomer changeover amongst the initial 2^+ level and datum level (v₂'). Their findings indicated that these values have distinct alterations in transitional areas, and exhibit contrasting patterns during phase transition at different orders. The results of their study (see inset to fig. 4(b) of [22]) were particularly significant for cases involving a small N_B. In their study, Rowe *et al.* [23] analyzed the ratio, $B_{4/2} = (BE2; 4^+ \rightarrow 2^+)/(BE2; 2^+ \rightarrow 0^+)$ of electromagnetic transition strengths in the IBA. This ratio shows a peak before reaching the critical area for the U(5)-SU(3) transformation, which is analogous to the peak observed in v_2 ' (see fig. 2a. of [23]). Yang and et al. [24] discovered that there is a persistent discrepancy in the transformations between U(5)-O(6) and U(5)-SU(3), as shown by the $B_{4/2}$ and the other B(E2)[†] ratio up to $N_B = 50$. However, such characteristics can be challenging to measure accurately, especially when dealing with elements far from stability, and they can have significant uncertainties. Moreover, alterations in structure typically result in minimal fluctuations of the $B_{4/2}$ ratio, typically falling within a narrow 1.4-1.7 range. McCutchan *et al.* [25] employed a modified IBA-1 Hamiltonian to examine the transition between isomers, isotopes, and the energy associated with bi-neutron segregation (S_{2n}) in even-even rare-earth nuclei from Gd-Hf; N = 86-104. They gave equal consideration to all ground-level, plus parity excitations and computed results for these nuclei. The results of their research showed that the series of isotopes divided into two separate directions: one consisting the isotopes of Gd- Er, while the next comprising the isotopes of Yb-Hf. Outcomes for Yb and Hf exhibit notable variations compared to earlier computations that overlooked the significance of the 0_2^+ levels. In their study, Bonatsos et al. [26] introduced a symmetry called X(5) symmetry, which represents a particular type of symmetry that can be observed in different systems such as molecules and nuclides during first order phase transitions. This symmetry specifically characterizes the changeover region from a vibrating state to a rotational state, where there are variations in the levels of freedom related to β and y. They presented their findings indicating that the ratio between the 6^+ energy level in the datum level and the first 0⁺ excited energy level (E_{61}^{+}/E_{02}^{+}) can be utilized as a measure to identify phase transitions. They supported their claim by analyzing empirical data on Nd-Dy, which are nuclei known to undergo firstorder transitions. Their analysis revealed that these nuclei exhibit precisely the same behavior as predicted by the IBA (Interacting Boson Approximation) for the E_{61}^{+}/E_{02}^{+} ratio. Bindra and Mittal [27-29] proposed that an uncomplicated representation of nuclear shapes could be achieved by graphing the Grodzins product (introduced by Grodzins in 1962) against the P-factor = $(N_p N_n / N_p + N_n)$, considering all recognized eveneven nuclei within the range of Z = 50 to 82 and N = 82 to 126. In their investigation, they also explored the correlation between the Grodzins systematic, represented by the increase in shape fluctuation energy product (ESF * B(E2)), and the rotational energy product (E_{ROT} * B(E2)), with the asymmetry parameter γ^0 within the major shell space of Z = 50 to 82 and N = 82 to 126. The asymmetry parameter γ^0 , ranging from

 0° to 60° , signifies the transition in nuclear structure from prolate to oblate shapes. They also emphasized significant anomalies observed in the phase transformation isotopes. While examining the relationship between shape fluctuation energy product (SFE * B(E2)) and rotational energy product (E_{ROT} * B(E2)) with valance nucleonic product (N_pN_n), they demonstrated that the nuclides exhibiting the highest deformations below Z < 76 undergo a transition towards a more spherical shape as Z goes > 76. This observation aligns with our findings regarding the transition of Gd-Hf (Z< 76) nuclear chains within the Interacting Boson Approximation (IBA) framework, as would be discussed ahead.

Following Bindra and Mittal [27-29], we here describe an order parameter $(E_4^+ * B(E2)\uparrow)$ that is remarkable for two reasons: (i) it can effectively depict the irregularities that appear in the proximity of the critical-point nuclei (Gd and Dy) at N = 90 vibrator-to-axial-rotor phase changeover region; (ii) it can precisely capture the variations in χ as the nuclei shift from the globular (U5) to distorted (SU(3) and O(6)) states within the IBA framework. Our study is the first to assess the utility of $(E_4^+ * B(E2)\uparrow)$ for ' χ ', and we have concluded that it is highly effective in representing these transformations. Our strategy will comprise simulating the transition zone with the IBA model, followed by an empirical examination of the IBA wave function calculations prior to and subsequent to the critical point.

II. THEORY

In order to understand the progression of the structural arrangement of atomic nuclides, which comprises of a limited number of nucleons, it is crucial to collect data regarding the systematic variations of measurable quantities that occur at or in the vicinity of these critical points. Scholten *et al.* [30] initially showcased the potentiality of IBM to effectively represent diverse nuclear structures by employing a simple Hamiltonian. This characteristic of IBM enables it to encompass a wide range of nuclei, as demonstrated in their observation of the isotopes of Sm. This article details the process of determining the transitions from spherical to deformed nuclear states using an uncomplicated bi-variable Hamiltonian. The calculations were performed for various rare-earth isotopes, and the resulting variables and observed quantities were studied to comprehend the changes in nuclear structures. The computations utilized the enhanced consistent Q formalism (ECQF) [31] having Hamiltonian [32, 33] within the framework of IBA-1.

$$\mathbf{H} = \mathbf{b}[(1 - \zeta) \mathbf{n}_{\mathrm{d}} - \zeta \cdot \mathbf{Q} \cdot \mathbf{Q}/4\mathbf{N}_{\mathrm{B}}] \quad (1)$$

Here $\mathbf{n}_{d} = d^{\dagger} \cdot d^{-}$ is the d boson-count operator, $\mathbf{Q} = (s^{\dagger}d^{-} + d^{\dagger}s) + \chi (d^{\dagger}d^{-})^{(2)}$ is the quadrupole operator, $\mathbf{N}_{\mathbf{B}}$ = valance boson number and **b** is a scaling factor. The Hamiltonian mentioned above includes a pair of variables, χ (ranging from 0 to -1.32) and ζ (ranging from 0 to 1). The three kinematic symmetries are presented in this formulation with (i) Any χ and $\zeta = 0$ for U(5) (ii) $\chi = -1.32$ and $\zeta = 1$ for SU(3) (iii) $\chi = 0$ and $\zeta = 1$ for O(6). The IBAR [34] code was used to carry out the calculations. Based on the obtained parameters, we have drawn an outline of each isotopic nuclear chain in the IBA variable space and presented it in the form of the IBA consistency triangle as depicted in figure 1.



Figure 1.The IBA consistency triangle; consistent boundaries are simplified in terms of the formulation of the Hamiltonian as given by the equation (1).

Our study took into account pairs of even-even atomic nuclei within the rare-earth zone for Z = 64-72; N = 86-104 and the information was extracted from the Nuclear Data Sheets [35] and McCutchan *et al.* [25]. Lately, there has been an increasing curiosity surrounding the analysis of the low energy excited levels of atomic nuclei. This interest stems from the emergence of dynamic symmetries like E(5) and X(5), as well as the compelling evidence indicating that specific nuclei bear a striking resemblance to these theoretical models [36, 37]. Figure 2 summarizes the key findings for each nucleus, specifically the parameter χ , while a more comprehensive breakdown of these parameters can be found in table 1. Generally, parameter χ

exhibit relatively uneven changes, which align with our expectations when explaining the random structural modifications that occur as the number of bosons is altered. Nevertheless, in certain chains of isotopes, a more random departure from the expected trend occurs in the development of the parameter, particularly when nearing the middle region of the shell structure. Such a variation may potentially suggest the presence of an alternative arrangement or structure. Usually, as the number of bosons increases, χ also increases for Gd-Er and the nuclei undergo a transition from vibrational spheroid to rotor one. This pattern is evident in these isotopic sequences until reaching N=92. For N values exceeding 92, the atomic nuclei of Gd-Er exhibit a growing χ , whereas Yb-Hf maintains a relatively steep χ representing a transformation from a rotor O(6) to a vibrator SU(3) limit, just as anticipated, until reaching the mid shell.



Figure 2.The variation of χ with boson number (N_B) in even-even nuclides within the rare-earth zone (N = 86-102 and Z = 64-72). Left: A clear 1st order shape transformation from U(5), for any values of χ , to SU(3) zone is evident in Gd-Er. Right: Steep χ for Yb-Hf nuclear chains ranging within O(6) to SU(3) vibrator limit. Intruder structural phase coexistence is evident for Yb-Hf at N_B~15 (N=100-102).

III. RESULTS AND DISCUSSION

Figure 3 illustrates the comparison between the calculated results of the Grodzins systematic (E_4^+ * $B(E2)\uparrow$) and the variable ' χ ' for the nuclear isotones Gd-Hf. The calculations were performed for values of boson number (N_B) up to 16. The curves for nuclear isotones of Gd-Er clearly demonstrate a noticeable 1st order shape transformation, signifying a shift from U(5) (any ' χ ') to SU(3) zone. The curves quickly enter O(6) boundary with $\chi \rightarrow 0$. The magnitude of χ initially appears significant for vibrational nuclei in the case of Gd and Dy isotopes, but it progressively tends towards -0.2 with the increase in N_B. The region of transformation becomes more distinct, occurring within a limited range of χ values, and the magnitude of the spike before the shape transformation increases. Despite, it is essential to note that there is a lack of initial data points for Gd. An intriguing aspect of the advancement of all isotopic chains is that they all pass through the phase transition region when reaching neutron count, N= 90 (see table 1). The chains of Gd-Er isotopes have been extensively studied and it has been observed that they undergo a transformation from a globular shape to a distorted shape. Specifically, the isotopes ¹⁵²Gd and ¹⁵⁴Dy are located near the point of transition [38-40] and exhibit characteristics that are consistent with the X (5) model. According to McCutchan *et al.* [25], the development of the 0_2^+ excited levels in Er-Yb nuclear chains for N~ 100 indicates the potential presence of an anomalous configuration. By considering the initial collective excited 0^+ states within the context of IBA, figure 2 (left) demonstrates a noticeable shift in the pattern of the first 0^+ excited level energy for Er at N_B=16 (N ~ 100). A similar shift is observed for Yb-Hf at NB~15; N~102 (fig. 2; right). Additionally, we also observed anomaly in the pattern of the parameters of these nuclei (fig. 3).



Figure 3. Left: The variation of $(E_4^+ * B(E2)\uparrow)$ with χ showing a clear transition from U(5)-SU(3). The curves quickly enter O(6) zone with $\chi \rightarrow 0$. Right: The Yb-Hf exhibiting a complete opposite trend with $\chi \sim 0$ for vibrators shifting to SU(3) value of -1.32 towards the mid shell.

In the Yb and Hf nuclear chains, we observe a completely different pattern where the value of χ is near zero for O(6) nuclei with vibrational properties, but it gradually approaches towards the value of -1.32 in the SU(3) zone towards the mid shell. The behavior of the Gd-Hf nuclear chains in terms of their parameters shows a significant deviation from the analysis made by Chou *et al.* [41]. This distinction can be concerning to the equal treatment of the 0_2^+ state and the 2^+ gamma state. When examining the behavior of $R_{4/2}$ and one neutron segregation energy (S_n), it becomes apparent that for nuclei which are positioned next to the U(5)-SU(3) edge of the triangular diagram indicating axial symmetry, such as Gd and Dy, the transformation from a globular to a distorted configuration occurs abruptly. The notable changes observed in the mentioned observables (fig. 3 left) provide support for this.

Table 1. Transitional isotopes within the rare earth region are pertinent to mention. It should be noted that the variables
were calculated while considering the first excited 0^+ states. A decreasing 0^+ energy for Gd-Er nuclei with increasing χ , for
N > 90, with a similar variation of $(E_4^+ B(E2))$ against χ , is supported by the observations of Iachello and Zamfir [22].
The energy values have been taken from [42], absolute (B(E2) \uparrow) values from Pretychenko <i>et al.</i> [43].

Nuclei	Ν	Α	NB	χ	(E ₄ ⁺ *B(E2)↑)
64Gd	88	152	10	-1.32	1261.50
64Gd	90	154	11	-1.10	1443.15
₆₄ Gd	92	156	12	-0.80	1331.14
₆₄ Gd	94	158	13	-0.80	1337.15
₆₄ Gd	96	160	14	-0.53	1304.15
64Gd	98	162	15	-0.30	1288.38
₆₆ Dy	86	154	10	-1.10	542.31
₆₆ Dy	88	156	11	-1.09	764.78
₆₆ Dy	90	158	12	-0.85	1499.54
66 Dy	92	160	13	-0.67	1477.86
₆₆ Dy	94	162	14	-0.49	1455.99
₆₆ Dy	96	164	15	-0.31	1421.30
₆₆ Dy	98	166	16	-0.26	1356.48
₆₈ Er	88	156	10	-0.67	1307.73
₆₈ Er	90	158	11	-0.61	1608.02
₆₈ Er	92	160	12	-0.60	1705.44
₆₈ Er	94	162	13	-0.53	1651.39
₆₈ Er	96	164	14	-0.37	1631.89
₆₈ Er	98	166	15	-0.31	1544.89
₆₈ Er	100	168	16	-0.36	1529.06
₇₀ Yb	88	158	9	-0.23	1561.61
₇₀ Yb	90	160	10	-0.35	1698.11
₇₀ Yb	92	162	11	-0.42	1720.27

₇₀ Yb	94	164	12	-0.52	1688.75
70Yb	96	166	13	-0.58	1731.71
70Yb	98	168	14	-0.61	1598.95
70Yb	100	170	15	-0.75	1606.31
70Yb	102	172	16	-1.20	1572.01
72 Hf	90	162	9	-0.37	984.82
72 Hf	92	164	10	-0.45	1256.47
72 Hf	94	166	11	-0.53	1646.61
$_{72}$ Hf	96	168	12	-0.60	1659.45
$_{72}$ Hf	98	170	13	-0.79	1705.22
72 Hf	100	172	14	-0.84	1382.30
72 Hf	102	174	15	-1.10	1451.21

While examining the nuclei under study, it was observed that all the chains initially exhibited vibrational characteristics with $R_{4/2}$ value close to 2.0. However, as the number of neutrons increased, these chains gradually transitioned towards rotational behavior, with an $R_{4/2}$ value of approximately 3.33. This pattern is clearly evident from the curves of figures 4, utilising the Gd-Yb chains as representative illustrations. In contrast to a non smooth change observed in Yb-Hf isotopes, the alteration in $R_{4/2}$ values is more sudden when examining isotopes of Gd-Er. While examining the relationship between the evolution of $(E_4^+ * B(E2)\uparrow)$ and χ , two distinct patterns are observed among the isotopic chains. As χ increases, the energy of the 0⁺ level in Gd, Dy, and Er nuclei with N > 90 decreases. A similar behavior is observed for $(E_4^+ * B(E2)\uparrow)$ plotted against χ (see table 1). These observations find support in the notable alterations observed in the aforementioned observables (fig. 4) in accordance with the observations of Iachello and Zamfir [22]. Our calculations successfully replicated these observed trends, as demonstrated by a disruption in the pattern of the parameters of the mentioned nuclei (see figures 2 and 3).



Figure 4. Portraying R_{4/2} values in support of sudden transitions in nuclear isotopes from Gd-Er on contrarily to a smooth transition observed in Yb-Hf isotopes.

In their work, Ramos *et al.* [44] demonstrated that they were able to identify parameters that accurately predict the energy spectra observed in experiments. However, these parameters significantly deviate from the experimental data when predicting the two neutron segregation energies (S_{2n}). As mentioned earlier, while the parameters can reasonably reproduce the energies and electromagnetic transition properties, a rigorous test of the applicability of the Hamiltonian to the entire isotopic chain would involve considering the one neutron segregation energies (S_{1n}). The Gd chain exhibits nonlinear behavior, while the Yb chain displays linear behavior, both of which can be reasonably described. The nonlinear behavior in the S_{1n} values of the Gd chain resembles the nonlinear behavior observed in the S_{2n} values of the Sm isotopic chain, which is also supported by Scholten *et al.* [30]. According to suggestions made by other researchers [9], a plateau-like pattern in the evolution of S_{2n} values (see fig.1; left of [9]) indicates a first-order phase transition. We have observed a similar behavior in the S_{1n} values (fig. 5), aligning with previous studies of Zamfir *et al.* [32] that have found evidence of such a transition in the Sm and Gd chains.



Figure 5. One neutron segregation energy in relation to neutron number N, replicating the observed transition parameters against U(5) spherical to distorted SU(3)- O(6) zones.

IV. CONCLUSION

There is a proposal to incorporate a novel symmetry X(5), into the critical point, which has not been described before. The intriguing observation is that every isotopic chain undergoes a phase shift when they reach neutron numbers 88 and 90, especially ¹⁵²Gd and ¹⁵⁴Dy. This discovery suggests that the new variable $(E_4^+ * B(E2) \uparrow)$ should be considered in conjunction with γ to understand this evolutionary aspect. In the region where a phase transition occurs, higher values of Z exhibit a greater degree of gammasoftness. In case of Gd, the initial nuclides in the sequence possess a high degree of y-stiffness, positioned on the U(5)-SU(3) edge of the triangular diagram. The level of gamma-softness shows a slight rise when considering the Dy and Er nuclides, and it becomes more pronounced when examining the Yb-Hf nuclides, which is positioned in close proximity to the U(5)-O(6) edge of the triangular diagram. Referring to the findings regarding the characteristics of S_n and $1R_{4/2}$ it seems that in case of nuclei positioned at the proximity of U(5)-SU(3) edge of the triangular diagram (indicating axial symmetry), like Gd and Dy, the shift from a globular shape to a distorted one occurs abruptly. The significant and sudden change observed in the aforementioned measurable quantity (fig. 4) stand in its support. As the value of Z rises and the atomic nuclei become increasingly gamma-soft, the smoother progression of γ (fig. 2 right) indicates that the phase transition is less sudden in its manifestation. The calculations conducted for even-even rare-earth nuclei with atomic numbers ranging from 64 to 72 and neutron numbers ranging from 86 to 104 focused equally on all down-lying, +ive parity excitations. These computations effectively replicate the energy levels of the primary bands and offer a satisfactory explanation of the strengths observed in the transitions between these energy levels beside S_n and $R_{4/2}$ values, representing additional variables, are also effectively explained. The observation reveals a division in isotopic chains, with one trajectory encompassing isotopes from Gd-Dy, while the next trajectory comprises isotopes from Yb-Hf. The findings for Yb-Hf exhibit notable distinctions compared to the previous calculations that assigned less significance to the more elevated excited levels.

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