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Structural evolution from shape invariants

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An overview of the concept of quadrupole shape invariants is given. Definitions and ways to derive shape invariants from data that were found in recent works are summarized, and the connection and sensitivity of shape invariants to the nuclear shape/phase transition is shown. First results of an ongoing survey of shape invariants for excited states are presented, investigating the critical point behavior as a function of angular momentum and energy. A manifestation of theoretical predictions appears to be found in the transitional Gd isotopes.

Keywords: Electromagnetic transitions; collective levels; collective models.

Se presenta una revisión del concepto de los invariantes de forma cuadrupolares, sus definiciones y las maneras de extraerlos de los datos experimentales. Se muestra la conexión y sensibilidad de invariantes de forma con las transiciones de fase en la física nuclear. Se discuten los primeros resultados de una investigación de invariantes de fase para estados excitados a través de un estudio del comportamiento del punto crítico como función del momento angular y la energía. Hay evidencia que las predicciones teóricas se manifiestan en los isótopos de Gd.

Descriptores: Transiciones electromagnéticas; excitaciones colectivas; modelos colectivos.

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1. Introduction

The well-known deformation parameters β and γ parametrize the shape of a nucleus like the shape of a liquid drop. They are used in geometrical models like that of Bohr and Mottelson [1] or the rigid triaxial rotor model (RTRM) by Davydov and Fillipov [2]. However, due to their geometrical origin, β and γ are model dependent and therefore values derived within different models are not trivially comparable.

An alternative approach for the description of the nuclear shape was introduced by Kumar [3], and later on was widely used and applied by Cline and co-workers (see, *e.g.* [4]). This approach used quadrupole shape invariants, which are higher order moments of the quadrupole operator in a given state, and will be introduced in more detail in Sec. 2.. Such shape invariants are not only calculable from every model giving E2 transition matrix elements, but can in principle also directly be measured in means of experimentally obtaining complete sets of E2 matrix elements.

The latter requirement makes the experimental determination of quadrupole shape invariants more than difficult, but we will see below that, in some cases, shape invariants can already be deduced with good accuracy from only few data [5]. This affords certain truncations to the pool of required matrix elements, by applying approximate selection rules, which were found to be valid within the so-called Q-phonon scheme [6, 7] for collective nuclei of various symmetries. Using such truncations and relations between shape invariants, in addition useful relations have been identified, resulting, *e.g.*, in a way to calculate the absolute value of the quadrupole moment of the first excited 2^+ state in even-even nuclei from other lifetime data. This will be discussed in Sec. 3.

As model independent quantities, quadrupole shape invariants can be calculated within geometrical models, therefore leading to expressions relating the lowest two invariants to the geometrical deformation parameters. However, we will see that those only give effective geometrical deformation parameters, as we deal with averages in a given state. In contrast, higher invariants relate to fluctuations in these parameters, making quadrupole shape invariants suitable for the description of rigid and non-rigid deformation, and therefore applicable to a wide range of nuclei.

This was shown [8] to be of special importance in the description of the nuclear shape/phase transition [9, 10], occurring as a function of the number of valence nucleons from spherical (vibrators) to deformed (rotors or γ-soft) nuclei [11, 12]. As discussed in section 4., certain invariants exhibit rapid changes in the vicinity of the nuclear shape/phase transition, therefore providing a way to experimentally survey the transition for a limited number of valence nucleons from E2 transition data, complementary to the investigation of level energies.

Many works focused on only the evolution of the ground state in even-even nuclei, but we now use quadrupole shape invariants to gain insight in the evolution of excited states. In Secs. 5 and 6 of we will show first results obtained within the ground state band and for the lowest two 0^+ states, which need to be explored in more detail in future works.

2. Quadrupole shape invariants

Quadrupole shape invariants are defined as higher order moments of the quadrupole operator in a given state. The lowest invariants are

$$q_2(J) = \langle J|(Q\cdot Q)|J\rangle \quad (1)$$

$$q_3(J) = \sqrt{\frac{35}{2}}\langle J|[QQQ]^{(0)}|J\rangle \tag{2}$$

$$q_4(J) = \langle J|(Q\cdot Q)(Q\cdot Q)|J\rangle \tag{3}$$

$$q_5(J) = \sqrt{\frac{35}{2}}\,\langle J|(Q\cdot Q)\,[QQQ]^{(0)}|J\rangle \tag{4}$$

$$q_6(J) = \frac{35}{2}\langle J|[QQQ]^{(0)}\,[QQQ]^{(0)}|J\rangle, \tag{5}$$

where Q is the quadrupole transition operator, brackets denote tensor coupling and a dot denotes a scalar product. Note that for q_4 we chose an intermediate coupling to spin zero, as we want to use it to measure fluctuations in q_2. However, other choices can be made and lead to interesting relations as demonstrated in Sec. 3. The expressions (1)-(5) can be converted into sums over E2 matrix elements using tensor coupling, the Wigner-Eckert theorem and the unitarity relation of Clebsch Gordan coefficients. For the lowest three invariants in the ground state, this procedure yields

$$q_2(0_1^+) = \sum_i \langle 0_1^+ \parallel Q \parallel 2_i^+\rangle\langle 2_i^+ \parallel Q \parallel 0_1^+\rangle \tag{6}$$

$$q_3(0_1^+) = \sqrt{\frac{7}{10}}\,\sum_{i,j}\langle 0_1^+ \parallel Q \parallel 2_i^+\rangle\langle 2_i^+ \parallel Q \parallel 2_j^+\rangle \cdot \langle 2_j^+ \parallel Q \parallel 0_1^+\rangle \tag{7}$$

$$q_4(0_1^+) = \sum_{i,j,k}\langle 0_1^+ \parallel Q \parallel 2_i^+\rangle\langle 2_i^+ \parallel Q \parallel 0_j^+\rangle \cdot \langle 0_j^+ \parallel Q \parallel 2_k^+\rangle \cdot \langle 2_k^+ \parallel Q \parallel 0_1^+\rangle\ . \tag{8}$$

We usually define [13] dimensionless shape parameters by dividing q_n by an appropriate power of q_2, which gives

$$K_n(J) = \frac{q_n(J)}{q_2(J)^{n/2}}\ \text{for}\ \ n \in \{3,4,5,6\}. \tag{9}$$

for any state.

The shape parameters K can be calculated within any model. The geometrical model, for example, leads to the expressions (omitting J for abbreviation)

$$q_2 = \left(\frac{3ZeR^2}{4\pi}\right)^2\,\langle\beta^2\rangle \equiv \left(\frac{3ZeR^2}{4\pi}\right)^2\,{\beta_{\text{eff}}}^2 \tag{10}$$

$$K_3 = \frac{\langle\beta^3\cos 3\gamma\rangle}{\langle\beta^2\rangle^{3/2}} \equiv \cos 3\gamma_{\text{eff}} \tag{11}$$

$$K_4 = \frac{\langle\beta^4\rangle}{\langle\beta^2\rangle^2} \tag{12}$$

$$K_6 = \frac{\langle\beta^6\cos^2 3\gamma\rangle}{\langle\beta^2\rangle^3}, \tag{13}$$

relating the shape parameters to the geometrical deformation parameters, or more precisely, to effective (non-rigid) deformation parameters [by Eqs. (10) and (11)] and fluctuations in those [from Eqs. (12) and (13)]. We note, that γ_{eff} gives a measure for triaxiality if the β-deformation is rigid and can be separated out.

The general behavior of the shape parameters K has been investigated for the ground state [13] and is shown in Fig. 1, showing results of calculations within the Interacting Boson Model (IBM-1) [14] for $N_B = 10$ bosons, using the extended consistent Q formalism (ECQF) [13, 15, 16]

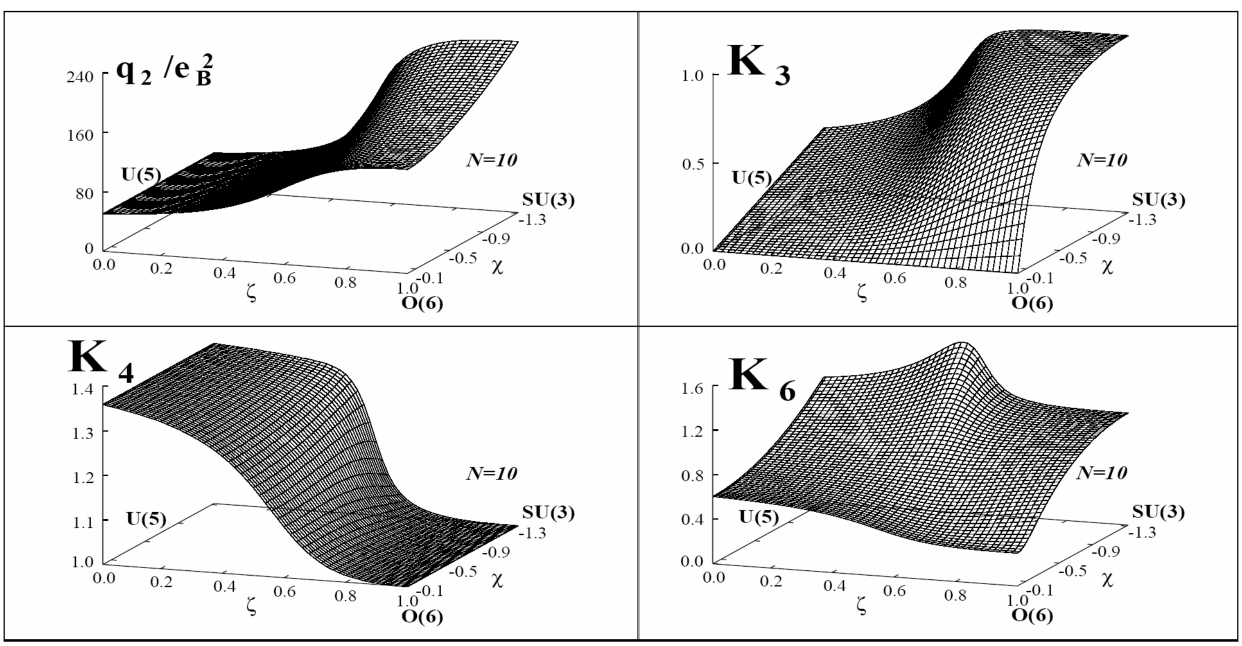

FIGURE 1. The relevant shape parameters q_2, K_3, K_4 and K_6, calculated for the ground state over the whole symmetry space spanned by the ECQF Hamiltonian in the IBM-1, using the parametrization of [13].

$$H_{IBM} = (1-\zeta)\, n_d - \frac{\zeta}{4N_B}\, Q^\chi \cdot Q^\chi , \quad (14)$$

omitting an absolute energy scale, and the quadrupole operator Q^χ which appears also in the E2 transition operator

$$T(E2)_{IBM} = e_B Q^\chi = e_B[(s^+\tilde{d} + d^+ s) + \chi(d^+\tilde{d})] , \quad (15)$$

n_d is the boson number operator, and e_B the effective charge. The limiting dynamical symmetry limits are denoted as U(5) (vibrator), SU(3) (axially symmetric rotor), and O(6) (γ-soft rotor)

3. Shape parameters from data

In general the derivation of quadrupole shape invariants from data affords the measurement of complete sets of E2 matrix elements. However, many of the involved matrix elements will be small and will not significantly contribute to the values of the invariants. In order to have a consistent way to truncate the sums given in Eqs. (6)-(8), it was shown [5, 17] that the application of the Q-phonon scheme [6, 7] is convenient and leads to good approximations.

In the Q-phonon scheme the first excited 2^+ state in even-even nuclei is given by acting on the ground state with the quadrupole operator Q, and n-phonon states are derived by acting on the ground state with Q n times, coupling the operators to angular momentum L,

$$|L^+, n\rangle = N^{(L,n)}(\underbrace{Q \ldots Q}_{n})^{(L)}|0_1^+\rangle , \quad (16)$$

where $N^{(L,n)}$ are normalization constants. As the E2 transition operator is Q, transitions between states are only allowed if they change the number of phonons by one, hence the selection rule $\Delta Q = 1$. It was shown in earlier works [18–20] that the the lowest excited states of even-even collective nuclei are rather pure Q-phonon configurations, regardless of the structure of a specific nucleus. Therefore, especially for the ground state, applying the Q-phonon selection rule to Eqs. (6)-(8) severely truncates the sums, and only few E2 matrix elements are left.

The simplest example is the shape invariant $q_2(0_1^+)$, for which only the matrix element to the 2_1^+ state is allowed in the truncation. Therefore, a good approximation is given by

$$q_2(0_1^+) \approx q_2^{appr.}(0_1^+) = B(E2; 0_1^+ \to 2_1^+) , \quad (17)$$

where we denote the used truncation as a first order approximation as a means of only allowing matrix elements with $\Delta Q = 1$ for transitions and $\Delta Q = 0$ for quadrupole moments.

The quadrupole shape invariant q_4 can be defined in different ways, as mentioned above, using different intermediate couplings of the quadrupole operators, e.g. for the ground state, as

$$q_{4,J}(0_1^+) = \langle 0_1^+|[QQ]^{(J)}[QQ]^{(J)}|0_1^+\rangle , \; J = 0, 2, 4 . \quad (18)$$

It was found [5] that the three different q_4 values from Eq. (18) are approximately equal, which is trivial in some models, while in the IBM-1 it is a $1/N$ or $1/N^2$ effect. This approximate identity lead to a useful relation between three B(E2) values, which is

$$B(E2; 2_1^+ \to 2_1^+) \approx B(E2; 4_1^+ \to 2_1^+) - B(E2; 2_2^+ \to 2_1^+) , \quad (19)$$

where the $B(E2; 2_1^+ \to 2_1^+)$ is directly proportional to the squared quadrupole moment $Q(2_1^+)^2$, using consistently

$$B(E2; J_i \to J_f) = \frac{1}{2J_i + 1}\, e^2\langle J_f||Q||J_i\rangle^2 . \quad (20)$$

The relation (19) was shown [5, 17] to be valid within few percent within the IBM-1 and the RTRM.

Another outcome of the approximate identity of the q_4 values and truncation of the Q-phonon scheme in first order is an approximation to the shape parameter $K_4(0_1^+)$, which is

$$K_4^{appr.}(0_1^+) = \frac{7}{10}\frac{B(E2; 4_1^+ \to 2_1^+)}{B(E2; 2_1^+ \to 0_1^+)}, \quad (21)$$

involving only the lowest two B(E2) values in the ground state band.

Applying the Q-phonon truncation to the shape parameter K_3, which relates to triaxiality via Eq. (11) showed [17] that the above first order approximation does not yield accurate values. In this case it is necessary to allow at most one matrix element in the sum with $\Delta Q = 2$, leading to an approximate value

$$K_3^{appr.}(0_1^+) = \sqrt{\frac{7}{10}}\mathrm{sign}(Q(2_1^+)) \left[\sqrt{\frac{B(E2; 2_1^+ \to 2_1^+)}{B(E2; 2_1^+ \to 0_1^+)}} - 2\frac{\sqrt{B(E2; 2_2^+ \to 0_1^+)B(E2; 2_2^+ \to 2_1^+)}}{B(E2; 2_1^+ \to 0_1^+)}\right] \quad (22)$$

involving four B(E2) values, one of which is the above mentioned quadrupole moment of the 2_1^+ state, which is the leading term. Using the technique described in section 4., but taking the derivative of K_3 with respect to the parameter χ which is inherent to the IBM-1 quadrupole operator, one can identify K_3 as a sensitive observable for the phase transition between prolate and oblate rotors, in which the O(6) dynamical symmetry limit of the IBM itself is the critical point [21].

4. Identification of critical points

One of the most striking features seen in Fig. 1 is the sharp drop of K_4 from vibrators toward the deformed limits, corresponding to the transition from β-soft to β-stable nuclei. This drop appears around $\zeta = 0.5$, which is the critical point between vibrators and deformed nuclei for an infinite number of valence nucleons. Due to the finite boson number the transition is smoothed out, which makes the definition of a critical point difficult.

In Ref. 8 it was suggested to identify the critical point in the realistic case of limited boson numbers with the point of steepest changes in corresponding observables, *e.g.* in K_4. It was found that this point corresponds well with the critical point found within the coherent state formalism of the IBM-1 [22, 23], where two coexisting minima of the ground state energy functional are degenerate.

Figure 2 shows the derivative of the shape parameter K_4, calculated within the IBM-1 between the U(5) (ζ=0) and SU(3) ($\zeta = 1$) dynamical symmetry limits. The derivative peaks at a value of ζ slightly larger than 0.5, reflecting the dependence of the exact location of the critical point (which is related to the X(5) critical point symmetry introduced by Iachello [10]) on the boson number. A similar analysis can be made for the shape invariant q_2, which rises from small values (small average deformations) in the vibrator limit to large values in the deformed limits (compare Fig. 1). This will be used in the analysis of shape invariants for excited states in the ground state band in Sec. 5.

5. The ground state band

We are currently carrying out calculations of shape parameters for excited states. First results are obtained for the ground state band. Figure 3 shows a plot similar to to Fig. 2, but for the derivative of q_2 for members of the ground state band up to $J = 10$ on the transition path U(5) to SU(3). For all states a qualitatively similar behavior is seen, while the absolute scale varies.

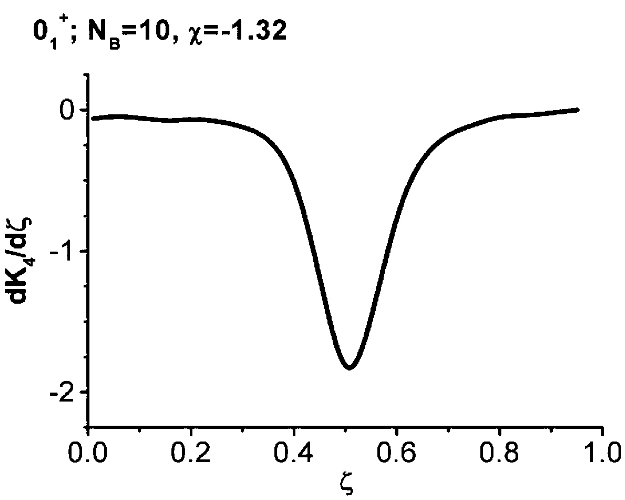

FIGURE 2. Derivative of K_4 with respect to the control parameter ζ, peaking at the point of steepest change in K_4. The calculation was done for $N_B = 10$ bosons fixing $\chi = -\sqrt{7}/2$ between the U(5) ($\zeta = 0$) and SU(3) ($\zeta = 1$) dynamical symmetry limits of the IBM-1.

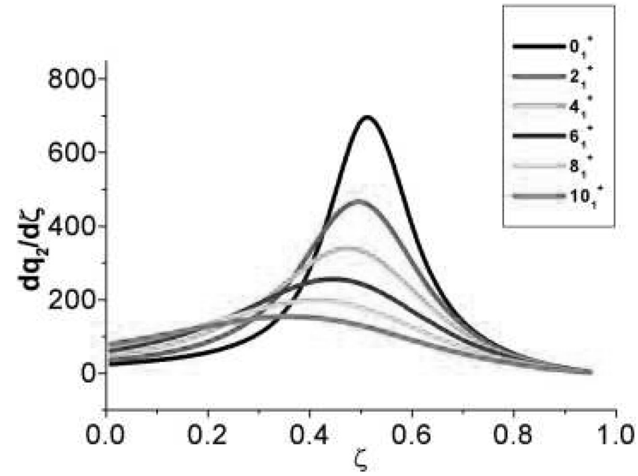

FIGURE 3. Derivative of q_2 with respect to the control parameter ζ, peaking at the point of steepest change in q_2. The calculation was done for $N_B = 10$ bosons fixing $\chi = -\sqrt{7}/2$ between the U(5) ($\zeta = 0$) and SU(3) ($\zeta = 1$) dynamical symmetry limits of the IBM-1. The line with the highest amplitude corresponds to the ground state, followed with decreasing amplitudes by the next members of the ground state band.

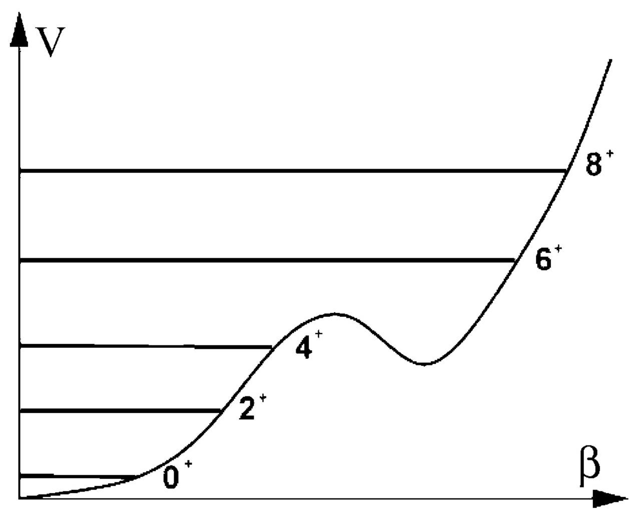

FIGURE 4. Schematic of the nuclear potential in the region where a coexistence of two minima occurs, as a function of the deformation parameter β.

The most important result is that the critical point of the transition, which corresponds to the maxima in the plotted curves, appears at decreasing values of the control parameter ζ, that means closer to the vibrator limit. It is not yet clear whether this is just a finite boson number effect that vanishes for $N_B \to \infty$. One possible qualitative interpretation may be that the lowering of a second, deformed, minimum of the potential when increasing ζ leads to a wider potential at higher energies, as depicted in Fig. 4. Higher lying states should be sensitive to a widening of the potential earlier than lower lying states.

These findings are currently being tested for large boson numbers, as well as for higher lying bands. In this way we

TABLE I. Approximate effective deformation parameters for the ground state and the first excited 0^+ state in the transitional Gd isotopes. For each state the value derived from data, as well as the value derived from IBM-1 fits are given.

	0_1^+		0_2^+	
	$\beta_{eff}^{appr.}$	$\beta_{eff}^{IBM,appr.}$	$\beta_{eff}^{appr.}$	$\beta_{eff}^{IBM,appr.}$
^{152}Gd	0.212(10)	0.216	0.22(1)	0.250
^{154}Gd	0.317(1)	0.320	0.26(1)	0.264

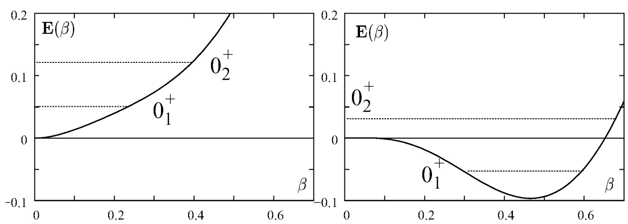

FIGURE 5. Schematic of the nuclear potential for a vibrator (left) and slightly behind the shape/phase transition to the rotational side (right), as a function of the deformation parameter β. Dotted lines denote the lowest 0^+ levels.

want to explore the phase transitional behavior of their band members as functions of spin, energy and number of valence nucleons.

6. Shrinking effect for 0^+ states

Another finding from the calculations for the ground state and the first excited 0^+ state is a shrinking effect in the β-deformation. From extensive fits to a large set of nuclei [24] within the IBM-1, parameters for the A=152,154 Gd isotopes are known. Using these parameters, we calculated shape parameters for those isotopes and find that the values of q_2, or in terms of the geometrical model the β-deformation, of the lowest two 0^+ states seem to reflect the change in the nuclear potential.

For the calculation of $q_2^{appr.}(0_2^+)$ following

$$q_2(0_n^+) = \sum_i B(E2; 0_n^+ \to 2_i^+) \tag{23}$$

the B(E2) transitions to the first three 2^+ states were taken into account in order to derive a first order approximation. Those correspond to the transition to the ground state band and the in-band transition. For the latter it was found that B(E2) values to the second and third excited 2^+ states had to be considered due to mixing effects.

Table I shows approximate effective β-deformation parameters, obtained from q_2 via Eqs. (17) and (10) for those nuclei. For the ground state one sees the typical drastic increase in deformation when passing the shape transition, increasing β_{eff} from about 0.21 to 0.32. This increase does not appear for the first excited 0^+ state, for which the deformation remains almost constant at about 0.25.

Comparing the deformations of 0^+ states within each isotope, they increase only slightly in the vibrational ^{152}Gd. In ^{154}Gd, the deformation of the excited state is lower than that of the ground state. In this case the ground state is in the deformed minimum. Data for both nuclei, which was taken from high precision experiments [25, 26], is included in Table I for both nuclei and seems to confirm the model predictions.

Again, a qualitative explanation for the effect may be found considering the nuclear potentials as sketched in Fig. 5. In the vibrational case, with a minimum of the potential at zero deformation, the effective deformation of the 0^+ states should be similar, somewhat larger for the excited state, corresponding to the findings for ^{152}Gd. When the ground state is in the deformed minimum, the excited 0^+ state may still reach zero deformation and therefore have a smaller effective deformation than that of the ground state, which may be the case in ^{154}Gd.

7. Summary

A review of results on quadrupole shape invariants and related shape parameters, obtained within recent years, was given. Shape parameters are model independent quantities and can be derived from E2 data. Using truncations implied by the Q-phonon scheme, the lowest shape parameters can be obtained from only few data for some states. Shape parameters are sensitive probes of the nuclear shape/phase transition, as was shown in earlier works for the ground state. A new study focuses on the systematic behavior of excited states. First results for the ground state band show a shift of the critical point on the vibrator/rotor transition toward the vibrator limit for higher members of the ground state band. A shrinking of the 0_2^+ state deformation relative to the ground state deformation is predicted, and an example was identified in the transitional Gd isotopes.

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