Quadrupole shape invariants in the interacting boson model

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In terms of the interacting boson model (IBM), shape invariants for the ground state, formed by quadrupole moments up to sixth order, are studied in the dynamical symmetry limits and over the whole structural range of the IBM-1. The results are related to the effective deformation parameters and their fluctuations in the geometrical model. New signatures that can distinguish vibrator and γ -soft rotor structures, and one that is related to shape coexistence, are identified.

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Nuclei are often regarded as drops of nuclear matter as in the geometrical model of Bohr and Mottelson. Having a view of nuclei as such geometrical objects leads directly to the importance of possible deformations of nuclei. The most important deformation of nuclei at low energies is the quadrupole deformation to which we restrict our discussion. These quadrupole deformations are of special interest as they enable us to make predictions of nuclear properties, such as energies or E2 transition strengths of the lowest excited states.

Conversely one can deduce information about nuclear deformations by observing E2 transition matrix elements. Indeed from a complete set of E2 matrix elements one can calculate model independent moments and higher order moments of the quadrupole operator, tensorially coupled to a scalar-the shape invariants. Shape invariants were first introduced by Kumar [1] and Cline [2] in the discussion of a large set of E2 matrix elements obtained in Coulomb excitation experiments. Calculating shape invariants in the geometrical model shows their connection to the deformation parameters β and γ used by Bohr and Mottelson or, to be more precise, to effective values $\beta_{\rm eff}$ and $\gamma_{\rm eff}$, and the fluctuations of those. Recently Jolos et al. [3,4] have introduced approximation formulas to the lowest shape invariants in the framework of the newly developed *Q*-phonon scheme [5-8]. These approximations now make it possible to determine approximate values of the shape invariants from data by using only a few absolute B(E2) values.

This is a substantial result since the advent of radioactive beams opens up entirely new nuclear regions for study but, at the same time, the very low intensities of such beams mean that data will be sparse and that nuclear structure information must be obtained from fewer and simpler-to-obtain data. Therefore, the approximations to the Q invariants are important. They allow estimates not only of basic deformation parameters such as β and γ , but also of higher moments, related to the stiffness of the potential in β and γ and to the amount of zero point motion. Such information has seldom if ever been available from any nuclear data. With these approximation formulas, they are now accessible from simple data.

It is therefore important to develop a global view of how these shape invariants behave as a function of structure so that they can be effectively used as signatures of structure. It is the purpose of this Rapid Communication to map out the behavior of the five essential invariants, as well as several related quantities, over the full range of nuclear structure. To do so we will use the algebraic interacting boson model (IBM) [9,10] to study the behavior of shape invariants in and between the dynamical symmetry limits of the IBM. Formulas will be given to transform the shape invariants into effective deformation parameters β and γ . The values derived from the algebraic model will be compared to values in the appropriate limiting cases of the geometrical model.

Shape invariants are formed by the isoscalar electric quadrupole operator, which is also the E2 transition operator in the consistent Q formalism (CQF) [11],

$$T(E2) = Q = e_B \ Q^{\text{IBM}},\tag{1}$$

where Q^{IBM} is the quadrupole operator in the IBM,

$$Q^{\rm IBM} = Q^{\chi} = s^+ \tilde{d} + d^+ s + \chi [d^+ \tilde{d}]^{(2)}, \qquad (2)$$

and e_B is the effective boson charge which is fixed for a given nucleus. We define moments up to sixth order of the quadrupole operator in the ground state as

$$q_2 = \langle 0_1^+ | (Q \cdot Q) | 0_1^+ \rangle, \tag{3}$$

$$q_{3} = \sqrt{\frac{35}{2}} |\langle 0_{1}^{+} | [QQQ]^{(0)} | 0_{1}^{+} \rangle|, \qquad (4)$$

$$q_4 = \langle 0_1^+ | (Q \cdot Q) (Q \cdot Q) | 0_1^+ \rangle, \tag{5}$$

$$q_{5} = \sqrt{\frac{35}{2}} |\langle 0_{1}^{+}| (Q \cdot Q) [QQQ]^{(0)} |0_{1}^{+} \rangle|, \qquad (6)$$

$$q_6 = \frac{35}{2} \langle 0_1^+ | [QQQ]^{(0)} [QQQ]^{(0)} | 0_1^+ \rangle, \tag{7}$$

where a dot denotes a scalar product and $[QQQ]^{(0)}$ abbreviates the tensor coupling $[Q \times [Q \times Q]^{(2)}]^{(0)}$. We should note that q_2 is equal to the total absolute E2 excitation strength from the ground state

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$$q_2 = \sum_j B(E2; 0_1^+ \to 2_j^+).$$
 (8)

 q_2 will be the only quantity in our discussion where an absolute value, namely the effective boson charge e_B , appears.

With the moments (3)-(7) we define the relative dimensionless shape invariants by normalizing to an appropriate power of q_2 ,

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

The quantities K_n do not depend on the effective boson charge e_B . The shape invariants K_n differ from earlier definitions of Jolos *et al.* [3] by normalization constants or tensor coupling. In the present definitions no value may become infinite and all shape invariants are exactly equal to unity in the limit of the rigid symmetric rotor or, in terms of the IBM, the SU(3) limit for any boson number N.

For the calculation of the shape invariants it is convenient to write the expressions for the quadrupole moments (3)–(7) as sums over *E*2 matrix elements. Therefore, the tensor properties of the quadrupole operator are taken into account and the unity operator $\mathbf{1}=\sum_{J,i,M}|J_iM\rangle\langle J_iM|$ is inserted between every pair of quadrupole operators. Using the Wigner-Eckert theorem and the unitarity relation of Clebsch Gordan coefficients it is possible to write the moments q_n as

$$q_{2} = \sum_{i} \langle 0_{1}^{+} \| Q \| 2_{i}^{+} \rangle \langle 2_{i}^{+} \| Q \| 0_{1}^{+} \rangle, \qquad (10)$$

$$q_{3} = \sqrt{\frac{7}{10}} \sum_{i,j} \langle 0_{1}^{+} \| Q \| 2_{i}^{+} \rangle \langle 2_{i}^{+} \| Q \| 2_{j}^{+} \rangle \langle 2_{j}^{+} \| Q \| 0_{1}^{+} \rangle \Big|,$$
(11)

$$q_{4} = \sum_{i,j,k} \langle 0_{1}^{+} \| Q \| 2_{i}^{+} \rangle \langle 2_{i}^{+} \| Q \| 0_{j}^{+} \rangle \langle 0_{j}^{+} \| Q \| 2_{k}^{+} \rangle \langle 2_{k}^{+} \| Q \| 0_{1}^{+} \rangle,$$
(12)

$$q_{5} = \sqrt{\frac{7}{10}} \left| \sum_{i,j,k,l} \langle 0_{1}^{+} \| Q \| 2_{i}^{+} \rangle \langle 2_{i}^{+} \| Q \| 2_{j}^{+} \rangle \langle 2_{j}^{+} \| Q \| 0_{k}^{+} \rangle \right. \\ \times \left. \langle 0_{k}^{+} \| Q \| 2_{l}^{+} \rangle \langle 2_{l}^{+} \| Q \| 0_{1}^{+} \rangle \right|,$$
(13)

$$q_{6} = \frac{7}{10} \sum_{i,j,k,l,m} \langle 0_{1}^{+} \| Q \| 2_{i}^{+} \rangle \langle 2_{i}^{+} \| Q \| 2_{j}^{+} \rangle \langle 2_{j}^{+} \| Q \| 0_{k}^{+} \rangle$$
$$\times \langle 0_{k}^{+} \| Q \| 2_{l}^{+} \rangle \langle 2_{l}^{+} \| Q \| 2_{m}^{+} \rangle \langle 2_{m}^{+} \| Q \| 0_{1}^{+} \rangle, \qquad (14)$$

involving reduced matrix elements between 0^+ and 2^+ states only. In general only the lowest states contribute to the sums because convergence of the *Q*-phonon expansion of nuclear states is fast [8]. Matrix elements between nuclear states that differ by several *Q* phonons are usually small [5].

In the model of a quadrupole deformed rotor analytical expressions for E2 matrix elements and thus for shape invariants can be obtained. In the rigid rotor the shape invari-

TABLE I. Shape invariants and fluctuations, calculated for $N = \infty$ in the *sd*-IBM-1 for the dynamical symmetry limits using analytical expressions. For comparison, corresponding values of an effective γ deformation are given.

$N = \infty$	<i>U</i> (5)	<i>SU</i> (3)	<i>O</i> (6)
$\gamma_{ m eff}$	30°	0°	30°
K_3	0	1	0
K_4	$\frac{7}{5}$	1	1
K_5	0	1	0
K_6	$\frac{\frac{21}{25}}{\frac{2}{5}}$	1	$\frac{1}{3}$
σ_{eta}	$\frac{2}{5}$	0	0
σ_{γ}	$\frac{21}{25}$	0	$\frac{1}{3}$

ants are functions of the fixed deformation parameters β and γ . If we assume a nonrigid deformation, we can give expressions for the shape invariants as

$$q_2 = \left(\frac{3ZeR^2}{4\pi}\right)^2 \langle \beta^2 \rangle \equiv \left(\frac{3ZeR^2}{4\pi}\right)^2 \beta_{\rm eff}^2, \qquad (15)$$

$$K_3 = \frac{\langle \beta^3 \cos 3\gamma \rangle}{\langle \beta^2 \rangle^{3/2}} \equiv \cos 3\gamma_{\rm eff}, \qquad (16)$$

$$K_4 = \frac{\langle \beta^4 \rangle}{\langle \beta^2 \rangle^2},\tag{17}$$

$$K_5 = \frac{\langle \beta^5 \cos 3\,\gamma \rangle}{\langle \beta^2 \rangle^{5/2}},\tag{18}$$

$$K_6 = \frac{\langle \beta^6 \cos^2 3\gamma \rangle}{\langle \beta^2 \rangle^3},\tag{19}$$

explicitly using expectation values of β and cos 3γ . We can define effective values of the deformation parameters β_{eff} and γ_{eff} by Eqs. (15) and (16). The parameter $\gamma_{\text{eff}} = \frac{1}{3} \arccos K_3$ is given in Table I for the appropriate dynamical symmetry limits of the IBM, where SU(3) corresponds to a symmetric rigid rotor, O(6) to a γ -soft nucleus with maximal triaxiality and U(5) to a vibrator.

The shape invariants are measures of effective deformation parameters and their fluctuations. This is made more explicit by defining the following quantities as measures of the fluctuations of β and cos 3γ :

$$\sigma_{\beta} = \frac{\langle \beta^4 \rangle - \langle \beta^2 \rangle^2}{\langle \beta^2 \rangle^2} = K_4 - 1, \qquad (20)$$

$$\sigma_{\gamma} = \frac{\langle \beta^{6} \cos^{2} 3 \gamma \rangle - \langle \beta^{3} \cos 3 \gamma \rangle^{2}}{\langle \beta^{2} \rangle^{3}} = K_{6} - K_{3}^{2}.$$
(21)

Using expressions (10)-(14), (20), (21) one can analytically calculate the shape invariants in the dynamical symme-

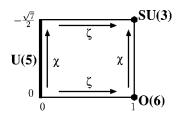


FIG. 1. The ECQF square for transition matrix elements in the IBM-1. U(5) converges to one single point for $N = \infty$.

try limits of the IBM-1. In this paper we will employ the extended consistent Q formalism (ECQF) [12] of the IBM-1, using the IBM-1 Hamiltonian

$$H_{\rm ECQF} = a \left[(1 - \zeta) n_d - \frac{\zeta}{4N} Q^{\chi} \cdot Q^{\chi} \right], \qquad (22)$$

with Q^{χ} taken from Eq. (2). This simple Hamiltonian contains three parameters (a, ζ, χ) . While one parameter (*a*) sets the absolute energy scale, the wave functions depend only on two structural constants (ζ, χ) . For a given nucleus the boson number *N* is fixed. The ECQF Hamiltonian covers the three dynamical symmetry limits as indicated in Fig. 1. We note that the structural parameter χ appearing in the shape invariants through the *E*2 transition operator is fixed in the SU(3) limit ($\chi = -\sqrt{7}/2$) and in the O(6) limit ($\chi=0$), while it is unspecified by the Hamiltonian in the U(5) limit. Therefore, shape invariants in the U(5) limit are functions of the structural parameter χ . The analytical expressions for the shape invariants and the fluctuations in the U(5) limit as functions of the boson number *N* and the structural parameter χ are

$$K_3^{U(5)} = \sqrt{\frac{7}{10}} \frac{1}{\sqrt{N}} |\chi|, \qquad (23)$$

$$K_4^{U(5)} = \frac{7}{5} \left(1 - \frac{2}{7N} \right), \tag{24}$$

$$K_5^{U(5)} = \sqrt{\frac{7}{2}} \frac{(11N-6)}{(5N)^{3/2}} |\chi|, \qquad (25)$$

$$K_6^{U(5)} = \frac{21}{25} \frac{(N-1)}{N^2} \left(3\chi^2 + N - 2 + \frac{5N\chi^2}{6(N-1)} \right), \quad (26)$$

$$\sigma_{\beta}^{U(5)} = \frac{2}{5} \left(1 - \frac{1}{N} \right), \tag{27}$$

$$\sigma_{\gamma}^{U(5)} = \frac{21}{25} \frac{(N-1)}{N^2} (3\chi^2 + N - 2).$$
 (28)

For completeness we also give K_6 as a function of the boson number N in the O(6) limit,

$$K_6^{O(6)} = \frac{1}{3} \frac{(N-2)(N-1)(N+5)(N+6)}{[N(N+4)]^2}.$$
 (29)

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These results enlarge the well-known symmetry triangle for wave functions of the IBM-1 to a structural ECQF square for shape invariants and thus for the interpretation of nuclear shapes. This fact is illustrated in Fig. 1. The use of a similar rectangular representation of the parameter space has also been suggested by Bucurescu *et al.* [13]. Known typical examples for particular points of the ECQF square are, e.g., ¹⁷²Yb for SU(3), ¹⁹⁶Pt for O(6), ¹¹⁶Cd for U(5) with $\chi=0$, and ¹⁵²Sm for large χ and moderate values of ζ (see [14–16] and the discussion below).

From Eqs. (23), (25), (26), and (28) we note that the necessary extension of the IBM-1 symmetry triangle to the ECQF square is a finite-*N* effect, because the shape invariants of U(5) wave functions converge in the limit $N \rightarrow \infty$ for any value of χ . Table I shows the values of the shape invariants and their fluctuations in the dynamical symmetry limits of the IBM-1 for an infinite boson number $N=\infty$. Only the quantities given in Eqs. (23)–(29) depend on the boson number *N*.

As we would expect the values of γ_{eff} in the symmetry limits are 0° and 30°, while the effective triaxiality fluctuates in the O(6) and the U(5) limits. In the SU(3) rigid rotor and $O(6) \gamma$ -soft limits the β deformation is rigid, while it fluctuates in the U(5) vibrator limit.

We have discussed the shape invariants and fluctuations in the dynamical symmetry limits of the IBM using analytical expressions. These values provide useful benchmarks for the geometrical interpretation of IBM ground state wave functions. However, the dynamical symmetry limits of the IBM and the corresponding geometrical models are idealized, analytically solvable limits. More accurate descriptions of the low energy structure of collective nuclei can usually be obtained by IBM Hamiltonians outside the dynamical symmetry limits. To gain insight into the structure of actual nuclei the quantities of interest have been calculated between the symmetry limits, using the ECQF Hamiltonian (22). The shape invariants and their fluctuations have been calculated gridwise over the whole IBM parameter space for N=10bosons as functions of the structural parameters ζ and χ . All calculations have been performed by diagonalizing the Hamiltonian numerically using the computer code PHINT [17]. Calculations of the shape invariants have been done by a FORTRAN code (QINVAR), which evaluates the PHINT output.

All quantities behave smoothly and one obtains an impression of how the quantities vary outside of the dynamical symmetry limits. Figure 2 represents the numerical results of this work presenting the variation of the most important quadrupole invariants over all ranges of structure. The behavior of the invariants, q_2 , K_3 - K_6 , between the symmetries is interesting. Strong variations towards and for deformed nuclei are typical. The invariant K_4 , which is related to fluctuations in β via Eq. (20), is one of the few observables that can distinguish U(5) from O(6). This can be useful in newly accessible exotic nuclei since K_4 can be approximately obtained from the simple expression [3]

$$K_4 \approx \frac{7}{10} \frac{B(E2; 4_1^+ \to 2_1^+)}{B(E2; 2_1^+ \to 0_1^+)} \equiv K_4^{\text{appr.}}, \qquad (30)$$

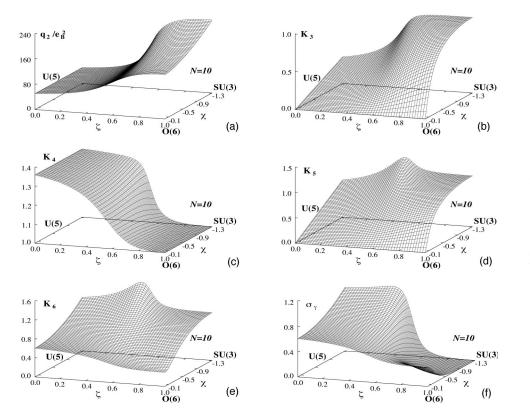


FIG. 2. (a)–(e) Shape invariants q_2 and K_3 - K_6 . (c) The invariant K_4 also determines the fluctuation $\sigma_\beta = K_4 - 1$. (f) The fluctuation σ_γ . All quantities shown in (a)–(f) are calculated gridwise over the ECQF parameter space of the IBM for N=10 bosons.

which involves two observables, easily measured, e.g., by Coulomb excitation experiments. The approximation (30) is valid within about 10% for the ECQF square and boson numbers $N \ge 5$. This was numerically checked for the whole ECQF square and for boson numbers N=5,7,10,16. For a detailed analysis an experimental value of $K_4^{\text{appr.}}$ can serve as a benchmark for starting points of numerical IBM calculations, which can be optimized to reproduce the measured transition strengths. The actual value of K_4 can then be determined from the complete set of calculated *E*2 transition matrix elements.

For large N, K_6 and σ_{γ} are quite different in U(5) and O(6) which is evident from Table I. The bottom right panel of Fig. 2 shows σ_{γ} , which gives the fluctuations in γ , gridwise over the full structural range. Note, however, that Fig. 2 is calculated for a finite boson number which lowers the value of K_6 and σ_{γ} in the U(5) and O(6) limits as seen from Eqs. (25), (28), and (29). In the SU(3) limit σ_{γ} vanishes, which characterizes the SU(3) limit as a model for a rigid rotor, also in the γ degree of freedom. In contrast, nonvanishing triaxiality fluctuations occur in the U(5) and O(6) limits, indicating that these limits and the whole transitional region between them model γ -soft nuclei.

Finally, we note that all shape invariants, especially σ_{γ} , change strongly between SU(3)- and U(5)-like values in an unusual region of the IBM-1 parameter space, namely for moderate values of ζ and $\chi = -\sqrt{7}/2$. Interestingly, this is just the region appropriate to the nucleus ¹⁵²Sm ($\zeta = 0.57$, $\chi = -\sqrt{7}/2$) [14,15]. The case of ¹⁵²Sm is currently under active discussion and it seems that it shows a certain degree of shape coexistence between spherical and deformed shapes with large effective triaxiality [16].

Above, we discussed the numerical calculation of the exact shape invariants within the *sd*-IBM-1 parameter space, using the ECQF Hamiltonian (22). One aspect of this work is to establish the shape invariants as a convenient link between the geometrical model and any other nuclear structure model which is able to calculate E2 transition matrix elements. Here we have chosen the algebraical IBM. Our ansatz is alternative to the intrinsic state formalism by Ginocchio and Kirson [18] which was used much earlier to link the IBM Hamiltonian to the geometrical Bohr Hamiltonian.

We note that the effective values of the shape parameters β_{eff} and γ_{eff} , in general, do not exactly coincide with the minima of a corresponding energy surface for the ground state in the deformation parameter plane. However, the shape invariants can easily be used to compare the predictions from different nuclear models in a geometrically transparent way.

In principle, the shape invariants can also be measured directly from extensive nuclear structure data, providing a direct test of nuclear structure models. Much more intriguing is the common case when only a few key observables, such as E2 branching ratios from low-lying 0^+ states and 2^+ states, are known experimentally and when a phenomenological nuclear structure model, such as the IBM, can be used to extrapolate the data to a complete set of E2 transition matrix elements.

To summarize, we have presented analytic expressions for moments up to sixth order of the quadrupole operator in the ground state and we have given definitions for the lowest shape invariants up to K_6 . The shape invariants were calculated analytically in the dynamical symmetry limits of the IBM-1. Formulas were given to derive effective deformation parameters and their fluctuations from shape invariants, and thus from IBM-1 calculations. A study, using the ECQF Hamiltonian (22), of the behavior of the shape invariants over a full range of structures, has been performed for the first time. It shows the smooth but yet widely varying behavior of the invariants. Thus they can be used to determine the properties of nuclei by comparing the calculated invariants to experimentally obtained values or to results of fits. Moreover, approximate values of these invariants can be obtained experimentally simply from B(E2) values involving just the 2_1^+ , 2_2^+ , and 4_1^+ states, and, for K_5 and K_6 , a B(E2) branching ratio from the appropriate excited 0^+ states.

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The invariant K_4 , as well as the fluctuation $\sigma_{\gamma} = K_6 - K_3^2$, are of special interest as they are observables that allow to distinguish between O(6) and U(5) symmetries which is rather difficult otherwise [19]. Finally, the values of σ_{γ} change most rapidly for IBM-1 Hamiltonians that show shape coexistence.

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